EVOLUTIONARY MARKOV CHAINS, POTENTIAL GAMES AND OPTIMIZATION UNDER THE LENS OF DYNAMICAL SYSTEMS

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To my parents Loukas and Maria,

my sister Theodora,

and the ones I lost along the way,

my grandmother Efthymia and my aunt Vivi.

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SUMMARY

The aim of this thesis is the analysis of complex systems that appear in different research fields such as evolution, optimization and game theory, *i.e.,* we focus on systems that describe the evolution of species, an algorithm which optimizes a smooth function defined in a convex domain or even the behavior of rational agents in potential games. The mathematical equations that describe the evolution of such systems are continuous or discrete dynamical systems (in particular they can be Markov chains). The challenging part in the analysis of these systems is that they live in high dimensional spaces, *i.e.,* they exhibit many degrees of freedom. Understanding their geometry is the main goal to analyze their long-term behavior, speed of convergence/mixing time (if convergence can be shown) and to perform average-case analysis. In particular, the stability of the equilibria (fixed points) of these systems play a crucial role in our attempt to characterize their structure. However, the existence of many equilibria (even uncountably many) makes the analysis more difficult. Using mathematical tools from dynamical systems theory, Markov chains, game theory and non-convex optimization, we have a series of results:

As far as evolution is concerned, (i) we show that mathematical models of haploid evolution imply the extinction of genetic diversity in the long term limit (for fixed fitness matrices) resolving a conjecture in genetics and moreover, (ii) we show that in case of diploid evolution the diversity usually persists, but it is NP-hard to predict it. Finally, (iii) we extend the results of haploid evolution when the fitness matrix changes per a Markov chain and we examine the role of mutation in the survival of the population.

Furthermore, we focus on a wide class of Markov chains, inspired by evolution.

These Markov chains are guided by a dynamical system defined in the simplex. Our key contribution is (iv) connecting the mixing time of these Markov chains and the geometry of the dynamical systems that guide them.

Last but not least, as far as game theory is concerned, (v) we propose a novel quantitative framework for analyzing the efficiency of potential games with many equilibria. The notion we use is not so pessimistic as price of anarchy and not so optimistic as price of stability; it captures the expected long-term performance of a system. Informally, we define the expected system performance as the weighted average of the social costs of all equilibria where the weight of each equilibrium is proportional to the (Lebesgue) measure of its region of attraction. Using replicator dynamics as our benchmark, we provide bounds of this notion for several classes of potential games.

Last but not least, using similar techniques, (vi) we show that gradient descent converges to local minima with probability one, for cost functions in several settings of interest, even when the set of critical points is uncountable.

CHAPTER I

INTRODUCTION

The thesis aims at the analysis of *complex systems* motivated by interdisciplinary areas such as *Evolution, Game Theory and Optimization.* Given a system, natural questions people address are: does the system reach a *steady/equilibrium* state, and if yes how *fast, i.e.,* what is the *speed of convergence*; if there are *multiple equilibria*, which is the "*right*" one; can the *long term behavior* of the system be predicted; what can be said about its *average performance*; is the system *robust* under noise. Theoretical computer science community is particularly interested in all these questions.

We will try to answer them for a variety of complex systems. All these systems are described mathematically by (discrete or continuous) dynamical systems. The branch of mathematics that tries to understand their behavior is called dynamical system theory and has its origins in Newtonian mechanics. The function (update rule) that describes mathematically a dynamical system is an implicit relation that gives the state of the system into the future (for short amount of time). This relation can be either a differential equation $\frac{d\mathbf{x}}{dt} = f(\mathbf{x})$ (continuous time) or difference equation $\mathbf{x}_{t+1} = g(\mathbf{x}_t)$ (discrete time). A dynamical system may have simple behavior and be easy to analyze (*e.g.,* when f, g is linear, when the system is gradient or hamiltonian, see Figure 2) or may have chaotic behavior (highly sensitive to initial conditions, see Figure 1). In section below, we provide all definitions, techniques and theorems, as far as dynamical systems are concerned, which are necessary for the rest of the thesis. Later on, we describe the evolutionary dynamics we particularly focus on, some basic definitions and tools for Markov chains, Game theory. The chapter ends with some notation and the organisation of this thesis.
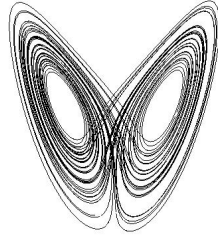
Figure 1: Lorenz attractor.

1.1 Dynamical systems: overview

1.1.1 Definitions

Continuous time dynamical systems. Let $f : \mathcal{S} \to \mathbb{R}^n$ be continuously differentiable with $\mathcal{S} \subset \mathbb{R}^n$, $\mathcal{S}$ an open set. An *autonomous continuous (time)* dynamical system is of the form

$$\frac{d\mathbf{x}}{dt} = f(\mathbf{x}). \tag{1}$$

Since f is continuously differentiable, the ordinary differential equation (1) along with the initial condition $\mathbf{x}(0) = \mathbf{x}_0 \in \mathcal{S}$ has a unique solution for $t \in \mathcal{I}(\mathbf{x}_0)$ (some time interval) and we can represent it by $\phi(t, \mathbf{x}_0)$, called the *flow* of the system. This is a generalization of Picard-Lindelöf theorem. $\phi_t(\mathbf{x}_0) := \phi(t, \mathbf{x}_0)$ corresponds to a function of time which captures the *trajectory* of the system with $\mathbf{x}_0$ the given starting point. The flow is continuously differentiable, its inverse exists (denoted by $\phi_{-t}(\mathbf{x}_0)$) and is also continuously differentiable, *i.e.,* the flow is a *diffeomorphism* in the so called maximal interval of existence $\mathcal{I}$. It is also true that $\phi_t \circ \phi_s = \phi_{t+s}$ for $t, s, t + s \in \mathcal{I}$ and therefore $\phi_k = \phi_1^k$ for $k \in \mathbb{N}$ (composition of ϕ_1 k times as long as $1, k \in \mathcal{I}$). $\mathbf{p} \in \mathcal{S}$ is called an *equilibrium* if $f(\mathbf{p}) = \mathbf{0}$. In that case, it holds that $\phi_t(\mathbf{p}) = \mathbf{p}$ for all $t \in \mathcal{I}$, *i.e.,* $\mathbf{p}$ is a *fixed point* of the function $\phi_t(\mathbf{x})$ for all $t \in \mathcal{I}$. Finally, a fixed point $\mathbf{p}$ is called *isolated* if there is a neighborhood U around $\mathbf{p}$ and $\mathbf{p}$ is the only fixed point in U.
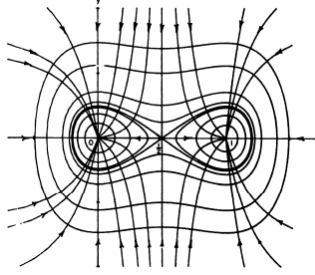
Figure 2: Gradient system.

Remark 1. *If f is globally Lipschitz[1], then the flow is defined for all $t \in \mathbb{R}$, i.e., $\mathcal{I} = \mathbb{R}$. One way to enforce the dynamical system to have a well-defined flow for all $t \in \mathbb{R}$ is to renormalize the vector field by $\|f(\mathbf{x})\| + 1$, i.e., the resulting dynamical system will be*

$$\frac{d\mathbf{x}}{dt} = \frac{f(\mathbf{x})}{\|f(\mathbf{x})\| + 1},$$ (2)

because the function becomes globally 1-Lipschitz. The two dynamical systems (before and after renormalization) are topologically equivalent ([110], p.184). Formally this means that there exists a homeomorphism H which maps trajectories of (1) onto trajectories of (2) and preserves their orientation by time. In words it means that the two systems have the same behavior/geometry (same fixed points, convergence properties).

Discrete time dynamical systems. Let $f : \mathcal{S} \to \mathbb{R}^n$ be a continuous function. An autonomous *discrete (time) dynamical system* is of the form

$$\mathbf{x}_{t+1} = f(\mathbf{x}_t),$$ (3)

with update rule f. The point $\mathbf{p}$ is called a *fixed point* or *equilibrium* of f if $f(\mathbf{p}) = \mathbf{p}$. A sequence $(f^t(\mathbf{x}_0))_{t \in \mathbb{N}}$ is called a *trajectory* of the dynamics with x_0 as starting point.

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[1]*A function is called globally Lipschitz or just Lipschitz if there exists a L so that for all $\mathbf{x}, \mathbf{y}$ it holds $\|f(\mathbf{x}) - f(\mathbf{y})\| \leq L \|\mathbf{x} - \mathbf{y}\|$. A function is locally Lipschitz if for each point $\mathbf{x}$ there is an ϵ-neighborhood of $\mathbf{x}$, and a constant $K(\mathbf{x}, \epsilon)$ so that f satisfies the Lipschitz condition for all $\mathbf{y}, \mathbf{z}$ in that neighborhood.*

Except of the notion of fixed point, there is the notion of periodic orbit or limit cycle. The definition below is about discrete time systems and is used in Chapter 5. [2]

Definition 1 (**Periodic orbits**). $C = \{\mathbf{x}_1, \ldots, \mathbf{x}_k\}$ *is called a periodic orbit of size* k *if* $\mathbf{x}_{i+1} = f(\mathbf{x}_i)$ *for* $1 \leq i \leq k-1$ *and* $f(\mathbf{x}_k) = \mathbf{x}_1$.

If a dynamical system converges in the sense that $\lim_{k \to \infty} f^k(\mathbf{x})$ (discrete case) or $\lim_{t \to \infty} \phi_t(\mathbf{x})$ (continuous case) exists, then the limit is an equilibrium point. In dynamical systems, we are interested in the set of initial conditions that converge to a particular equilibrium point. This is captured by the notion of the *region of attraction* of an equilibrium point. Formally the region of attraction of a fixed point $\mathbf{p}$ is $R_{\mathbf{p}} = \{\mathbf{x} \in \mathcal{S} : \lim_{t \to \infty} \phi_t(\mathbf{x}) = \mathbf{p}\}$ for continuous and apparently for discrete is $R_{\mathbf{p}} = \{\mathbf{x} \in \mathcal{S} : \lim_{k \to \infty} f^k(\mathbf{x}) = \mathbf{p}\}$. But *how can one show convergence?* This will be partially answered in the next section.

1.1.2 Convergence and stability

Lyapunov functions and convergence. One way to show that a dynamical system converges, is via *Lyapunov type functions.* A Lyapunov (or potential) type[3] function $V : \mathcal{S} \to \mathbb{R}$ is a function that strictly decreases along every non-trivial trajectory of the dynamical system. Formally, for continuous time dynamical systems it holds that $\frac{dV}{dt} \leq 0$ with equality only when $f(\mathbf{x}) = \mathbf{0}$. For discrete time dynamical systems, it is true that $V(\mathbf{x}) \geq V(f(\mathbf{x}))$ with equality only at fixed points. Intuitively, a Lyapunov function is an energy function of the system.

Therefore, given a dynamical system, one has to come up with a Lyapunov function to show convergence; this is a hard task in general, especially for discrete dynamical systems. Nevertheless, using the theorem below and by doing reverse engineering,

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[2]There exists the analogue notion for continuous time systems.
[3]We use the word type because this is not the formal definition of a Lyapunov function, but a generalized refinement.

we are able to construct Lyapunov functions for specific (discrete time) evolutionary dynamics that appear in Chapters 4 and 5. It turns out that the dynamical systems we are looking at in these specific chapters have the same structure with the ones that are induced by the following theorem.

Theorem 1.1 (**Baum and Eagon Inequality** [14]). *Let $P(\mathbf{x}) = P(\{x_{ij}\})$ be a polynomial with nonnegative coefficients homogeneous of degree d in its variables $\{x_{ij}\}$. Let $\mathbf{x} = \{x_{ij}\}$ be any point of the domain $D : x_{ij} \geq 0, \sum_{j=1}^{q_i} x_{ij} = 1, i = l, \ldots, p, j = l, \ldots, q_i$. For $\mathbf{x} = \{x_{ij}\} \in D$, let $\Xi(\mathbf{x}) = \Xi\{x_{ij}\}$ denote the point of D whose i, j coordinate is*

$$\Xi(\mathbf{x})_{ij} = \left(x_{ij} \frac{\partial P}{\partial x_{ij}} \bigg|_{(\mathbf{x})} \right) \cdot \left(\sum_{j=1}^{q_i} x_{ij} \frac{\partial P}{\partial x_{ij}} \bigg|_{(\mathbf{x})} \right)^{-1}.$$

Then $P(\Xi(\mathbf{x})) > P(\mathbf{x})$ unless $\Xi(\mathbf{x}) = \mathbf{x}$.

Local behavior. Assume now that for a fixed point $\mathbf{p}$, we use Taylor's theorem (around $\mathbf{p}$) and we get

$$f(\mathbf{x}) = \mathbf{p} + J(\mathbf{p})(\mathbf{x} - \mathbf{p}) + o(\|\mathbf{x} - \mathbf{p}\|).$$

It follows that the linear function $\mathbf{p} + J(\mathbf{p})(\mathbf{x} - \mathbf{p})$ is a good approximation to the (nonlinear) function $f(\mathbf{x})$ in the neighborhood of the fixed point $\mathbf{p}$. It is very natural to expect the behavior of the system near the fixed point $\mathbf{p}$ is (well) approximated by the behavior of the linear system with matrix the Jacobian of f at $\mathbf{p}$. Analyzing a linear dynamical system is very standard; can be done by spectral analysis of the underlying matrix. So it seems that the we can say something about the behavior of the system, at least locally around the fixed points via analysis of the linearized system. Below, we give some definitions due to Lyapunov, based on the local behavior of dynamical systems around fixed points.

Definition 2 (**Stable**). *Let $\mathcal{S} \subseteq \mathbb{R}^n$ be an open set. A fixed point $\mathbf{p}$ of (1) is called stable if for every $\epsilon > 0$, there exists a $\delta = \delta(\epsilon) > 0$ such that for all $\mathbf{x}$ with*

$\|\mathbf{x} - \mathbf{p}\| < \delta$ we have that $\|\phi_t(\mathbf{x}) - \mathbf{p}\| < \epsilon$ for every $t \geq 0$. For discrete time systems (3), a fixed point $\mathbf{p}$ is called stable if for every $\epsilon > 0$, there exists a $\delta = \delta(\epsilon) > 0$ such that for all $\mathbf{x}$ with $\|\mathbf{x} - \mathbf{p}\| < \delta$ we have that $\|f^k(\mathbf{x}) - \mathbf{p}\| < \epsilon$ for every $k \geq 0$. Otherwise it is called unstable.

In words, a fixed point $\mathbf{p}$ is stable so that, if the starting point of the dynamics is sufficiently close to $\mathbf{p}$, then the dynamics remains close to $\mathbf{p}$ for all times.

Definition 3 (**Asymptotically stable**). *Let $\mathcal{S} \subseteq \mathbb{R}^n$ be an open set. A fixed point $\mathbf{p}$ of (1) is called asymptotically stable if it is stable and there exists a $\delta > 0$ such that for all $\mathbf{x}$ with $\|\mathbf{x} - \mathbf{p}\| < \delta$ we have that $\|\phi_t(\mathbf{x}) - \mathbf{p}\| \to 0$ as $t \to \infty$. For discrete time systems (3), a fixed point $\mathbf{p}$ is called asymptotically stable if it is stable and there exists a $\delta > 0$ such that for all $\mathbf{x}$ with $\|\mathbf{x} - \mathbf{p}\| < \delta$ we have that $\|f^k(\mathbf{x}) - \mathbf{p}\| \to 0$ as $k \to \infty$.*

In words, a fixed point $\mathbf{p}$ is asymptotically stable so that, if the starting point of the dynamics is sufficiently close to $\mathbf{p}$, then the dynamics converge to $\mathbf{p}$ as $t \to \infty$. This is a stronger notion than the notion of a stable fixed point.

Arguably one of the most important theorems in dynamical systems is the next theorem and is used extensively in this thesis. It connects the stability of a fixed point $\mathbf{p}$ with the spectral properties of the Jacobian matrix at $\mathbf{p}$.

Theorem 1.2 (**Eigenvalues and stability** [110]). *As far as continuous dynamical systems are concerned (1), at fixed point $\mathbf{p}$ if $J(\mathbf{p})$ has at least one eigenvalue with positive real part, then $\mathbf{p}$ is unstable. If all the eigenvalues have real part negative then $\mathbf{p}$ is asymptotically stable. Moreover, for discrete dynamical systems (3), at fixed point $\mathbf{p}$ if $J(\mathbf{p})$ has at least one eigenvalue with absolute value > 1, then $\mathbf{p}$ is unstable. If all the eigenvalues have absolute value < 1 then it is asymptotically stable.*

In Chapters 2, 4 and 6 we use the following refinement of stability.

Definition 4 (**Linearly stable**). *For continuous time dynamical systems (1), a fixed point* $\mathbf{p}$ *is called linearly stable, if the eigenvalues of* $J(\mathbf{p})$ *of* f *have real part at most zero. Otherwise, it is called linearly unstable. Analogously, for discrete time dynamical systems (3), a fixed point* $\mathbf{p}$ *is called linearly stable, if the eigenvalues of* $J(\mathbf{p})$ *of* f *are at most* 1 *in absolute value. Otherwise, it is called linearly unstable.*

Center-stable manifold theorem. The Center-stable Manifold Theorem 1.3 mentioned below is one of the most important results in the local qualitative theory of continuous and discrete dynamical systems. It is written in terms of discrete time systems; we will explain in a moment how to use it for continuous time systems. The theorem shows that near a fixed point $\mathbf{p}$, a nonlinear system has center-stable and unstable manifolds S and U tangent at $\mathbf{p}$ to the center-stable and unstable subspaces $E^s \oplus E^c$ and E^u of the linearized system $\mathbf{x}_{k+1} = \mathbf{p} + J(\mathbf{p})(\mathbf{x}_k - \mathbf{p})$. Furthermore, S and U are of the same dimensions as $E^s \oplus E^c$ and E^u and the set of starting points in a neighborhood of $\mathbf{p}$ so that the dynamics converges to $\mathbf{p}$ lies on S. As far as continuous dynamical systems are concerned, we work with the function $\phi_1(\mathbf{x})$ (setting $t = 1$, this is called *time one map*). Hence the same theorem holds for continuous time dynamical systems, but the eigenspaces (described below) correspond to eigenvalues with real part negative, zero and positive respectively[4]. We use Center-stable Manifold Theorem in a way to prove that the set of initial conditions that satisfy some property is of measure zero (see Theorems 2.8, 3.6 and 6.4).

Theorem 1.3 (**Center-stable Manifold Theorem** [128]). *Let* $\mathbf{p}$ *be a fixed point for the* C^r *local diffeomorphism* $f : U \to \mathbb{R}^n$ *where* $U \subset \mathbb{R}^n$ *is an open neighborhood of* $\mathbf{p}$ *in* $\mathbb{R}^n$ *and* $r \geq 1$. *Let* $E^s \oplus E^c \oplus E^u$ *be the invariant splitting of* $\mathbb{R}^n$ *into generalized eigenspaces of* $J(\mathbf{p})$ *corresponding to eigenvalues of absolute value less than one, equal to one, and greater than one. To the* $J(\mathbf{p})$ *invariant subspace* $E^s \oplus E^c$ *there is an*

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[4]The version for continuous dynamical systems is used in Chapter 6

associated local h invariant C^r embedded disc W_{loc}^{sc} tangent to the linear subspace at **p** *and a ball B around* **p** *such that:*

$$f(W_{loc}^{sc}) \cap B \subset W_{loc}^{sc}. \text{ If } f^n(\mathbf{x}) \in B \text{ for all } n \geq 0, \text{ then } \mathbf{x} \in W_{loc}^{sc}. \tag{4}$$

We suggest the reader to see [110] for more information on dynamical systems. Below we give a brief introduction to evolutionary dynamical systems.

1.2 Evolution and dynamical systems

Evolutionary dynamical systems are central to the sciences due to their versatility in modeling a wide variety of biological, social and cultural phenomena [100]. Such dynamics are often used to capture the deterministic, *infinite population* setting, and are typically the first step in our understanding of seemingly complex evolutionary processes.

The mathematical introduction of (infinite population) evolutionary processes is dating back to the work of Fisher, Haldane, and Wright in the beginning of the twentieth century. These processes to a large extent are simple, almost toy-like, alas concrete. One example is the replicator equations, first introduced by Fisher [51] in 30's for genotype evolution, the simplest form (continuous/ discrete) of which is the following:

$$\dot{x}_i(t) = x_i(t)((A\mathbf{x}(t))_i - \mathbf{x}(t)^\top A\mathbf{x}(t)) \text{ (cont.)}, \ x_i(t+1) = x_i(t)\frac{(A\mathbf{x}(t))_i}{\mathbf{x}(t)^\top A\mathbf{x}(t)} \text{ (discrete)},$$

where A is a payoff matrix (generally non-negative), **x** a vector that lies in simplex and $(A\mathbf{x})_i$ denotes $\sum_j A_{ij}x_j$. Observe that in the nonlinear dynamics above, simplex is invariant (if we start from a probability distribution, the vector remains a probability distribution). This dynamics is called replicator dynamics and has been used numerous times (biology, evolution, game theory, genetic algorithms).

Theoretical computer science community is particularly interested in evolution. Valiant [134] started viewing evolution through the lens of computation and after

that we have witnessed an accumulation of papers and problem proposals [79, 136, 135, 135, 39]. In [24, 23], a surprisingly strong connection was discovered between standard models of evolution in mathematical biology and Multiplicative Weights Updates Algorithm, a ubiquitous model of online learning and optimization. These papers establish that mathematical models of biological evolution are tantamount to applying MWUA[5], on coordination games. This connection allows for introducing insights from the study of game theoretic dynamics into the field of mathematical biology. The aforementioned papers are a stepping stone for our results in Chapters 2, 3 and 4.

In Chapter 2 we show that mathematical models of haploid[6] evolution imply the extinction of genetic diversity in the long term limit, a widely believed conjecture in genetics [12]. In game theoretic terms we show that in the case of coordination games, under minimal genericity assumptions, (modified) discrete replicator dynamics converge to pure Nash equilibria for all but a zero measure of initial conditions.

Moreover, in Chapter 3 our contribution is to establish complexity theoretic hardness results implying that even in the textbook case of single locus (gene) diploid models, predicting whether diversity survives (in the limit) or not given its fitness landscape is algorithmically intractable.

Last but not least, in Chapter 4 we study the role of mutation in changing environments in the presence of sexual reproduction. Following [139], we model changing environments via a Markov chain, with the states representing environments, each with its own fitness matrix. In this setting, we show that in the absence of mutation, the population goes extinct, but in the presence of mutation, the population survives with positive probability.

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[5]Multiplicative weights update algorithm.
[6]See Section A.1 for (non-technical) definition of biological terms.

All the above mentioned results assume that the population size is infinite (continuum of individuals). However, real populations are finite and often lend themselves to substantial stochastic effects (such as random drift) and it is often important to understand these effects as the population size varies. Hence, stochastic or *finite population* versions of evolutionary dynamical systems are appealed to in order to study such phenomena. While there are many ways to translate a deterministic dynamical system into a stochastic one, one thing remains common: the mathematical analysis becomes much harder as differential equations are easier to analyze and understand than stochastic processes.

One such stochastic version, motivated by the Wright-Fisher model in population genetics, whose deterministic version is Eigen's evolution equations [43], was studied by Dixit *et al.* [39]. Here, the population is fixed to a size N and there are m types of individuals. The process has 3 stages. In the replication (R) stage, every individual of type i in the current population is replaced by a_i individuals of type i and an intermediate population is created. In the selection (S) stage, the population is culled back to size N by sampling with replacement N individuals from this intermediate population. Finally, we have the mutation (M) stage, where each individual is mutated in this intermediate population independently and stochastically according to some matrix Q of size $m \times m$. Q_{ij} corresponds to the probability an individual of type i to change his type to j. This RSM process is a Markov chain with state space $\{\mathbf{x} \in \mathbb{N}^m$ so that $\sum_{i=1}^m x_i = N\}$. However, the number of states in the RSM process is roughly N^m (when m is small compared to N), and a mixing time that grows too fast as a function of the size of the state space can therefore be prohibitively large.

In Chapter 5 we develop techniques for bounding the mixing time of a wide class of Markov chains (where the previous process is included) called evolutionary. Essentially, we make a novel connection between evolutionary Markov chains and dynamical

systems on the probability simplex. This allows us to use the local and global stability properties of the fixed points of such dynamical systems and prove several results. Roughly we show that if there exists one stable fixed point in the dynamical system, then the chain is rapidly mixing ($O(\log N)$ mixing time), otherwise the mixing time is slow ($e^{\Omega(N)}$ mixing time). In section below, we give all the necessary definitions and facts about Markov chains that will be used in Chapter 5.

1.3   Markov chains basics

A Markov chain is a random process that undergoes transitions from one configuration to another on a (finite) state space Ω. The process is *memoryless*, *i.e.*, the probability of moving from one configuration to another depends only on the current configuration (not on history). Formally, a Markov chain is a sequence of random variables $\mathbf{X}^{(0)}, \mathbf{X}^{(1)}, \mathbf{X}^{(2)}, \ldots$ satisfying the *Markov property*, namely that the probability of moving to next state depends only on the present state and not on the previous states

$$\mathbb{P}\left[\mathbf{X}^{(t+1)} = \mathbf{x} | \mathbf{X}^{(1)} = \mathbf{x}_1, \ldots, \mathbf{X}^{(t)} = \mathbf{x}_t\right] = \mathbb{P}\left[\mathbf{X}^{(t+1)} = \mathbf{x} | \mathbf{X}^{(t)} = \mathbf{x}_t\right]. \tag{5}$$

A time-homogeneous Markov chain, which has the property that the r.h.s of (5) is the same for all t, is associated with a transition matrix $P = \{P(\mathbf{x}, \mathbf{y})\}$, where each entry corresponds to the probability with which to move from one state to another. Formally it holds

$$P(\mathbf{x}, \mathbf{y}) = \mathbb{P}\left[\mathbf{X}^{(t+1)} = \mathbf{y} \mid \mathbf{X}^{(t)} = \mathbf{x}\right],$$

for all $\mathbf{x}, \mathbf{y} \in \Omega$ and t.

We focus on the class of *ergodic* Markov chains. A Markov chain is called ergodic if there exists a time $t \in \mathbb{N}$ so that $P^t(\mathbf{x}, \mathbf{y}) > 0$ for all $\mathbf{x}, \mathbf{y} \in \Omega$. For finite (state) Markov chains, ergodicity is equivalent to irreducibility and aperiodicity. A Markov chain is *irreducible* if for any two states $\mathbf{x}, \mathbf{y} \in \Omega$, there exists an integer t so that

$P^t(\mathbf{x}, \mathbf{y}) > 0$, *i.e.,* it is possible to get to any state from any state and is called *aperiodic* if for all $\mathbf{x}$ it holds that $\gcd\{t : P^t(\mathbf{x}, \mathbf{x}) > 0\} = 1$. [7]

A stationary distribution π is defined to be invariant with respect to the transition matrix P, *i.e.,* it satisfies $\pi = \pi P$. It can be shown that an ergodic Markov chain has a unique *stationary distribution* π and converges to it. This is a very useful fact in algorithms and theoretical computer science. One easy case in order to compute π is when the Markov chain is *reversible*. A Markov chain is said to be *reversible* if there is a distribution π which satisfies the detailed balanced equations, namely

$$\text{for all } \mathbf{x}, \mathbf{y} \text{ we have } \pi_\mathbf{x} P(\mathbf{x}, \mathbf{y}) = \pi_\mathbf{y} P(\mathbf{y}, \mathbf{x}).$$

In this case, it can be easily checked that π is a stationary distribution.

One way to sample from a distribution π is to create an ergodic Markov chain that converges to π and this is commonly used in theoretical computer science and machine learning. For the sampling to be efficient, the underlying Markov chain must converge fast to the stationary distribution π. Chapter 5 is devoted to bounding the time a Markov chain needs to get close to the stationary distribution (with respect to some metric between distributions), for a specific class of Markov chains inspired by evolution.

1.3.1 Mixing time and coupling method

Mixing time. As mentioned above, an ergodic Markov chain converges to a unique stationary distribution π. Since we talk about convergence for distributions, we need to define an appropriate metric. The most commonly used is the total variation distance (essentially ℓ_1 distance).

Definition 5 (Total variation distance (TV)). *For distributions μ and ν on Ω,*

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[7] Therefore if a Markov chain has loops, *i.e.,* $P(\mathbf{x}, \mathbf{x}) > 0$ for all $\mathbf{x}$, then it is aperiodic.

their variation distance is defined as

$$\|\mu - \nu\|_{\mathrm{TV}} = \frac{1}{2} \sum_{\mathbf{x} \in \Omega} |\mu(\mathbf{x}) - \nu(\mathbf{x})| = \max_{S \subseteq \Omega} \mu(S) - \nu(S). \qquad (6)$$

We are now ready to define the mixing time of an ergodic Markov chain, notion that captures how much time the chain needs to get close to the stationary distribution.

Definition 6 (**Mixing time** [75]). *Let $\mathcal{M}$ be an ergodic Markov chain on a finite state space Ω with stationary distribution π. Then, the* mixing time $t_{\mathrm{mix}}(\varepsilon)$ *is defined as the smallest time such that for any starting state $\mathbf{X}^{(0)}$, the distribution of the state $\mathbf{X}^{(t)}$ at time t is within total variation distance ε of π. The term mixing time is also used for $t_{\mathrm{mix}}(\epsilon)$ for a* fixed *value of $\varepsilon < 1/2$.*

We say that a Markov chain is *rapidly mixing* (or mixes rapidly) if the mixing time is polynomial in $\log |\Omega|$ and slowly mixing if it is exponential in $\log |\Omega|$. A *phase transition* occurs when a small change in a parameter such as temperature, learning, mutation parameter, causes a large-scale change to the system. Classic example in nature is water; when it is heated and temperature reaches 100 degree Celsius, the water changes from liquid to gas. In terms of Markov chains, a phase transition occurs when a small change in a parameter, changes the mixing from rapid to slow or vice-versa. In Section 5.7.4 we provide a phase transition result for the mixing time of a specific Markov chain that describes evolution of grammar acquisition.

Coupling method. It is clear that the mixing time is a very important notion, both from theoretical and practical perspective, and a lot of research focuses on bounding the mixing time for specific classes of Markov chains (*e.g.,* glauber dynamics). One of the most common techniques for rigorously proving bounds on the mixing time is coupling.

Definition 7 (**Coupling**). *A coupling for distributions μ, ν on finite Ω, is a joint*

distribution ξ on $\Omega \times \Omega$ so that [8]

$$\text{For all } \mathbf{x} \in \Omega, \sum_{\mathbf{y} \in \Omega} \xi(\mathbf{x}, \mathbf{y}) = \mu(\mathbf{x}) \text{ and}$$

$$\text{For all } \mathbf{y} \in \Omega, \sum_{\mathbf{x} \in \Omega} \xi(\mathbf{x}, \mathbf{y}) = \nu(\mathbf{y}).$$

There always exists an optimal coupling which exactly captures the total variation distance. The following lemma is used extensively in this thesis.

Lemma 1.4 (Coupling lemma [4]**).** *Let μ, ν be two probability distributions on Ω. Then,*

$$\|\mu - \nu\|_{\text{TV}} = \min_{\xi} \mathbb{P}_{(\mathbf{X},\mathbf{Y}) \sim \xi} \left[\mathbf{X} \neq \mathbf{Y}\right],$$

where the minimum is taken over all valid couplings $\mathcal{C}$ of μ and ν. The expression $(\mathbf{X}, \mathbf{Y}) \sim \xi$ means that random variable $(\mathbf{X}, \mathbf{Y})$ is chosen from the distribution ξ. Therefore for a given coupling ξ' it also holds that

$$\|\mu - \nu\|_{\text{TV}} \leq \mathbb{P}_{(\mathbf{X},\mathbf{Y}) \sim \xi'} \left[\mathbf{X} \neq \mathbf{Y}\right].$$

The general technique to bound the mixing time of a Markov chain is the following: One considers two arbitrary starting states $\mathbf{X}^{(0)}$ and $\mathbf{Y}^{(0)}$. Assume he is able to construct a coupling ξ for two stochastic processes $\mathbf{X}$ and $\mathbf{Y}$ which are started at $\mathbf{X}^{(0)}$ and $\mathbf{Y}^{(0)}$ and as long as $\mathbf{Y}^{(t_0)} = \mathbf{Y}^{(t_0)}$ for some $t_0 \in \mathbb{N}$ then $\mathbf{Y}^{(t)} = \mathbf{Y}^{(t)}$ for all $t \geq t_0$. Let T be the first (random) time such that $\mathbf{X}^{(T)} = \mathbf{Y}^{(T)}$. From coupling lemma 1.4, if it can be shown that $\mathbb{P}\left[T > t\right] \leq 1/4$ for some $t \in \mathbb{N}$ and for every pair of starting states then

$$\left\|P^t(\mathbf{X}^{(0)}, .) - P^t(\mathbf{Y}^{(0)}, .)\right\|_{\text{TV}} = \left\|\mathbf{X}^{(t)} - \mathbf{Y}^{(t)}\right\|_{\text{TV}}$$
$$\leq \mathbb{P}\left[\mathbf{X}^{(t)} \neq \mathbf{Y}^{(t)}\right]$$
$$\leq \frac{1}{4},$$

---

[8] *We say distribution ξ satisfies the marginals.*

and hence $t_{\text{mix}}(1/4) \leq t$ since

$$\max_{\mathbf{x}\in\Omega}\left\|P^t(\mathbf{x},.)-\pi\right\|_{\text{TV}} \leq \max_{\mathbf{x},\mathbf{y}\in\Omega}\left\|P^t(\mathbf{x},.)-P^t(\mathbf{y},.)\right\|_{\text{TV}},$$

where π is the stationary distribution.

Remark 2. *Typically in theoretical computer science we consider $t_{\text{mix}}(1/4)$ as the mixing time, i.e., for $\epsilon = \frac{1}{4}$. It is well-known that if one is willing to pay an additional factor of $\log 1/\delta$, one can bring down the error from $1/4$ to δ for any $\delta > 0$; see [75].*

1.4   Game theory and equilibrium selection

Nash's theorem [94] on the existence of fixed points in game theoretic dynamics ushered in an exciting new era in the study of economics. At a high level, the inception of the Nash equilibrium concept allowed, to a large degree, the disentanglement between the study of complex behavioral dynamics and the study of games. Equilibria could be concisely described, independently from the dynamics that gave rise to them, as solutions of algebraic equations. Crucially, their definition was simple, intuitive, analytically tractable in many practical instances of small games, and arguably instructive about real life behavior. The notion of a solution to (general) games, which was introduced by the work of von Neumann in the special case of zero-sum games [138], would be solidified as a key landmark of economic thought. This mapping from games to their solutions, *i.e.,* the set of equilibria, grounded economic theory in a solid foundation and allowed for a whole new class of questions in regards to numerous properties of these sets including their geometry, computability, and resulting agent utilities.

Unfortunately, unlike von Neumann's essentially unique behavioral solution to zero-sum games, it became immediately clear that Nash equilibrium fell short from

its role as a universal solution concept in a crucial way. It is non-unique. It is straightforward to find games[9] with constant number of agents, strategies and uncountably many distinct equilibria with different properties in terms of support sizes, symmetries, efficiency, and practically any other conceivable attribute of interest. This raises a natural question. *How should we analyze games with multiple Nash equilibria?*

The centrality of the general equilibrium selection problem can hardly be overestimated. Indeed, according to Ariel Rubinstein "No other task may be more significant within game theory. A successful theory of this type may change all of economic theory." Accordingly, a wide range of radically different approaches to this challenge has been explored by economists, social scientists, and computer scientists alike. Despite their differing points of view, they share a common high level goal. The goal is to reduce the number of admissible equilibria and, if possible, effectively pinpoint a single one as target for analytical inquiry. This way, the multi-valued equilibrium correspondence becomes a simple function and prediction uncertainty vanishes. Although no single approach stands out as providing the definitive answer, each has allowed for significant headway in specific classes of interesting games, and some have sprung forth standalone lines of inquiry. Next, we mention two approaches that have inspired our work (Chapter 6): risk dominance and price of anarchy analysis.

Risk dominance is an equilibrium refinement process that centers around uncertainty about opponent behavior, introduced by Harsanyi and Selten [60]. A Nash equilibrium is considered *risk dominant* if it has the largest basin of attraction (*i.e.,* less risky)[10]. The benchmark example is the Stag Hunt game, shown in figure 10(a) of Chapter 6. In such symmetric 2x2 coordination games a strategy is risk dominant if it is a best response to the uniformly random strategy of the opponent.

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[9]An example of such a game can be found in Section 6.7.2, Lemma 6.27.

[10]Although risk dominance [60] was originally introduced as a hypothetical model of the method by which perfectly rational players select their actions, it may also be interpreted [91] as the result of evolutionary processes.

Price of anarchy [72] follows a much more quantitative approach (see also Definitions 9, 10). The point of view here is that of optimization and the focus is on extremal equilibria. Price of anarchy, defined as the ratio between the social welfare of the worst equilibrium and that of the optimum tries to capture the loss in efficiency due to the lack of centralized authority.

A plethora of similar concepts, based on normalized ratios, has been defined (*e.g., price of stability* [5] focuses on best case equilibria). Tight bounds on these quantities have been established for large classes of games [29, 120]. However, these bounds do not necessarily reflect the whole picture. They usually correspond to highly artificial instances. Even in these bad instances, typically there exist sizable gaps between their price of anarchy and price of stability, allowing for the possibility of significantly tighter analysis of system performance. More to the point, worst case equilibria maybe unlikely in themselves by having a negligible basin of attraction [70].

Based on geometric characterizations of dynamical systems such as *point-wise convergence, computing regions of attraction* and *system invariants*[11], in Chapter 6 we propose a novel quantitative framework for analyzing the efficiency of potential games with many equilibria. The predictions of different equilibria are weighted by their probability to arise under evolutionary dynamics (replicator dynamics) given random initial conditions. This average case analysis is shown to offer the possibility of novel insights in classic game theoretic challenges, including quantifying the risk dominance in stag-hunt games and allowing for more nuanced performance analysis in networked coordination and congestion games with large gaps between price of stability and price of anarchy.

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[11]Invariant functions remain constant along every system trajectory.

1.4.1 Two-player Games and Nash equilibrium

In this section we provide some necessary definitions and facts about two-player games where each player has finitely many pure strategies (moves). This part is necessary for Chapters 2, 3 and 6. Let S_i, $i = 1, 2$ be the set of strategies for player i, and let $m := |S_1|$ and $n := |S_2|$. Then a two-player game can be represented by two payoff matrices A and B of dimension $m \times n$, where payoff to the players are A_{ij} and B_{ij} respectively if the first-player plays i and the second plays j.

Players may randomize among their strategies. The set of mixed strategies for the first player is $\Delta_m = \{\mathbf{x} = (x_1, \dots, x_m) \mid \mathbf{x} \geq 0, \sum_{i=1}^m x_i = 1\}$, and for the second player is $\Delta_n = \{\mathbf{y} = (y_1, \dots, y_n) \mid \mathbf{y} \geq 0, \sum_{j=1}^n y_j = 1\}$. By *mixed* strategy (or fixed point) we mean strictly mixed strategy (or fixed point), *i.e.*, $\mathbf{x}$ such that $|SP(\mathbf{x})| > 1$, and non-mixed are called *pure* (deterministic).

The expected payoffs of the first-player and second-player from a mixed-strategy $(\mathbf{x}, \mathbf{y}) \in \Delta_m \times \Delta_n$ are, respectively

$$\sum_{i,j} A_{ij} x_i y_j = \mathbf{x}^\top A \mathbf{y} \quad \text{and} \quad \sum_{i,j} B_{ij} x_i y_j = \mathbf{x}^\top B \mathbf{y}$$

Definition 8 (**Nash equilibrium (NE)** [98]). *A strategy profile is said to be a Nash equilibrium (NE) strategy profile if no player achieves a better payoff by a unilateral deviation [94]. Formally for two-player games, $(\mathbf{x}, \mathbf{y}) \in \Delta_m \times \Delta_n$ is a NE iff $\forall \mathbf{x}' \in \Delta_m$, $\mathbf{x}^\top A \mathbf{y} \geq \mathbf{x}'^\top A \mathbf{y}$ and $\forall \mathbf{y}' \in \Delta_n$, $\mathbf{x}^\top B \mathbf{y} \geq \mathbf{x}^\top B \mathbf{y}'$.* [12]

There is also the notion of strict Nash equilibrium which is used in Chapter 3.

Definition 9 (**Strict Nash equilibrium**). *NE $\mathbf{x}$ is **strict** if $\forall k \notin SP(\mathbf{x})$, $(A\mathbf{x})_k < (A\mathbf{x})_i$, where $i \in SP(\mathbf{x})$.*

Given strategy $\mathbf{y}$ for the second-player, the first-player gets $(A\mathbf{y})_k$ from her k-th strategy. Clearly, her best strategies are $\arg\max_k (A\mathbf{y})_k$, and a mixed strategy fetches

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[12] *In a similar way, NE is defined for more players, given a utility function for each player.*

the maximum payoff only if she randomizes among her best strategies. Similarly, given $\mathbf{x}$ for the first-player, the second-player gets $(\mathbf{x}^\top B)_k$ from k-th strategy, and same conclusion applies. These can be equivalently stated as the following complementarity type conditions. Let $(\mathbf{x}, \mathbf{y})$ be a Nash equilibrium, then it holds

$$
\begin{aligned}
\forall i \in S_1, \ x_i > 0 &\Rightarrow (A\mathbf{y})_i = \max_{k \in S_1}(A\mathbf{y})_k \\
\forall j \in S_2, \ y_j > 0 &\Rightarrow (\mathbf{x}^\top B)_j = \max_{k \in S_2}(\mathbf{x}^\top B)_k.
\end{aligned} \tag{7}
$$

We end this section by giving the definition of symmetric and coordination games. Important part of Chapter 6 is devoted to analyze the efficiency of equilibria in coordination games.

Symmetric Game. Game (A, B) is said to be symmetric if $B = A^\top$. In a symmetric game the strategy sets of both the players are identical, *i.e.*, $m = n$, and $S_1 = S_2$. We use n, S and Δ_n to denote number of strategies, the strategy set and the mixed strategy set respectively of the players in such a game. A Nash equilibrium profile $(\mathbf{x}, \mathbf{y}) \in \Delta_n \times \Delta_n$ is called *symmetric* if $\mathbf{x} = \mathbf{y}$. Note that at a symmetric strategy profile $(\mathbf{x}, \mathbf{x})$ both the players get payoff $\mathbf{x}^\top A \mathbf{x}$. Using (7) it follows that $(\mathbf{x}, \mathbf{x})$ is a symmetric NE of game $(A, A^\top)$, with payoff $\mathbf{x}^\top A \mathbf{x}$ to both players, if and only if,

$$
\forall i \in S, x_i > 0 \Rightarrow (A\mathbf{x})_i = \max_k (A\mathbf{x})_k \tag{8}
$$

Coordination Game. In a *coordination* game $B = A$, *i.e.*, both the players get the same payoff regardless of who is playing what. Note that such a game always has a pure equilibrium, namely $\arg\max_{(i,j)} A_{ij}$.

1.4.2 Replicator on congestion/network coordination games

In this section we provide the definitions of congestion and network coordination games, one of the most well-studied classes of games. Congestion and network coordination games are potential games. This means that there exists a single global function Φ called the potential (depending on the strategies players choose) so that

if a player changes his strategy unilaterally, the change in his payoff is equal to the change in Φ. This Φ is essentially the analogue of a Lyapunov function and is used to prove convergence to Nash equilibria in many (game) dynamics. Local optima of Φ are Nash equilibria, and it is also true that potential games have at least a pure Nash equilibrium (easy to prove via potential arguments).

Later in the section, we describe the equations of (continuous replicator dynamics) for congestion and coordination games, as have appeared in [70]. Replicator dynamics is a learning dynamics and describes the rational behavior of the players in a game. As we will see in Chapter 6, replicator dynamics in congestion and network coordination games, has some nice properties concerning convergence and stability. Additionally, we give the definition of price of anarchy and the notation we use for the rest of thesis concerning game theory (especially in Chapter 6).

Congestion Games. A congestion game (Rosenthal [119]) is defined by the tuple $(\mathcal{N}; \mathcal{E}; (S_i)_{i \in \mathcal{N}}; (c_e)_{e \in \mathcal{E}})$ where $\mathcal{N}$ is the set of *agents* (with $N = |\mathcal{N}|$), $\mathcal{E}$ is a set of *resources* (also known as *edges* or *bins* or *facilities*), and each player i has a set S_i of subsets of $\mathcal{E}$ ($S_i \subseteq 2^{\mathcal{E}}$). Each strategy $s_i \in S_i$ is a set of edges (a *path*), and c_e is a cost (negative utility) function associated with facility e. We will also use small greek characters like γ, δ to denote different strategies/paths. For a strategy profile $\mathbf{s} = (s_1, s_2, \ldots, s_N)$, the cost of player i is given by $c_i(\mathbf{s}) = \sum_{e \in s_i} c_e(\ell_e(\mathbf{s}))$, where $\ell_e(\mathbf{s})$ is the number of players using e in $\mathbf{s}$ (the load of edge e). In linear congestion games, the latency functions are of the form $c_e(x) = a_e x + b_e$ where $a_e, b_e \geq 0$. Measures of social cost ($sc(\mathbf{s})$) include the makespan, which is equal to the cost of the most expensive path and the sum of the costs of all the agents.

Network (Polymatrix) Coordination Games. A coordination (or partnership) game is a two player game where in each strategy outcome both agents receive the same utility. In other words, if we flip the sign of the utility of the first agent then we get a zero-sum game. An N-player polymatrix (network) coordination game is

defined by an undirected graph $G(V, E)$ with $|V| = N$ vertices and each vertex corresponds to a player. An edge $(i, j) \in E(G)$ corresponds to a coordination game between players i, j. We assume that we have the same strategy space S for every edge. Let A_{ij} be the payoff matrix for the game between players i, j and $A_{ij}^{\gamma\delta}$ be the payoff for both (coordination) if i, j choose strategies γ, δ respectively. The set of players will be denoted by N and the set of neighbors of player i will be denoted by $N(i)$. For a strategy profile $\mathbf{s} = (s_1, s_2, \ldots, s_N)$, the utility of player i is given by $u_i(\mathbf{s}) = \sum_{j \in N(i)} A_{ij}^{s_i s_j}$. The social welfare of a state $\mathbf{s}$ corresponds to the sum of the utilities of all the agents $sw(\mathbf{s}) = \sum_{i \in V} u_i(\mathbf{s})$.

The *price of anarchy* is defined as:

$$\mathrm{PoA} = \frac{\max_{\mathbf{s} \in \mathrm{NE}} \mathrm{Social\ Cost}(\mathbf{s})}{\min_{\mathbf{s}^* \in \times_i S_i} \mathrm{Social\ Cost}(\mathbf{s}^*)}, \tag{9}$$

for cost functions and similarly

$$\mathrm{PoA} = \frac{\max_{\mathbf{s}^* \in \times_i S_i} \mathrm{Social\ Welfare}(\mathbf{s}^*)}{\min_{\mathbf{s} \in \mathrm{NE}} \mathrm{Social\ Welfare}(\mathbf{s})}, \tag{10}$$

for utilities. [13]

We denote by $\Delta(S_i) = \{\mathbf{p} \geq \mathbf{0} : \sum_{\gamma} p_{i\gamma} = 1\}$ the set of mixed (randomized) strategies of player i and $\Delta = \times_i \Delta(S_i)$ the set of mixed strategies of all players. For congestion games we use $c_{i\gamma} = \mathbb{E}_{s_{-i} \sim \mathbf{p}_{-i}} c_i(\gamma, \mathbf{s}_{-i})$ to denote the expected cost of player i given that he chooses strategy γ and $\hat{c}_i = \sum_{\delta \in S_i} p_{i\delta} c_{i\delta}$ to denote his expected cost. Similarly, for network coordination games we use $u_{i\gamma} = \mathbb{E}_{s_{-i} \sim \mathbf{p}_{-i}} u_i(\gamma, \mathbf{s}_{-i})$ to denote the expected utility of player i given that he chooses strategy γ and $\hat{u}_i = \sum_{\delta \in S_i} p_{i\delta} u_{i\delta}$ to denote his expected utility.

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[13]NE denotes the set of Nash equilibria.

1.4.3   Continuous replicator dynamics

Replicator dynamics [132, 125, 70] is described by the following system of differential equations, adjusted to congestion and network coordination games respectively:

$$\frac{dp_{i\gamma}}{dt} = p_{i\gamma}\big(\hat{c}_i - c_{i\gamma}\big), \quad \frac{dp_{i\gamma}}{dt} = p_{i\gamma}\big(u_{i\gamma} - \hat{u}_i\big) \tag{11}$$

for each $i \in \mathcal{N}$, $\gamma \in S_i$. Observe that if $\hat{c}_i > c_{i\gamma}$ then $\frac{dp_{i\gamma}}{dt} > 0$, *i.e.*, $p_{i\gamma}$ is increasing with respect to time, thus player i tends to increase the probability he chooses strategy γ. Similarly if $\hat{c}_i < c_{i\gamma}$ then $\frac{dp_{i\gamma}}{dt} < 0$, *i.e.*, $p_{i\gamma}$ is decreasing w.r.t time, thus player i tends to decrease the probability he chooses strategy γ. [14] Replicator dynamics capture similar rational behavior in the case of network coordination games.

Remark 3 (**Nash equilibria $\subseteq$ Fixed points**). *An interesting observation about the replicator is that its fixed points are exactly the set of randomized strategies such that each agent experiences equal costs across all strategies he chooses with positive probability. This is a generalization of the notion of Nash equilibrium, since equilibria furthermore require that any strategy that is played with zero probability must have expected cost at least as high as those strategies which are played with positive probability.*

1.5   Notation and organisation

Notation. Throughout this thesis we use the following notation: We use boldface letters, *e.g.*, $\mathbf{x}$, to denote column vectors and denote a vector's i-th coordinate by x_i. We use $\mathbf{x}_{-i}$ to denote $\mathbf{x}$ after removing coordinate i-th. For two vectors $\mathbf{x}, \mathbf{y}$, $(\mathbf{x}; \mathbf{y})$ denotes the concatenation of them. To denote a row vector we use $\mathbf{x}^\top$. The set $\{1, \ldots, n\}$ is denoted by $[1 : n]$ or $[n]$ and *int* S is the interior of set S.

We denote the probability simplex on a set of size n as Δ_n. Time indices are denoted by (super)scripts. Thus, a time indexed scalar s at time t is denoted as $s^{(t)}$, s^t

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[14]Replicator dynamics describes rational behavior in a sense.

or $s(t)$ while a time indexed vector $\mathbf{x}$ at time t is denotes as $\mathbf{x}^{(t)}$, $\mathbf{x}^t$ or $\mathbf{x}(t)$. The letters $\mathbf{X}$ and $\mathbf{Y}$ (with time (super)scripts and coordinate subscripts, as appropriate) will be used to denote random vectors. Scalar random vectors and matrices are denoted by capital letters. Boldface $\mathbf{1}$ denotes a vector all whose entries are 1. Moreover we denote by $\mathbb{R}, \mathbb{N}, \mathbb{Z}$ the set of reals, naturals and integers respectively.

For any square matrix A, we denote by $\mathrm{sp}\,(A), \|A\|_1, \|A\|_2$, the spectral radius, $1 \to 1$ norm and *operator norm* of A respectively. Define $A_{\max}, A_{\min}$ the largest, smallest entry in matrix A and $(A\mathbf{x})_i := \sum_j A_{ij} x_j$. We also use $\|\mathbf{x}\|_2$, $\|\mathbf{x}\|_1$, $\|\mathbf{x}\|$ or $\|\mathbf{x}\|_\infty$ for the $\ell_2, \ell_1, \ell_\infty$ norm of vector $\mathbf{x}$ respectively.

By $\nabla^2 f(\mathbf{x})$ we denote the Hessian of a twice differentiable function $f : \mathcal{E} \to \mathbb{R}$, for some set $\mathcal{E} \subseteq \mathbb{R}^n$. For a function f, by f^n we denote the composition of f with itself n times, namely $\underbrace{f \circ f \circ \cdots \circ f}_{n \text{ times}}$. We use $J(\mathbf{x})$ [15] to denote the Jacobian matrix (of some function clear from the context) at the point $\mathbf{x}$.

Organisation. The thesis is organised as follows: In Chapter 2 we show that (i) mathematical models of haploid evolution imply the extinction of genetic diversity in the long term limit. In Chapter 3 we focus on diploid evolution and show that (ii) diversity might persist in the limit but is NP-hard to predict that. Moreover, in Chapter 4 we complement our results on haploid evolution by analyzing the role of mutation in the survival of the population if the environments change. Furthermore, in Chapter 5 we provide (iii) a connection between dynamical systems and the mixing time of a wide class of Markov chains inspired by evolution. In Chapter 6 we propose (iv) a novel framework to analyze the efficiency of potential games with many Nash equilibria. Finally, in Chapter 7, using the machinery developed in Chapter 2, we show (v) that gradient descent converges to minimizers with probability 1.

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[15] In some cases we also use $\mathbb{J}^\mathbf{x}, \mathcal{J}^\mathbf{x}$.

CHAPTER II

EVOLUTIONARY DYNAMICS IN HAPLOIDS

2.1 Introduction

Decoding the mechanisms of biological evolution has been one of the most in-
spiring contests for the human mind. The modern theory of population genetics has
been derived by combining the Darwinian concept of natural selection and Mendelian
genetics. Detailed experimental studies of a species of fruit fly, Drosophila, allowed
for a unified understanding of evolution that encompasses both the Darwinian view
of continuous evolutionary improvements and the discrete nature of Mendelian genet-
ics. The key insight is that evolution relies on the progressive selection of organisms
with advantageous mutations. This understanding has lead to precise mathematical
formulations of such evolutionary mechanisms, dating back to the work of Fisher,
Haldane, and Wright [18] in the beginning of the twentieth century.

The existence of dynamical models of genotypic evolution, however, does not offer
by itself clear, concise insights about the future states of the phenotypic landscape[1].
Which allele combinations, and as a result, which attributes will take over? Predic-
tion of the evolution of the phenotypic landscape is a key, alas not well understood,
question in the study of biological systems [145].

Despite the advent of detailed mathematical models, still at the forefront of our
understanding lie experimental studies and simulations. Of course, this is to some
extent inevitable since the involved dynamical systems are nonlinear and hence a
complete theoretical understanding of all related questions seems intractable [126, 40].
Nevertheless, some rather useful qualitative statements have been established.

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[1]See Section A.1 for (non-technical) definition of biological terms.

Nagylaki [92] showed that, when mutations do not affect reproduction success by a lot[2], the system state converges quickly to the so-called Wright manifold, where the distribution of genotypes is a product distribution of the allele frequencies in the population. In this case, in order to keep track of the distribution of genotypes in the population it suffices to record the distribution of the different alleles for each gene. The overall distribution of genotypes can be recovered by simply taking products of the allele frequencies. Nagylaki *et al.* [93] have also shown that under hyperbolicity assumptions (*e.g.,* isolated equilibria) such systems converge.

Chastain *et al.* [23] have built on Nagylaki's work by establishing an informative connection between these mathematical models of population genetics and the multiplicative update algorithm (MWUA). MWUA is a ubiquitous online learning dynamics [8], which is known to enjoy numerous connections to biologically relevant mathematical models. Specifically, its continuous time limit is equivalent to the replicator dynamics (in its standard continuous form) [70] and its equivalent up to a smooth change of variables to the Lotka-Volterra equations [61]. In [23] another strong such connection was established. Specifically, under the assumption of weak selection standard models of population genetics are shown to be closely related to applying *discrete* replicator dynamics on a coordination game (see Meir and Parkes [87] paper for a more detailed examination of this connection). Discrete replicator dynamics (MWUA variant), which Chastain *et al.* refer to as discrete MWUA, is already a well established dynamics in the literature of mathematical biology and evolutionary game theory [82, 61] under the name discrete (time, version of) replicator dynamics and to avoid confusion we will refer to it by its standard name.

The coordination game is as follows: Each gene is an agent and its available strategies are its alleles. Any combination of strategies/alleles (one for each gene/agent)

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[2]This is referred to as the weak selection regime and it corresponds to a well supported principle known as Kimura's neutral theory.

gives rise to a specific genotype/individual. The common utility of each gene/agent at that genotype/outcome is equal to the fitness of that phenotype. In the weak selection regime this is a number in $[1 - s, 1 + s]$ for some small $s > 0$. If we interpret the frequency of the allele in the population as mixed (randomized) strategies in this game then the population genetics model reduces to each agent/gene updating their distribution according to discrete replicator dynamics.

In discrete replicator dynamics the rate of increase of the probability of a given strategy is directly proportional to its current expected utility. In population genetic terms, this expected utility reflects the average fitness of a specific allele when matched with the current mixture of alleles of the other genes. Livnat *et al.* [78] coined the term mixability to refer to this beneficial attribute. In other words, an allele with high mixability achieves high fitness when paired against the current allele distribution. Naturally, this trait is not a standalone characteristic of an allele but depends on the current state of the system. An allele that enjoys a high mixability in one distribution of alleles, might exhibit a low mixability in another. So, although mixability offers a palpable interpretation of how evolutionary models behaves in a single time step, *it does not offer insights about the long term behavior.*

Game theory, however, can provide us with clues about the long term behavior as well. Specifically, discrete replicator dynamics converges to sets of fixed points in variants of coordination games [82] (see also Chapter 6). This allows for a concise characterization of the possible limit points of the population genetics model, since they coincide with the set of equilibria (fixed points). In [24] it was observed that random two agent coordination games (in the weak selection payoff regime) exhibit (in expectation) exponentially many such mixed strategies. The abundance of such mixed Nash equilibria seems like a strong indicator that (i) the long term system behavior will result in a state of high genetic variance (highly mixed population), (ii) we cannot even efficiently enumerate the set of all biologically relevant limiting behaviors, let

alone predict them. We show that this intuition does not reflect accurately the dynamical system behavior.

Our contribution. We show that given a generic two agent coordination games, starting from all but a zero measure of initial conditions, discrete MWUA converges to pure, strict Nash equilibria (see Theorem 2.9). The genericity assumption is minimal and merely requires that any row/column of the payoff matrix have distinct entries. This genericity assumption, is trivially satisfied with probability one, if the entries of the matrix are i.i.d from a distribution that is continuous and symmetric around zero, say uniform in $[-1, 1]$ as in the full version of [24]. This class of games contains instances with uncountably many Nash equilibria, *e.g.,* if the payoff matrix is $A = \begin{pmatrix} 1 & 4 \\ 4 & 1 \\ 2 & 3 \end{pmatrix}$ for both. Our results carry over even if the game has uncountably many Nash equilibria.

Biological Interpretation. Our work sheds new light on the role of natural selection in haploid genetics. We show that natural selection acts as an antagonistic process to the preservation of genetic diversity. The long term preservation of genetic diversity needs to be safeguarded by evolutionary mechanisms which are orthogonal to natural selection such as mutations and speciation (see Chapter 4 mutations and dynamic environments). This view, although may appear linguistically puzzling at first, is completely compatible with the mixability interpretation of [78, 23]. Mixability implies that good "mixer" alleles, *i.e.,* alleles that enjoy high fitness in the current genotypic landscape) gain an evolutionary advantage over their competition. On the other hand, the preservation of mixed populations relies on this evolutionary race between alleles having no clear long term winner with the average-over-time mixability of two, or more, alleles being roughly equal (in game theoretic terms, in order for two strategies to be played with positive probability by the same agent in

the long run, it must be the case that the time-average expected utilities of these two strategies are roughly equal. The time average here is over the history of play so far). As with actual races, ties are rare and hence mixability leads to non-mixed populations in the long run. According to recent PNAS commentary [12] some of the points in [23] raised questions when compared against commonly held beliefs in mathematical biology.

> "Chastain *et al.* suggest that the representation of selection as (partially) maximizing entropy may help us understand how selection maintains diversity. However, it is widely believed that selection on haploids (the relevant case here) cannot maintain a stable polymorphic equilibrium. There seems to be no formal proof of this in the population genetic literature..."

Our argument above helps bridge this gap between belief and theory.

2.2 Related work

The earliest connection, to our knowledge, between MWUA and genetics lies in [70], where such a connection is established between MWUA (in its usual exponential form) and replicator dynamics [132, 125], one of the most basic tools in mathematical ecology, genetics, and mathematical theory of selection and evolution. Specifically, MWUA is up to first order approximation equivalent to replicator dynamics. Since the MWUA variant examined in [23] is an approximation of its standard exponential form, these results follow a unified theme. MWUA in its classic form is up to first order approximation equivalent to models of evolution. The MWUA variant examined in [23] was introduced by Losert and Akin in [82] in a paper that also brings biology and game theory together. Specifically, they prove the first point-wise convergence to equilibria for a class of evolutionary dynamics resolving an open question at the time. We build on the techniques of this paper, while also exploiting the (in)stability analysis of mixed equilibria along the lines of [70]. The connection between MWUA and

replicator dynamics by [70] also immediately implies connections between MWUA and mathematical ecology. This is because replicator dynamics is known to be equivalent (up to a diffeomorphism) to the classic prey/predator population models of Lotka-Voltera [61].

As a result of the discrete nature of MWUA, its game theoretic analysis tends to be trickier than that of its continuous time variant, the replicator. Analyzed settings of this family of dynamics include zero-sum games [3, 123], congestion games [70], games with non-converging behavior [37, 57, 11] and as well as families of network coordination games (see Chapter 6). New techniques can predict analytically the limit point of replicator systems starting from randomly chosen initial condition. This approach is referred to as average case analysis of game dynamics (Chapter 6).

2.3 Technical Overview

Technically, our result is based mostly on two prior works. In [70] the generic instability of mixed Nash was established for other variants of MWUA, including the replicator equation. Our instability analysis follows along similar lines. Any linearly stable equilibrium is shown to be a weakly stable Nash equilibrium [70]. A weakly stable Nash is a Nash equilibrium that satisfies the extra property that if you force any single randomizing agent to play any strategy in his current support with probability one, all other agents remain indifferent between the strategies in their support. This is a strong refinement of the Nash equilibrium property and in two agent coordination games under our genericity assumption it coincides with the notion of pure Nash. Since mixed equilibria are linearly unstable, by applying the Center-Stable Manifold Theorem 1.3 we establish that locally the set of initial conditions that converge to such an equilibrium is of measure zero. To translate this to a global statement about the size of the region of attraction technical smoothness conditions must be established about the discrete time map. For continuous time systems, such as the replicator

[70], these are standard. Our analysis does not require any additive noise. Also, our system is deterministic, implying a stronger convergence result.

In the case of coordination games with isolated equilibria our theorem follows by combining the zero measure regions of attraction of all unstable equilibria via union bound arguments. The case of uncountably infinite equilibria is tricky and requires specialized arguments. Intuitively the problem lies on the fact that a) black box union bound arguments do not suffice, b) the standard convergence results in potential games merely imply convergence to equilibrium sets, *i.e.,* the distance of the state from the set of equilibria goes to zero, instead of the stronger point-wise convergence, *i.e.,* every trajectory has a unique (equilibrium) limit point. Set-wise convergence allows for complicated non-local trajectories that weave infinitely often in and out of the neighborhood of an equilibrium making topological arguments hard. Once point-wise convergence has been established (Theorem 2.3), the continuum of equilibria can be chopped down into countable many pieces via Lindelöf's lemma A.1 and once again standard union bound arguments suffice. Nagylaki *et al.* point-wise convergence result [93] does not apply here, because their hyperbolicity assumption is not satisfied. Further, assuming $s \to 0$, they analyze a continuous time dynamical system governed by a differential equation. Unlike Nagylaki the system we analyze is discrete MWUA, and establish point-wise convergence to pure Nash equilibria almost always following the work of Losert and Akin [82], even if hyperbolicity is not satisfied (uncountably many equilibria).

We close the chapter with some technical observations about the speed of divergence from the set of unstable equilibria as well as discussing an average case analysis approach for predicting the probabilities that we converge to any of the pure equilibria given a random initial condition (this approach is analyzed in detail and for many classes of games in Chapter 6). We believe that these observations could stimulate future work in the area.

2.4 Preliminaries

In this section we formally describe the dynamics under consideration, and its equivalence with MWUA in evolution. Moreover, we describe some known results about this dynamics, shown by Losert and Akin [82].

2.4.1 Haploid evolution and MWUA

Chastain *et al.* [23] observed that the update rule derived by Nagylaki [92] for allele frequencies, during evolutionary process under weak selection, is exactly multiplicative weight update algorithm (MWUA) applied on coordination game, where genes are players and alleles are their strategies. Formally, if fitness values of a genome defined by a combination of alleles (strategy profile) is from $[1-s,\ 1+s]$ for a small $s > 0$ (weak selection), then for the two-gene (two-player) case such a fitness matrix can be written as $B = \mathbf{1}_{m \times n} + \epsilon C^3$, where each $C_{ij} \in \mathbb{R}$ and $\epsilon \ll 1$. This, defines a coordination game (B, B). Further, the change in allele frequencies in each new generation is as per the following rule:

$$\forall i,\ x_i(t+1) = \frac{x_i(t)(1 + \epsilon(C\mathbf{y}(t))_i)}{1 + \epsilon \mathbf{x}(t)^\top C \mathbf{y}(t)};\ \forall j,\ y_j(t+1) = \frac{y_j(t)(1 + \epsilon(C^\top \mathbf{x}(t))_j)}{1 + \epsilon \mathbf{x}(t)^\top C \mathbf{y}(t)}. \quad (12)$$

Using the fact that $B = \mathbf{1}_{m \times n} + \epsilon C$, this can be reformulated as,

$$\frac{x_i(t)(1 + \epsilon(C\mathbf{y}(t))_i)}{1 + \epsilon \mathbf{x}(t)^\top C \mathbf{y}(t)} = x_i(t) \frac{(B\mathbf{y}(t))_i}{\mathbf{x}(t)^\top B \mathbf{y}(t)};\quad \frac{y_j(t)(1 + \epsilon(C^\top \mathbf{x}(t))_j)}{1 + \epsilon \mathbf{x}(t)^\top C \mathbf{y}(t)} = y_j(t) \frac{(B^\top \mathbf{x}(t))_j}{\mathbf{x}(t)^\top B \mathbf{y}(t)}.$$

We study convergence of discrete MWUA through this reformulation, *i.e.,* discrete replicator dynamics. In general, given a game $(A, B)^4$ consider the update rule (map) $f : \Delta_m \times \Delta_n \to \Delta_m \times \Delta_n$,

$$\text{For } (\mathbf{x}, \mathbf{y}) \in \Delta_m \times \Delta_n \quad \text{if } (\mathbf{x}', \mathbf{y}') = f(\mathbf{x}, \mathbf{y}), \quad \text{then} \quad \begin{array}{l} \forall i \in S_1, \quad x_i' = x_i \frac{(A\mathbf{y})_i}{\mathbf{x}^\top A \mathbf{y}}, \\[2mm] \forall j \in S_2, \quad y_j' = y_j \frac{(\mathbf{x}^\top B)_j}{\mathbf{x}^\top B \mathbf{y}}. \end{array}$$

$$(13)$$

---

[3] m, n are the number of alleles (strategies) for first and second gene (player) respectively.
[4] A, B have size $m \times n$.

Clearly, $\mathbf{x}' \in \Delta_m, \mathbf{y}' \in \Delta_n$, and therefore f is well-defined. Starting with $(\mathbf{x}(0), \mathbf{y}(0))$, the strategy profile at time $t \geq 1$ is $(\mathbf{x}(t), \mathbf{y}(t)) = f(\mathbf{x}(t-1), \mathbf{y}(t-1)) = f^t(\mathbf{x}(0), \mathbf{y}(0))$.

2.4.2 Losert and Akin

Losert and Akin showed a very interesting result on the convergence of discrete replicator dynamics when applied on evolutionary games [18] with positive matrix. These games are symmetric games, where pure strategies are species and the player is playing against itself, *i.e.*, symmetric strategy $(\mathbf{x} = \mathbf{y})$. Consider a $k \times k$ positive matrix A, and the following dynamics, called discrete replicator dynamics, starting with $\mathbf{z}(0) \in \Delta_k$

$$z_i(t+1) = z_i(t)\frac{(A\mathbf{z}(t))_i}{\mathbf{z}(t)^\top A\mathbf{z}(t)}. \tag{14}$$

Clearly, $\mathbf{z}(t+1) \in \Delta_k$, $\forall t \geq 1$. Thus, there is a map $f_s : \Delta_k \to \Delta_k$ corresponding to the above dynamics, where if $\mathbf{z}' = f_s(\mathbf{z})$ then $z_i' = z_i\frac{(A\mathbf{z})_i}{\mathbf{z}^\top A\mathbf{z}}$, implying

$$\mathbf{z}(t+1) = f_s(\mathbf{z}(t)) = f_s^{t+1}(\mathbf{z}(0)). \tag{15}$$

If $\mathbf{z}(t)$ is a fixed point of f_s then $\mathbf{z}(t') = \mathbf{z}(t)$, $\forall t' \geq t$. Losert and Akin [82] proved that the above dynamical system converges point-wise to fixed point, and that map f is a diffeomorphism in an open set that contains Δ_k. Formally:

Theorem 2.1 (Convergence and diffeomorhism [82]**).** *Let $\{\mathbf{z}(t)\}$ be an orbit for the dynamic of (14). As $t \to \infty$, $\mathbf{z}(t)$ converges to a unique fixed point $\mathbf{q}$. Additionally, the map f_s corresponding to (14) is a diffeomorphism in an neighborhood of Δ_k.*

2.5 Proving the result

2.5.1 Point-wise convergence and diffeomorphism

In this section we show that the discrete replicator dynamics of (13), when applied to a two-player coordination game (B, B), converges point-wise to a fixed point of f under weak selection. Further, map f is diffeomorphism. Essentially we will reduce

the problem to applying discrete replicator dynamics on symmetric game with positive matrix and then use the result of Losert and Akin [82] (Theorem 2.1).

Under weak selection regime we have $B_{ij} \in [1-s, 1+s]$, $\forall (i,j)$, for some $s < 1$. Let $\epsilon < 1 - s$, and consider the following matrix

$$A = \begin{pmatrix} \boldsymbol{\epsilon}_{m \times m} & B - \epsilon \\ B^\top - \epsilon & \boldsymbol{\epsilon}_{n \times n} \end{pmatrix}. \tag{16}$$

We will show that applying dynamics of (13) on game $(B, B^\top)$ starting at $(\mathbf{x}(0), \mathbf{y}(0))$ is same as applying (14) on game $(A, A^\top)$ starting at $\mathbf{z}(0) = (\frac{\mathbf{x}(0)}{2}, \frac{\mathbf{y}(0)}{2})$.

Lemma 2.2 (Reduction to replicator dynamics). *Given* $(\mathbf{x}(0), \mathbf{y}(0)) \in \Delta_m \times \Delta_n$, *let* $\mathbf{z}(0) = (\frac{\mathbf{x}(0)}{2}, \frac{\mathbf{y}(0)}{2})$, *then* $\forall t \geq 0$, $(\mathbf{x}(t), \mathbf{y}(t)) = 2 \cdot \mathbf{z}(t)$, *where* $\mathbf{x}(t)$ *and* $\mathbf{y}(t)$ *are as per (13) and* $\mathbf{z}(t)$ *is as per (14).*

Proof. We will show the result by induction. By hypothesis the base case of $t = 0$ holds. Suppose, it holds up to time t, then let $\mathbf{x} = \mathbf{x}(t+1)$, $\mathbf{y} = \mathbf{y}(t+1)$ and $(\mathbf{x}', \mathbf{y}') = \mathbf{z}(t+1)$. Now, $\forall i \leq m+n$, $z_i(t+1) = z_i(t) \frac{(A\mathbf{z}(t))_i}{\mathbf{z}(t)^\top A \mathbf{z}(t)}$ together with $\mathbf{z}(t) = \frac{1}{2}(\mathbf{x}(t), \mathbf{y}(t))$ gives us

$$\forall i \leq m, x_i' = \frac{x_i(t)}{2} \frac{\frac{\epsilon \sum_i x_i(t)}{2} + \frac{(B\mathbf{y}(t))_i}{2} - \frac{\epsilon \sum_j y_j(t)}{2}}{\frac{\mathbf{x}(t)^\top B \mathbf{y}(t)}{4} + \frac{\mathbf{y}(t) B^\top \mathbf{x}(t)}{4}} = \frac{2 x_i(t)}{4} \frac{(B\mathbf{y}(t))_i}{\mathbf{x}(t)^\top B \mathbf{y}(t)} = \frac{x_i}{2}.$$

Similarly, we can show that $\forall j \leq n$, $y_j' = \frac{y_j}{2}$, and the lemma follows. $\qquad\square$

Lemma 2.2 establishes equivalence between games (B, B) and $(A, A^\top)$ in terms of dynamics, and thus the next theorem follows using Theorem 2.1.

Theorem 2.3 (Convergence and diffeomorphism for haploid evolution). *Let* $\{\mathbf{x}(t), \mathbf{y}(t)\}$ *be an orbit for the dynamic of (13). As t approaches ∞, $(\mathbf{x}(t), \mathbf{y}(t))$ converges to a unique fixed point $(\mathbf{p}, \mathbf{q})$. Additionally, the map F corresponding to (13) is a diffeomorphism in an neighborhood of $\Delta_m \times \Delta_n$.*

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2.5.2 Convergence to pure NE almost always

In Section 2.5.1 we saw that dynamics of (13) converges to a fixed point regardless of where we start in coordination games with weak selection. However, which equilibrium it converges to depends on the starting point. In this section we show that it almost always converge to a pure Nash equilibrium under mild genericity assumptions on the game matrix. In the light of the known fact that a coordination game (B, B), where B_{ij}s are chosen uniformly at random from $[1-s, 1+s]$, may have exponentially many mixed NE [24], this result comes as a surprise.

To show the result, we use the concept of weakly stable Nash equilibrium [70]. This is a refinement of the classic notion of equilibrium and we show that for coordination games it coincides with pure NE under some mild assumptions. Further, we connect them to *stable* fixed points of f (13) by showing that all stable fixed points of f are weakly stable NE. Finally, using the Center-Stable Manifold Theorem 1.3 we show that dynamics defined by f converges to stable fixed points except for a zero measure set of starting points.

Definition 10 (**Weakly stable NE**)**.** *A Nash equilibrium* $(\mathbf{x}, \mathbf{y})$ *is called* weakly stable *if fixing one of the players to choosing a pure strategy in the support of her strategy with probability one, leaves the other player indifferent between the strategies in his support, e.g., let T_1 and T_2 are supports of $\mathbf{x}$ and $\mathbf{y}$ respectively, then for any $i \in T_1$ if the first player plays i with probability one then the second player is indifferent between all the strategies of T_2, and vice-versa.*

Note that pure NE are always weakly stable, and coordination games always have pure NE. Further, for a mixed-equilibrium to be weakly stable, for any $i \in T_1$ all the B_{ij}'s corresponding to $j \in T_2$ are the same. Thus, the next lemma follows.

Lemma 2.4 (**Weakly stable NE implies pure**)**.** *If coordinates of a row or a column of B are all distinct, then every weakly stable equilibrium is a pure NE.*

Proof. To the contrary suppose $(\mathbf{x}, \mathbf{y})$ is a mixed weakly stable NE, then for $T_1 = \{i \mid x_i > 0\}$ and $T_2 = \{j \mid y_j > 0\}$ we have $\forall i \in T_1$, $B_{ij} = B_{ij'}$, $\forall j \neq j' \in T_2$, a contradiction. $\qquad\square$

Remark 4. *We note that the games analyzed in [24], where entries of matrix B are chosen uniformly at random from the interval $[1 - s, 1 + s]$, will have distinct entries in each of its rows/columns with probability one, and thereby due to Lemma 2.4 all its weakly stable NE are pure NE.*

Stability of a fixed point is defined based on eigenvalues of Jacobian matrix evaluated at the fixed point. So let us first describe the Jacobian matrix of function f. We denote this matrix by J which is $m + n \times m + n$, and let f_k denote the function that outputs k-th coordinate of f. Then, $\forall i \neq i' \leq m$ and $\forall j \neq j' \leq n$

$$J_{ii} = \frac{df_i}{dx_i} = \frac{(By)_i}{x^\top By} - x_i \left(\frac{(By)_i}{x^\top By} \right)^2, \qquad J_{(m+j)(m+j)} = \frac{df_{m+j}}{dy_j} = \frac{(B^\top x)_i}{x^\top By} - y_i \left(\frac{(B^\top x)_i}{x^\top By} \right)^2,$$

$$J_{ii'} = \frac{df_i}{dx_{i'}} = -x_i \frac{(By)_i \cdot (By)_{i'}}{(x^\top By)^2}, \qquad J_{(m+j)(m+j')} = \frac{df_{m+j}}{dy_{j'}} = -y_j \frac{(B^\top x)_j \cdot (B^\top x)_{j'}}{(x^\top By)^2},$$

$$J_{i(m+j)} = \frac{df_i}{dy_j} = x_i \frac{B_{ij} \cdot (x^\top By) - (By)_i (B^\top x)_j}{(x^\top By)^2}, \quad J_{(m+j)i} = \frac{df_{m+j}}{dx_i} = y_j \frac{B_{ij} \cdot (x^\top By) - (B^\top x)_j (By)_i}{(x^\top By)^2}.$$

Now in order to use Center-Stable Manifold Theorem (see Theorem 1.3), we need a map whose domain is full-dimensional around the fixed point. However, an n-dimensional simplex (Δ_n) in $\mathbb{R}^n$ has dimension $n - 1$, and therefore the domain of f, namely $\Delta_m \times \Delta_n$ is of dimension $m + n - 2$ in space $\mathbb{R}^{m+n}$. Therefore, we need to take a projection of the domain space and accordingly redefine the map f. We note that the projection we take will be fixed point dependent; this is to keep of the proof of Lemma 2.6 relatively less involved later.

Let $\mathbf{r} = (\mathbf{p}, \mathbf{q})$ be a fixed point of map f in $\Delta_m \times \Delta_n$. Define $i(\mathbf{r})$ and $j(\mathbf{r})$ to be coordinates of $\mathbf{p}$ and $\mathbf{q}$ respectively that are non-zero, *i.e.,* $p_{i(\mathbf{r})} > 0$ and $q_{j(\mathbf{r})} > 0$. Consider the mapping $z_\mathbf{r} : R^{m+n} \to R^{m+n-2}$ so that we exclude from each player $1, 2$ the variables $x_{i(\mathbf{r})}, y_{j(\mathbf{r})}$ respectively. We substitute the variables $x_{i(\mathbf{r})}$ with $1 - \sum_{i \neq i(\mathbf{r})} x_i$ and $y_{j(\mathbf{r})}$ with $1 - \sum_{j \neq j(\mathbf{r})} y_j$. Consider map f under the projection $z_\mathbf{r}$, and let

$J^{\mathbf{r}}$ denote the *projected Jacobian* at $\mathbf{r}$. Then, $\forall i, i' \in [m] \backslash \{i(\mathbf{r})\}$ and $\forall j, j' \in [n] \backslash \{j(\mathbf{r})\}$ we get that

$$
\begin{aligned}
J^{\mathbf{r}}_{ii} &= \frac{(By)_i}{x^\top By} - x_i \left(\frac{(By)_i}{x^\top By} \right)^2 + x_i \frac{(By)_i \cdot (By)_{i(\mathbf{r})}}{(x^\top By)^2}, \\
J^{\mathbf{r}}_{(m+j)(m+j)} &= \frac{(B^\top x)_j}{x^\top By} - y_j \left(\frac{(B^\top x)_j}{x^\top By} \right)^2 + y_j \frac{(B^\top x)_j \cdot (B^\top x)_{j(\mathbf{r})}}{(x^\top By)^2}, \\
J^{\mathbf{r}}_{ii'} &= -x_i \frac{(By)_i \cdot (By)_{i'}}{(x^\top By)^2} + x_i \frac{(By)_i \cdot (By)_{i(\mathbf{r})}}{(x^\top By)^2}, \\
J^{\mathbf{r}}_{(m+j)(m+j')} &= -y_j \frac{(B^\top x)_j \cdot (B^\top x)_{j'}}{(x^\top By)^2} + y_j \frac{(B^\top x)_j \cdot (B^\top x)_{j(\mathbf{r})}}{(x^\top By)^2}, \\
J^{\mathbf{r}}_{i(m+j)} &= x_i \frac{B_{ij} \cdot (x^\top By) - (By)_i (B^\top x)_j}{(x^\top By)^2} - x_i \frac{B_{ij(\mathbf{r})} \cdot (x^\top By) - (By)_i (B^\top x)_{j(\mathbf{r})}}{(x^\top By)^2}, \\
J^{\mathbf{r}}_{(m+j)i} &= y_j \frac{B_{ij} \cdot (x^\top By) - (B^\top x)_j (By)_i}{(x^\top By)^2} - y_j \frac{B_{i(\mathbf{r})j} \cdot (x^\top By) - (B^\top x)_j (By)_{i(\mathbf{r})}}{(x^\top By)^2}.
\end{aligned}
\tag{17}
$$

The characteristic polynomial of $J^{\mathbf{r}}$ at $\mathbf{r}$ is

$$
\prod_{i: p_i = 0} \left(\lambda - \frac{(B\mathbf{q})_i}{\mathbf{p}^\top B\mathbf{q}} \right) \prod_{j: q_j = 0} \left(\lambda - \frac{(B^\top \mathbf{p})_j}{\mathbf{p}^\top B\mathbf{q}} \right) \times det(\lambda I - \mathbb{J}^{\mathbf{r}}),
$$

where $\mathbb{J}^{\mathbf{r}}$ corresponds to $J^{\mathbf{r}}$ at $\mathbf{r}$ by deleting rows i, columns j with $p_i = 0$ and $q_j = 0$.

Lemma 2.5 (Linearly stable implies NE). *Every linearly stable fixed point is a Nash Equilibrium.*

Proof. Assume that a linearly stable fixed point $\mathbf{r}$ is not a Nash equilibrium. Without loss of generality suppose player $t = 1$ can deviate and gain. Since $\mathbf{r}$ is a fixed point of map f, $\forall p_i > 0 \Rightarrow (B\mathbf{q})_i = \mathbf{p}^\top B\mathbf{q}$. Hence, there exists a strategy $i \leq m$ such that $p_i = 0$ and $(B\mathbf{q})_i > \mathbf{p}^\top B\mathbf{q}$. Then the characteristic polynomial has $\frac{(B\mathbf{q})_i}{\mathbf{p}^\top B\mathbf{q}} > 1$ as a root, a contradiction. □

We are going to show that the dynamics of (13) converge to linearly stable fixed point except for measure zero starting conditions. However, what we want is that it almost always converge to weakly stable NE. So, let us first establish relation between stable fixed points and weakly stable NE.

Lemma 2.6 (Linearly stable implies weakly stable NE). *Every linearly stable fixed point is a weakly stable Nash equilibrium.*

Proof. Let $k \times k$ be the size of matrix $\mathbb{J}^{\mathbf{r}}$. If $k = 0$ then the equilibrium is pure and therefore is stable. For the case when $k > 0$, let $T_{\mathbf{p}}$ and $T_{\mathbf{q}}$ be the support of $\mathbf{p}$ and $\mathbf{q}$ respectively, *i.e.*, $T_{\mathbf{p}} = \{i \mid p_i > 0\}$ and similarly $T_{\mathbf{q}}$. If we show that $\forall i, i' \in T_{\mathbf{p}}$ and $\forall j, j' \in T_{\mathbf{q}}$, $M^{i,i',j,j'} = (B_{ij} - B_{i'j}) - (B_{ij'} - B_{i'j'}) = 0$, then using argument similar to Theorem 3.8 in [70], the lemma follows. We show this using the expression of $tr((\mathbb{J}^{\mathbf{r}})^2)$ (tr denotes the trace).

Claim 2.7. $tr((\mathbb{J}^{\mathbf{r}})^2) =$

$$k + \frac{1}{(\mathbf{p}^\top B \mathbf{q})^2} \sum_{\substack{i<i':i,i'\neq i(\mathbf{r}) \\ j<j':j,j'\neq j(\mathbf{r})}} p_i q_j p_{i'} q_{j'} (M^{i,i',j,j'})^2 + \frac{1}{(\mathbf{p}^\top B \mathbf{q})^2} \sum_{\substack{i:i\neq i(\mathbf{r}) \\ j:j\neq j(\mathbf{r})}} p_i q_j p_{i(\mathbf{r})} q_{j(\mathbf{r})} (M^{i,i(\mathbf{r}),j,j(\mathbf{r})})^2$$

$$+ \frac{1}{(\mathbf{p}^\top B \mathbf{q})^2} \sum_{\substack{j<j':j,j'\neq j(\mathbf{r}) \\ i:i\neq i(\mathbf{r})}} p_i p_{i(\mathbf{r})} q_j q_{j'} (M^{i,i(\mathbf{r}),j,j'})^2 + \frac{1}{(\mathbf{p}^\top B \mathbf{q})^2} \sum_{\substack{j:j\neq j(\mathbf{r}) \\ i<i':i,i'\neq i(\mathbf{r})}} p_i p_{i'} q_j q_{j(\mathbf{r})} (M^{i,i',j,j(\mathbf{r})})^2.$$

Proof of Claim. Since $\mathbb{J}^{\mathbf{r}}_{ii'} = 0$, $\mathbb{J}^{\mathbf{r}}_{(m+j)(m+j')} = 0$ for $i \neq i'$ and $j \neq j'$, and $\mathbb{J}^{\mathbf{r}}_{ii} = 1$, $\mathbb{J}^{\mathbf{r}}_{(m+j)(m+j)} = 1$ we get that

$$tr((\mathbb{J}^{\mathbf{r}})^2) = k + \sum_{i,j} \mathbb{J}^{\mathbf{r}}_{i(m+j)} \mathbb{J}^{\mathbf{r}}_{(m+j)i}.$$

We consider the following cases:

- Let $i < i'$ with $i, i' \neq i(\mathbf{r})$ and $j < j'$ with $j, j' \neq j(\mathbf{r})$ and we examine the term $\frac{1}{(\mathbf{p}^\top B \mathbf{q})^2} p_i q_j p_{i'} q_{j'}$ in the sum and we get that it appears with

$$[[M^{i,i',j,j(\mathbf{r})}] \times [M^{i,i(\mathbf{r}),j,j'}] + [M^{i,i',j,j(\mathbf{r})}] \times [M^{i(\mathbf{r}),i',j,j'}]$$

$$+[M^{i,i',j(\mathbf{r}),j'}] \times [M^{i,i(\mathbf{r}),j,j'}] + [M^{i,i',j(\mathbf{r}),j'}] \times [M^{i(\mathbf{r}),i',j,j'}]$$

$$=(M^{i,i',j,j'})^2.$$

- Let $i \neq i(\mathbf{r})$ and $j \neq j(\mathbf{r})$. The term $\frac{1}{(\mathbf{p}^\top B \mathbf{q})^2} p_i q_j p_{i(\mathbf{r})} q_{j(\mathbf{r})}$ in the sum appears in multiplication with $(M^{i,i(\mathbf{r}),j,j(\mathbf{r})})^2$.

- Let $i < i'$ with $i, i' \neq i(\mathbf{r})$ and $j \neq j(\mathbf{r})$. The term $\frac{1}{(\mathbf{p}^\top B \mathbf{q})^2} p_i q_j p_{i'} q_{j(\mathbf{r})}$ in the sum

appears with

$$[M^{i,i',j,j(\mathbf{r})}] \times [M^{i,i(\mathbf{r}),j,j(\mathbf{r})}] + [M^{i,i',j,j(\mathbf{r})}] \times [M^{i(\mathbf{r}),i',j,j(\mathbf{r})}]$$
$$= (M^{i,i',j,j(\mathbf{r})})^2.$$

- Similarly to the previous case, for $j < j'$ with $j, j' \neq j(\mathbf{r})$ and $i \neq i(\mathbf{r})$. The term $\frac{1}{(\mathbf{p}^\top B \mathbf{q})^2} p_i q_j p_{i(\mathbf{r})} q_{j'}$ in the sum appears with $(M^{i,i(\mathbf{r}),j,j'})^2$.

$\square$

The trace of $(\mathbb{J}^\mathbf{r})^2$ can not be larger than k, otherwise there exists an eigenvalue with absolute value greater than one contradicting $\mathbf{r}$ being a stable fixed point. From the above claim, it is clear that $tr((\mathbb{J}^\mathbf{r})^2) \geq k$ and it is exactly k if and only if $M^{i,i',j,j'} = 0$, $\forall i, i' \in T_1$ and $j, j' \in T_2$, and the lemma follows. $\square$

We show that except for zero measure starting points $(\mathbf{x}(0), \mathbf{y}(0))$ the dynamics of (13) converges to stable fixed points using the Center-Stable Manifold Theorem 1.3, which proves the next theorem.

Theorem 2.8 (**Replicator converges to stable fixed points**). *The set of initial conditions in $\Delta_m \times \Delta_n$ so that the dynamical system with Equations (13) converges to unstable fixed points has measure zero.*

Proof. To prove Theorem 2.8, we will make use of Center-Stable manifold theorem (Theorem 1.3). First we need to project the domain to a lower dimensional space. We consider the (diffeomorphism) function g that is a projection of the points $(\mathbf{x}, \mathbf{y}) \in \mathbb{R}^{m+n}$ to $\mathbb{R}^{m+n-2}$ by excluding a specific (the "first") variable for each player (we know that the probabilities must sum up to one for each player). Let $N = m + n$, then we denote this projection of $\Delta := \Delta_m \times \Delta_n$ by $g(\Delta)$, *i.e.*, $(\mathbf{x}, \mathbf{y}) \rightarrow_g (\mathbf{x}', \mathbf{y}')$ where $\mathbf{x}' = (x_2, \ldots, x_n)$ and $\mathbf{y}' = (y_2, \ldots, y_n)$. Further, recall the fixed point dependent projection function $z_\mathbf{r}$ defined in Section 2.5.2, where we remove $x_{i(\mathbf{r})}$ and $y_{j(\mathbf{r})}$.

Let f be the update of dynamical system (13). For an unstable fixed point $\mathbf{r}$ we consider the function $\psi_{\mathbf{r}}(\mathbf{v}) = z_{\mathbf{r}} \circ f \circ z_{\mathbf{r}}^{-1}(\mathbf{v})$ which is diffeomorphism (due to theorem 2.3 in a neighborhood of $g(\Delta)$), with $\mathbf{v} \in R^{N-2}$. Let $B_{\mathbf{r}}$ be the (open) ball derived from Theorem 1.3 and we consider the union of these balls (transformed in $\mathbb{R}^{N-2}$)

$$A = \cup_{\mathbf{r}} A_{\mathbf{r}},$$

where $A_{\mathbf{r}} = g(z_{\mathbf{r}}^{-1}(B_{\mathbf{r}}))$ ($z_{\mathbf{r}}^{-1}$ "returns" the set $B_{\mathbf{r}}$ back to $\mathbb{R}^N$). Set $A_{\mathbf{r}}$ is an open subset of $\mathbb{R}^{N-2}$ (by continuity of $z_{\mathbf{r}}$ and g being diffeomorphism). Due to the Lindelöf's Lemma A.1, we can find a countable subcover for A, *i.e.,* there exists fixed points $\mathbf{r}_1, \mathbf{r}_2, \ldots$ such that $A = \cup_{m=1}^{\infty} A_{\mathbf{r}_m}$.

For a $t \in \mathbb{N}$ let $\psi_{t,\mathbf{r}}(\mathbf{v})$ the point after t iteration of dynamics (13), starting with $\mathbf{v}$, under projection $z_{\mathbf{r}}$, *i.e.,* $\psi_{t,\mathbf{r}}(\mathbf{v}) = z_{\mathbf{r}} \circ f^t \circ z_{\mathbf{r}}^{-1}(\mathbf{v})$. If point $\mathbf{v} \in g(\Delta)$ (which corresponds to $g^{-1}(\mathbf{v})$ in our original Δ) has as unstable fixed point as a limit, there must exist a t_0 and m so that $\psi_{t,\mathbf{r}_m} \circ z_{\mathbf{r}_m} \circ g^{-1}(\mathbf{v}) \in B_{\mathbf{r}_m}$ for all $t \geq t_0$ (we have point-wise convergence from Theorem 2.3) and therefore again from Theorem 1.3 and the fact that $g(\Delta)$ is invariant we get that $\psi_{t_0,\mathbf{r}_m} \circ z_{\mathbf{r}_m} \circ g^{-1}(\mathbf{v}) \in W_{loc}^{sc}(\mathbf{r}_m)$, hence $\mathbf{v} \in g \circ z_{\mathbf{r}_m}^{-1} \circ \psi_{t_0,\mathbf{r}_m}^{-1}(W_{loc}^{sc}(\mathbf{r}_m) \cap z_{\mathbf{r}_m}(\Delta))$. Hence the set of points in $g(\Delta)$ whose ω-limit has an unstable equilibrium is a subset of

$$C = \cup_{m=1}^{\infty} \cup_{t=1}^{\infty} g \circ z_{\mathbf{r}_m}^{-1} \circ \psi_{t,\mathbf{r}_m}^{-1}(W_{loc}^{sc}(\mathbf{r}_m) \cap z_{\mathbf{r}_m}(\Delta)). \tag{18}$$

Since $\mathbf{r}_m$ is linearly unstable, it holds that $dim(E^u) \geq 1$, and therefore dimension of $W_{loc}^{sc}(\mathbf{r}_m)$ is at most $N-3$. Thus, the set $W_{loc}^{sc}(\mathbf{r}_m) \cap z_{\mathbf{r}_m}(\Delta)$ has Lebesgue measure zero in $\mathbb{R}^{N-2}$. Finally since $g \circ z_{\mathbf{r}_m}^{-1} \circ \psi_{t,\mathbf{r}_m}^{-1} : \mathbb{R}^{N-2} \to \mathbb{R}^{N-2}$ is continuously differentiable (in a neighborhood of $g(\Delta)$, by Theorem 2.3), $\psi_{t,\mathbf{r}_m}$ is C^1 and locally Lipschitz (see p.71 in [110]). Therefore using Lemma A.2, it preserves the null-sets, and thereby we get that C is a countable union of measure zero sets, *i.e.,* is measure zero as well, and Theorem 2.8 follows. $\square$

Theorem 2.8 together with Lemmas 2.4 and 2.6 gives the following main result.

Theorem 2.9 (**Main Theorem - Convergence to pure**). *For all but measure zero initial conditions in $\Delta_m \times \Delta_n$, the dynamical system (13) when applied to a coordination game (B, B) with $B_{ij} \in [1 - s, 1 + s]$, $\forall (i, j)$ for $s < 1$, converges to weakly stable Nash equilibria. Furthermore, assuming that entries in each row and column of B are distinct, it converges to pure Nash equilibria.*

2.6 *Figure of stable/unstable manifolds in simple example*

Figure 3 corresponds to a two agent coordination game with payoff structure $B = \begin{pmatrix} 1 & 0 \\ 0 & 3 \end{pmatrix}$. Since this game has two agents with two strategies each, in order to capture the state space of game it suffices to describe one number for each agent, namely the probability with which he will play his first strategy. This game has three Nash equilibria, two pure ones $(0, 0), (1, 1)$ and a mixed one $\left(\frac{3}{4}, \frac{3}{4}\right)$. We depict them using small circles in the figure. The mixed equilibrium has a stable manifold of zero measure that we depict with a black line. In contrast, each pure Nash equilibrium has region of attraction of positive measure. The stable manifold of the mixed NE separates the regions of attraction of the two pure equilibria. The $(0, 0)$ equilibrium has larger region of attraction, represented by darker region in the figure. It is the risk dominant equilibrium of the game. In Chapter 6 we provide techniques to compute such objects (stable manifolds, volumes of region of attraction) analytically.
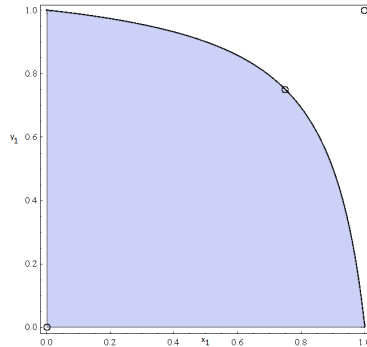
Figure 3: Regions of attraction for $B = [1\ 0; 0\ 3]$, where $\circ$ correspond to NE points.

2.7 Discussion

Building on the observation of [23] that the process of natural selection under weak selection regime can be modeled as discrete Multiplicative weight update dynamics on coordination games, we showed that it converges to pure NE almost always in the case of two-player games. As a consequence natural selection alone seem to lead to extinction of genetic diversity in the long term limit, a widely believed conjecture of haploid genetics [12]. Thus, the long term preservation of genetic diversity must be safeguarded by evolutionary mechanisms which are orthogonal to natural selection such as mutations and speciation (see Chapter 4). This calls for modeling and study of these latter phenomenon in game theoretic terms under discrete replicator dynamics. Additionally below we observe that in some special cases, (i) the rate of convergence of discrete replicator dynamics is doubly exponentially fast in some special cases, and (ii) the expected fitness of the resulting population, starting with a random distribution, under such dynamics is constant factor away from the optimum fitness. It will be interesting to get similar results for the general case of two-player coordination games.

Rate of Convergence. Let's consider a special case where B is a square diagonal matrix. In that case, starting from any point $(\mathbf{x}(0), \mathbf{y}(0))$ observe that after one time step, we get that $\mathbf{x}(1) = \mathbf{y}(1)$ $(i.e., f(\mathbf{x}(0)) = f(\mathbf{y}(0)))$. Therefore without loss of generality let us assume that $\mathbf{x}(0) = \mathbf{y}(0)$. Then both the players get the same payoff from each of their pure strategies in the first play as $B = B^\top$. And thus it follows that $f^n(\mathbf{x}(0)) = f^n(\mathbf{y}(0))$ for all $n \geq 1$. Let $U_i(t)$ be the payoff that both gets from their i-th strategy at time t (both will get the same payoff). Suppose for $i \neq j$ we have $U_i(0) = cU_j(0)$, then

$$\frac{U_i(t)}{U_j(t)} = \left(\frac{B_{ii}x_i(t-1)}{B_{jj}x_j(t-1)} \right)^2 = \left(\frac{U_i(t-1)}{U_j(t-1)} \right)^2 = \left(\frac{U_i(0)}{U_j(0)} \right)^{2^t} = c^{2^t}.$$

Thus the ratio between payoffs from each pure strategy increases doubly exponentially, and the next lemma follows.

Lemma 2.10 (**Rate of convergence**). *If $z = \min_j \frac{U_{i^*}(0)}{U_j(0)}$ where $i^* \in \arg\max_k U_k(0)$, we get that after $O(\log\log \frac{1}{z\epsilon})$ we are ϵ-close to a Nash equilibrium with support $\arg\max_k U_k(0)$ (in terms of the total variation distance).*

2.8 Conclusion and remarks

The results of this chapter appear in [84] and it is joint work with Ruta Mehta and Georgios Piliouras. We show that standard mathematical models of haploid evolution imply the extinction of genetic diversity in the long term limit. This reflects a widely believed conjecture in population genetics [12]. We prove this via recent established connections between game theory, learning theory and genetics [24, 23]. Specifically, in game theoretic terms we show that in the case of coordination games, under minimal genericity assumptions, discrete MWUA converges to pure Nash equilibria for all but a zero measure of initial conditions. This result holds despite the fact that mixed Nash equilibria can be exponentially (or even uncountably) many, completely dominating in number the set of pure Nash equilibria. Thus, in haploid organisms the long term preservation of genetic diversity needs to be safeguarded by other evolutionary mechanisms such as mutations and speciation (see Chapter 4 for mutations and dynamic environments).

The intersection between computer science, genetics and game theory has already provided some unexpected results and interesting novel connections. As these connections become clearer, new questions emerge alongside the possibility of transferring knowledge between these areas. In Section 2.7 we raised some novel questions that have to do with speed of dynamics as well as the possibility of understanding the evolution of biological systems given random initial conditions. Such an approach can be thought of as a middle ground between price of anarchy (worst case scenario) and price of stability (best case scenario) in game theory. We believe that this approach can also be useful from the standard game theoretic lens (see Chapter 6).

CHAPTER III

COMPLEXITY OF GENETIC DIVERSITY IN DIPLOIDS

3.1 Introduction

The beauty and complexity of natural ecosystems have always been a source of fascination and inspiration for the human mind. The exquisite biodiversity of Galapagos' ecosystem, in fact, inspired Darwin to propose his theory of natural selection as an explanatory mechanism for the origin and evolution of species. This revolutionary idea can be encapsulated in the catch phrase "survival of the fittest"[1]. Natural selection promotes the survival of those genetic traits that provide to their carriers an evolutionary advantage.

Arguably, the most influential result in the area of mathematical biology is Fisher's fundamental theorem of natural selection (1930) [51]. It states that the rate of increase in fitness of any organism at any time is equal to its genetic variance in fitness at that time. In the classical model of population genetics (Fisher-Wright-Haldane, discrete or continuous version) of single locus (one gene) multi-allele diploid models it implies that the average fitness of the species populations is always strictly increasing unless we are at an equilibrium. In fact, convergence to equilibrium is point-wise[2] even if there exist continuum of equilibria (see [82] and references therein). This strong result was used in the previous chapter to show Theorem 2.9 (essentially by reducing the haploid dynamics to the classic replicator dynamics). Theorem 2.9 states that in haploids systems all mixed (polymorphic) equilibria are unstable and evolution converges to monomorphic states. However, in the case of diploid systems the answer

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[1]The phrase "survival of the fittest" was coined by Herbert Spencer.

[2]From dynamical systems perspective, this establishes that the average fitness acts as a Lyapunov function for the system and that every trajectory converges to an equilibrium.

to *whether diversity survives or not* depends crucially on the geometry of the fitness landscape.

Besides the purely dynamical systems interpretation, an alternative, more palpable, game theoretic interpretation of these (diploid) genetic systems is possible. Specifically, these systems can be interpreted as symmetric coordination/partnership two-agent games where both agents, starting with the same mixed initial strategy and applying (discrete) replicator dynamics. The analogies are as follows (this is very close to the interpretation we see in the previous chapter due to Chastain *et al.* [23]): The two players are two gene locations on a chromosome pair, and the alleles are their strategies. When both players choose a strategy, say i and j, an individual (i, j) is defined whose fitness, say A_{ij}, is the payoff to both players, hence we have a coordination game. Furthermore, allele pairs are unordered so we have $A_{ij} = A_{ji}$, *i.e.*, A is symmetric and so is the game. The frequencies of the alleles in the initial population, namely $\mathbf{x} := (x_1, ..., x_n) \in \Delta_n$ [3] of n different alleles, corresponds to the initial common mixed strategy of both players. In each generation, every individual from the population mates with another individual picked at random from the population, and the updates of the mixed strategies/allele frequencies are captured by replicator dynamics, *i.e.*,

$$x_i' = x_i \frac{\sum_j A_{ij} x_j}{\mathbf{x}^\top A \mathbf{x}}, \tag{19}$$

where x_i' is the proportion of allele i in the next generation (for details see Section 3.4). In game theoretic language, the fundamental theorem of natural selection implies that the social welfare $\mathbf{x}^\top A \mathbf{x}$ (average fitness in biology terms) of the game acts as potential for the game dynamics. This implies convergence to fixed points of the dynamics (see Theorem 2.1). Fixed points are superset of Nash equilibria where each strategy played with positive probability fetches the same average payoff.

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[3]Recall that Δ_n denotes the simplex of dimension n.

We say that population is genetically diverse if at least two alleles have non-zero proportion in the population, *i.e.,* allele frequencies form a mixed (polymorphic) strategy. The game theoretic results do not provide insight on the *survival of genetic diversity.* One way to formalize this question is *whether there exists a mixed fixed point that the dynamics converges to with positive probability*, given a uniformly random starting point in Δ_n. The answer to this question for the minimal case of $n = 2$ alleles (alleles b/B, individuals $bb/bB/BB$) is textbook knowledge and can be traced back to the classic work of Kalmus (1945) [64]. The intuitive answer here is that diversity can survive when the heterozygote individuals (see A.1 for terms used in biology), bB, have a fitness advantage. Intuitively, this can be explained by the fact that even if evolution tries to dominate the genetic landscape by bB individuals, the random genetic mixing during reproduction will always produce some bb, BB individuals, so the equilibrium that this process is bound to reach will be mixed. On the other hand, it is trivial to create instances where homozygote individuals are the dominant species regardless of the initial condition.

As we increase the size/complexity of the fitness landscape, not only is not clear that a tight characterization of the diversity-inducing fitness landscape exists (a question about global stability of nonlinear dynamical systems), but also, it is even less clear whether one can decide efficiently whether such conditions are satisfied by a given fitness landscape (a computational complexity consideration). How can one address this challenge and moreover, *how can one account for the apparent genetic diversity of the ecosystems around us?*

Our contribution. In a nutshell, we establish that the decision version of the problem is computationally hard (see Theorems 3.27, 3.33), by sandwiching limit points of the dynamics between various stability notions (Theorem 3.1 or 3.11). This core result is shown to be robust across a number of directions. Deciding the existence of

stable (mixed) polymorphic equilibria remains hard under a host of different definitions of stability examined in the dynamical systems literature. The hardness results persist even if we restrict the set of allowable landscape instances to reflect typical instance characteristics (see Theorem 3.31). Despite the hardness of the decision problems, randomly chosen fitness landscapes are shown to support polymorphism with significant probability (at least $^1/_3$, see Theorem 3.17). The game theoretic interpretation of our results allow for proving hardness results for understanding standard game theoretic dynamics in symmetric coordination games. We believe that this is an important result of independent interest as it points out at a different source of complexity in understanding social dynamics.

3.2   Related work

Analyzing limit sets of dynamical systems is a critical step towards understanding the behavior of processes that are inherently dynamic, like evolution. There has been an upsurge in studying the complexity of computing these sets. Quite few works study such questions for dynamical systems governed by arbitrary continuous functions or ordinary differential equations [66, 65, 131]. Limit cycles are inherently connected to dynamical systems and recent works by Papadimitriou and Vishnoi [107] showed that computing a point on an approximate limit cycle is PSPACE-complete. On the positive side, in Chapter 5 we will show that a class of evolutionary Markov chains mix rapidly, where techniques from dynamical systems are used.

The complexity of checking if a game has an evolutionary stable strategy (ESS) has been studied first by Nissan and then by Etessami and Lochbihler [97, 46] and has been nailed down to be Σ_2^P-complete by Conitzer [31]. These decision problems are completely orthogonal to understanding the persistence of genetic diversity. Finally, another recent related result [116] gives connections between computational complexity and ecology/evolution.

3.3 Technical overview

To study survival of diversity in diploidy, we need to characterize limiting population under evolutionary pressure. We focus on the simplest case of single locus (one gene) species. For this case, evolution under natural selection has been shown to follow replicator dynamics in symmetric two-player coordination games ([82], Equations (14)), where the genes on two chromosomes are players and alleles are their strategies as described in the introduction. Losert and Akin established point-wise convergence for this dynamics through a potential function argument [82] (for more information see Theorem 2.1); here average fitness $\mathbf{x}^\top A \mathbf{x}$ is the potential. The limiting population corresponds to fixed points, and so to make predictions about diversity (if the limiting population has support size at least 2) we need to characterize and compute these limiting fixed points.

Let $\mathcal{L}$ denote the set of fixed points with region of attraction of positive (Lebesgue) measure. Hence, given a random starting point replicator dynamics converges to such a fixed point with positive probability. It seems that an exact characterization of $\mathcal{L}$ is unlikely because we do not know necessary and sufficient conditions so that a fixed point has a region of attraction of positive measure. Instead we try to capture it as closely as possible through different stability notions. First we consider two standard notions defined by Lyapunov, the *stable* and *asymptotically stable* fixed point (see Introduction). If we start close to a stable fixed point then we stay close forever, while in case of asymptotically stable fixed point furthermore the dynamics converges to it (see Section 3.4.2). Thus *set of asymptotically stable* $\subseteq \mathcal{L}$ follows, *i.e.,* an asymptotically stable fixed point has region of attraction of positive measure (*e.g.,* a small ball around the fixed point).

Certain properties of these stability notions using the absolute eigenvalues (EVal) of the Jacobian of the update rule (function) of the dynamics are well known: if the Jacobian at a fixed point has an Eval > 1 then the fixed point is *un-stable* (not *stable*),

and if all Eval < 1 then it is asymptotically stable. The case when all Eval ≤ 1 with equality holding for some, is the ambiguous one. In that case we can say nothing about the stability because the Jacobian does not suffice. We call these fixed points *linearly stable* (Definition 4). At a fixed point, say $\mathbf{x}$, if some EVal > 1 then the direction of corresponding eigenvector is repelling, and therefore any starting vector with a component of this vector can never converge to $\mathbf{x}$. Thus points converging to $\mathbf{x}$ can not have positive measure. Using this as an intuition we show that $\mathcal{L} \subseteq$ *set of linearly stable* fixed points. In other words the set of initial points so that the dynamics converges to linearly *un*-stable fixed points has zero measure (Theorem 3.6). This theorem is heavily utilized to understand (non-)existence of diversity.

Efficient computation requires efficient verification. However, note that whether a given fixed point is (asymptotically) stable or not does not seem easy to verify. To achieve this, one of the contributions of this chapter is the definition of two more notions: *Nash stable* and *strict Nash stable* [4]. It is easy to see that NE of the corresponding coordination game described in introduction are fixed points of the replicator dynamics (Equations (19),(20)) but not vice-versa. Keeping this in mind we define Nash stable fixed point, which is a NE and the sub-matrix corresponding to its support satisfies certain negative semi-definiteness. The latter condition is derived from the fact that stability is related to local optima of $\mathbf{x}^\top A \mathbf{x}$ and also from Sylvester's law of inertia [99] (see Section 3.5 and proofs). For strict Nash stable both conditions are strict, namely strict NE and negative definite. Combining all of these notions we show the following:

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[4] These two notions are not the same as evolutionary stable strategies/states.

Theorem 3.1 (Relations between stability notions).

$$\textit{Strict Nash stable} \subseteq \textit{Asymptotically stable} \subseteq \mathcal{L} \subseteq \textit{linearly stable} = \textit{Nash stable}$$

$$\cap |$$

$$\textit{stable} \subseteq \textit{linearly stable} = \textit{Nash stable}$$

We note that the sets asymptotically stable, stable, $\mathcal{L}$ and linearly stable of Theorem 3.1 do not coincide in general. The example below makes the statement clear.

Example. Let x_{t+1} be the next step for the following update rules:

$$f(x_t) = \frac{1}{2}x_t, \; g(x_t) = x_t - \frac{1}{2}x_t^2, \; h(x_t) = x_t + \frac{x_t^3}{2}, \; d(x_t) = x_t.$$

Then for dynamics governed by f, 0 is asymptotically stable, stable and linearly stable, and hence is also in $\mathcal{L}$. While for g it is linearly stable and is in $\mathcal{L}$, but is not stable or asymptotically stable. For d it is linearly stable and stable, but not asymptotically stable and is not in $\mathcal{L}$. Finally, for h it is only linearly stable, and does not belong to any other class[5].

Our primary goal was to see if diversity is going to survive. We formalize this by checking whether set $\mathcal{L}$ contains a mixed point, *i.e.,* where more than one alleles have non-zero proportion, implying that diversity survives with some positive probability, where the randomness is w.r.t the random initial $\mathbf{x} \in \Delta_m$. In Section 3.7 we show that for all five notions of stability, checking existence of mixed fixed point is NP-hard. This gives NP-hardness for checking survival of diversity as well.

Theorem 3.2 (Informal - Hard to predict diversity). *Given a symmetric matrix A, it is NP-hard to check if replicator dynamics with payoff A has mixed (asymptotically) stable, linear-stable, or (strict) Nash stable fixed points. A common reduction for all together with Theorem 3.1 will imply that it is NP-hard to check whether diversity survives for a given fitness matrix.*

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[5]We also note that generically these sets coincide for replicator dynamics. It can be shown [83] that given a fitness matrix, its entries can be perturbed to ensure that fixed points are *hyperbolic*. Formally, if we consider the dynamics as an operator (called *Fisher* operator) then the set of hyperbolic operators is dense in the space of Fisher operators.

Our reductions are from k-**clique** - given an undirected graph check if it has a clique of size k; a well known NP-hard problem. Given an instance G of k-*clique*, we will construct a symmetric matrix A as shown in Figure 4, and consider coordination game (A, A). We show that if G has a clique of size k then (A, A) has a mixed strict Nash stable equilibrium, and if (A, A) has a mixed Nash stable equilibrium then G has a clique of size k. This together with the fact that all other

Figure 4: See Equations (24).

notions of stability including our target set $\mathcal{L}$ are sandwiched between strict Nash stable and Nash stable equilibria implies checking existence of mixed fixed point for any notions of the (strict) Nash stable, (asymptotically) stable, linearly stable, and $\mathcal{L}$ is NP-hard.

The main idea in the construction of matrix A (Figure 4) is to use modified version of adjacency matrix E of the graph as one of the blocks in the payoff matrix such that, (i) clique of size k or more implies a stable Nash equilibrium in that block, and (ii) all stable mixed equilibria are only in that block. Here E' is modification of E where off-diagonal zeros are replaced with $-h$; h is a large (polynomial-size) number.

The fitness matrix created for hardness results is very specific, while one could argue that real-life fitness matrices may be more random. *So is it easy to check survival of diversity for a typical matrix? Or is it easy to check if a given allele survives?* We answer negatively for both of these.

There has been a lot of work on NP-hardness for decision versions of Nash equilibrium in general games [59, 32, 124, 56], where finding one equilibrium is also PPAD-hard [25]. Whereas to the best of our knowledge these are the first NP-hardness results for coordination games, where finding one Nash equilibrium is easy, and therefore may be of independent interest. Finally in Section 3.6 we show that even though checking is hard, on average things are not that bad.

Theorem 3.3 (**Informal - Survival with constant probability**). *If the entries of a fitness matrix are i.i.d. on an atomless distribution then with significantly high*

probability, at least ¹/₃, diversity will surely survive.

Sure survival happens if every fixed point in $\mathcal{L}$ is mixed. We show that this fact is ensured if every diagonal entry (i, i) of the fitness matrix is dominated by some entry in its row or column. Next we lower bound the probability of latter *by a constant* for a random symmetric matrix (from atomless distribution) of *any size*. The tricky part is to avoid correlations arising due to symmetry and we achieve this using an inclusion-exclusion argument.

3.4   Preliminaries

In this section we formally describe the diploid dynamics, which is exactly discrete replicator dynamics as described in Section 2.4.2, Equations (14).

3.4.1   Infinite population dynamics for diploids

Consider a diploid single locus species, in other words species with chromosome pair and single gene. Every gene has a set of representative alleles, like gene for eye color has different alleles for brown, black and blue eyes. Let n be the number of alleles for the single gene of our species, and let these be numbered $1, \ldots, n$. An individual is represented by an unordered pair of alleles (i, j), and we denote its fitness by A_{ij}. The fitness represents its ability to reproduce during a mating. In every generation two individuals are picked uniformly at random from the population, say (i, j) and (i', j'), and they mate. The allele pair of the offspring can be any of the four possible combinations, namely $(i, i'), (i, j'), (i', j), (j, j')$, with equal probability[6]. Let X_i be a random variable that denotes the proportion of the population with allele i. After one generation, the expected number of offsprings with allele i is proportional to $X_i \cdot X_i \cdot (A\mathbf{X})_i + 2\frac{1}{2}(1 - X_i)X_i \cdot (A\mathbf{X})_i = X_i(A\mathbf{X})_i$ (X_i^2 stands for the probability that first individual has both his alleles i, *i.e.,* is represented by (i, i) - and thus the

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[6]Punnett Square.   See http://www.nature.com/scitable/topicpage/inheritance-of-traits-by-offspring-follows-predictable-6524925 for a nice article.

offspring will inherit allele i - and $2\frac{1}{2}(1 - X_i)X_i$ stands for the probability that the first individual has allele i exactly once in his representation and the offspring will inherit). Hence, if $\mathbf{X}$ denote the frequencies of the alleles in the population in the next generation (random variables)

$$E[X_i'|\mathbf{X}] = \frac{X_i(A\mathbf{X})_i}{\mathbf{X}^\top A\mathbf{X}}.$$

We focus on the *deterministic* version of the equations above, which captures the infinite population model. Thus if $\mathbf{x} \in \Delta_n$ represents the proportions of alleles in the current population, under the evolutionary process of natural-selection (the reproduction happens as described) this proportion changes as per the following multivariate function $f : \Delta_n \to \Delta_n$ under the infinite population model [82]; discrete replicator dynamics (Chapter 2, Equations (14)).

$$\mathbf{x}' = f(\mathbf{x}) \quad \text{where} \quad x_i' = f_i(\mathbf{x}) = x_i\frac{(A\mathbf{x})_i}{\mathbf{x}^\top A\mathbf{x}}, \quad \forall i \in [n] \tag{20}$$

where $\mathbf{x}'$ are the proportions of the next generation. f is a continuous function with convex, compact domain (= range), and therefore always has a fixed point [63]. Further, limit points of f have to be fixed points.

3.4.2 Stability and eigenvalues

By Definition 3 it follows that if $\mathbf{x}$ is asymptotically stable with respect to dynamics f (20), then the set of initial conditions in Δ so that the dynamics converge to $\mathbf{x}$ has positive measure. Using the fact that under f the potential function $\pi(\mathbf{x}) = \mathbf{x}^\top A\mathbf{x}$ strictly decreases unless $\mathbf{x}$ is a fixed point, the next theorem was derived in [83].

Theorem 3.4 (Stable fixed points $\Leftrightarrow$ local minima [83], § 9.4.7)**.** *A fixed point* $\mathbf{r}$ *of dynamics (20) is stable if and only if it is a local maximum of* π*, and is asymptotically stable if and only if it is a strict local maximum.*

As the domain of π is closed and bounded, there exists a global maximum of π in Δ_n, which by Theorem 3.4 is a stable fixed point, and therefore its existence follows.

However, existence of asymptotically stable fixed point is not guaranteed, for example if $A = [1]_{m \times n}$ then no $\mathbf{x} \in \Delta_n$ is attracting under f.

To analyze limiting points of f with respect to the notion of stability in terms of perturbation resistant, we need to use the eigenvalues of the Jacobian of f at fixed points. Let $J^{\mathbf{r}}$ denote the Jacobian at $\mathbf{r} \in \Delta_n$. The following theorem in dynamics/control theory relates (asymptotically) stable fixed points with the eigenvalue of its Jacobian. Theorem 1.2 implies that eigenvalues of the Jacobian at a stable fixed point have absolute value at most 1, however the converse may not hold. Below we provide the equations of the Jacobian.

Equations of Jacobian. Since f is defined on n variables while its domain is Δ_n which is of $n - 1$ dimension, we consider a projected Jacobian by replacing a strategy t with $x_t > 0$ by $1 - \sum_{i \neq t} x_i$ in f.

$$J_{ii}^{\mathbf{x}} = \frac{(A\mathbf{x})_i}{\mathbf{x}^\top A \mathbf{x}} + x_i \frac{(A_{ii} - A_{it})(\mathbf{x}^\top A \mathbf{x}) - 2(A\mathbf{x})_i((A\mathbf{x})_i - (A\mathbf{x})_t)}{(\mathbf{x}^\top A \mathbf{x})^2},$$

$$J_{ij}^{\mathbf{x}} = x_i \frac{(A_{ij} - A_{it})(\mathbf{x}^\top A \mathbf{x}) - 2(A\mathbf{x})_i((A\mathbf{x})_j - (A\mathbf{x})_t)}{(\mathbf{x}^\top A \mathbf{x})^2}.$$

If $\mathbf{x}$ is a fixed point of f, then using Remark 3.5 below the above simplifies to,

$$J_{ii}^{\mathbf{x}} = 1 + x_i \frac{(A_{ii} - A_{it})}{\mathbf{x}^\top A \mathbf{x}} \text{ if } x_i > 0 \quad \text{and} \quad J_{ii}^{\mathbf{x}} = \frac{(A\mathbf{x})_i}{\mathbf{x}^\top A \mathbf{x}} \text{ if } x_i = 0,$$

$$J_{ij}^{\mathbf{x}} = x_i \frac{A_{ij} - A_{it}}{\mathbf{x}^\top A \mathbf{x}} \text{ if } x_i, x_j > 0 \quad \text{and} \quad J_{ij}^{\mathbf{x}} = 0 \text{ if } x_i = 0.$$

Fact 3.5. *Profile* $\mathbf{x}$ *is a fixed point of* f *iff* $\forall i \in [n], \ x_i > 0 \Rightarrow (A\mathbf{x})_i = \mathbf{x}^\top A \mathbf{x}$.

Using properties of $J^{\mathbf{x}}$ and [82], we prove next:

Theorem 3.6 (Replicator converges to stable fixed points). *The set of initial conditions in* Δ_n *so that the dynamics (20) converge to linearly unstable fixed points has measure zero.*

Proof. This is an application of Center-stable Manifold Theorem 1.3 and the proof is similar to that of Theorem 2.9. To use Center-stable Manifold Theorem we need

to project the map of the dynamics (20) to a lower dimensional space. We consider the (diffeomorphism) function g that is a projection of the points $\mathbf{x} \in \mathbb{R}^n$ to $\mathbb{R}^{n-1}$ by excluding a specific (the "first") variable. We denote this projection of Δ_n by $g(\Delta_n)$, i.e., $\mathbf{x} \rightarrow_g (\mathbf{x}')$ where $\mathbf{x}' = (x_2, \ldots, x_n)$. Further, we define the fixed point dependent projection function $z_{\mathbf{r}}$ where we remove one variable x_t so that $\mathbf{r}_t > 0$ (like function g but the removed strategy must be chosen with positive probability at $\mathbf{r}$).

Let f be the map of dynamical system (20). For a linearly unstable fixed point $\mathbf{r}$ we consider the function $\psi_{\mathbf{r}}(\mathbf{v}) = z_{\mathbf{r}} \circ f \circ z_{\mathbf{r}}^{-1}(\mathbf{v})$ which is C^1 local diffeomorphism (due to the point-wise convergence of f, i.e., Theorem 2.1, we know that the rule of the dynamical system is a diffeomorphism), with $\mathbf{v} \in R^{n-1}$. Let $B_{\mathbf{r}}$ be the ball derived from Theorem 1.3 and consider the union of these balls (transformed in $\mathbb{R}^{n-1}$)

$$A = \cup_{\mathbf{r}} A_{\mathbf{r}},$$

where $A_{\mathbf{r}} = g(z_{\mathbf{r}}^{-1}(B_{\mathbf{r}}))$ ($z_{\mathbf{r}}^{-1}$ "returns" the set $B_{\mathbf{r}}$ back to $\mathbb{R}^n$). Set $A_{\mathbf{r}}$ is an open subset of $\mathbb{R}^{n-1}$ (by continuity of $z_{\mathbf{r}}$). Due to the Lindelőf's Lemma A.1, we can find a countable subcover for A, i.e., there exists fixed points $\mathbf{r}_1, \mathbf{r}_2, \ldots$ such that $A = \cup_{m=1}^{\infty} A_{\mathbf{r}_m}$.

For a $t \in \mathbb{N}$ let $\psi_{t,\mathbf{r}}(\mathbf{v})$ the point after t iteration of dynamics (20), starting with $\mathbf{v}$, under projection $z_{\mathbf{r}}$, i.e., $\psi_{t,\mathbf{r}}(\mathbf{v}) = z_{\mathbf{r}} \circ f^t \circ z_{\mathbf{r}}^{-1}(\mathbf{v})$. If point $\mathbf{v} \in g(\Delta_n)$ (which corresponds to $g^{-1}(\mathbf{v})$ in our original Δ_n) has a linearly unstable fixed point as a limit, there must exist a t_0 and m so that $\psi_{t,\mathbf{r}_m} \circ z_{\mathbf{r}_m} \circ g^{-1}(\mathbf{v}) \in B_{\mathbf{r}_m}$ for all $t \geq t_0$ (we have point-wise convergence from Theorem 2.1) and therefore again from Theorem 1.3 and the fact that $g(\Delta_n)$ is invariant we get that $\psi_{t_0,\mathbf{r}_m} \circ z_{\mathbf{r}_m} \circ g^{-1}(\mathbf{v}) \in W_{loc}^{sc}(\mathbf{r}_m)$, hence $\mathbf{v} \in g \circ z_{\mathbf{r}_m}^{-1} \circ \psi_{t_0,\mathbf{r}_m}^{-1}(W_{loc}^{sc}(\mathbf{r}_m) \cap z_{\mathbf{r}_m}(\Delta_n))$. Hence the set of points in $g(\Delta_n)$ whose ω-limit has a linearly unstable equilibrium is a subset of

$$C = \cup_{m=1}^{\infty} \cup_{t=1}^{\infty} g \circ z_{\mathbf{r}_m}^{-1} \circ \psi_{t,\mathbf{r}_m}^{-1}(W_{loc}^{sc}(\mathbf{r}_m) \cap z_{\mathbf{r}_m}(\Delta_n)). \tag{21}$$

Since $\mathbf{r}_m$ is linearly unstable, it holds that $dim(E^u) \geq 1$, and therefore dimension

of $W_{loc}^{sc}(\mathbf{r}_m)$ is at most $n-2$. Thus, the set $W_{loc}^{sc}(\mathbf{r}_m) \cap z_{\mathbf{r}_m}(\Delta_n)$ has Lebesgue measure zero in $\mathbb{R}^{n-1}$. Finally since $g \circ z_{\mathbf{r}_m}^{-1} \circ \psi_{t,\mathbf{r}_m}^{-1} : \mathbb{R}^{n-1} \to \mathbb{R}^{n-1}$ is continuously differentiable (in a neighborhood of $g(\Delta_n)$, by Theorem 2.1), $\psi_{t,\mathbf{r}_m}$ is C^1 and locally Lipschitz (see [110] p.71). Therefore using Lemma A.2 below it preserves the null-sets, and thereby we get that C is a countable union of measure zero sets, *i.e.,* is measure zero as well, and Theorem 3.6 follows. $\qquad\square$

In Theorem 3.6 we manage to discard only those fixed points whose Jacobian has eigenvalue with absolute value > 1, while characterizing limiting points of f; the latter is finally used to argue about the survival of diversity.

3.5 Convergence, stability, and characterization

As established in Section 3.4.1, evolution in single locus diploid species is governed by dynamics f of (20). Understanding survival of diversity requires to analyze the following set,

$$\mathcal{L} = \{\mathbf{x} \in \Delta_n \mid \text{positive measure of starting points converge to } \mathbf{x} \text{ under } f\}. \quad (22)$$

By Definition 3 it follows that asymptotically stable $\subseteq \mathcal{L}$. In addition, the characterization of linearly stable fixed point from Theorem 3.6 implies $\mathcal{L} \subseteq$ linearly stable. In this section we try to characterize $\mathcal{L}$ using various notions of stability, which have game theoretic and combinatorial interpretation. These notions sandwich set-wise the classic notions of stability given in the preliminaries, and thereby give us a partial characterization of $\mathcal{L}$. This characterization turns out to be crucial for our hardness results as well as results on survival in random instances.

Given a symmetric matrix A, a two-player game (A, A) forms a symmetric coordination game. We identify special symmetric NE of this game to characterize stable fixed points of f. Given a profile $\mathbf{x} \in \Delta_n$, define a transformed matrix $T(A, \mathbf{x})$ of

dimension $(k-1) \times (k-1)$, where $k = |SP(\mathbf{x})|$, as follows.

Let $SP(\mathbf{x}) = \{i_1, \ldots, i_k\}$, $B = T(A, \mathbf{x})$. $\forall a, b < k$, $B_{ab} = A_{i_a i_b} + A_{i_k i_k} - A_{i_a i_k} - A_{i_k i_b}$.

$$(23)$$

Since A is symmetric it is easy to check that B is also symmetric, and therefore has real eigenvalues. Recall the Definition 9 of strict symmetric NE.

Definition 11 (**Notion of (strict) Nash stable**). *A strategy* $\mathbf{x}$ *is called (strict) Nash stable if it is a (strict) symmetric NE of the game* (A, A)*, and* $T(A, \mathbf{x})$ *is negative (definite) semi-definite.*

Lemma 3.7. *For any given* $\mathbf{x} \in \Delta_n$*,* $T(A, \mathbf{x})$ *is negative (definite) semi-definite iff* $(\mathbf{y}^\top A \mathbf{y} < 0)$ $\mathbf{y}^\top A \mathbf{y} \leq 0$*,* $\forall y \in \mathbb{R}^n$ *such that* $\sum_i y_i = 0$ *and* $x_i = 0 \Rightarrow y_i = 0$*.*

Proof. It suffices to assume that $\mathbf{x}$ is fully mixed. Let $\mathbf{z}$ be any vector with $\sum_i z_i = 0$ and define the vector $\mathbf{w} = (z_1 - z_n, \ldots, z_{n-1} - z_n)$ with support $n-1$. It is clear that $\mathbf{z}^\top A \mathbf{z} \leq 0$ iff $\mathbf{w}^\top T(A, \mathbf{x}) \mathbf{w} \leq 0$. So if $\mathbf{z}^\top A \mathbf{z} \leq 0$ for all $\mathbf{z}$ with $\sum_i z_i = 0$ then $T(A, \mathbf{x})$ is negative semidefinite. If there exists a $\mathbf{z}$ with $\sum_i z_i = 0$ s.t $\mathbf{z}^\top A \mathbf{z} > 0$ then $\mathbf{w}^\top T(A, \mathbf{x}) \mathbf{w} > 0$, so $T(A, \mathbf{x})$ is not negative semidefinite. $\square$

Since stable fixed points are local optima, we map them to Nash stable strategies.

Lemma 3.8 (**Stable fixed point implies Nash stable**). *Every stable fixed point* $\mathbf{r}$ *of* f *is a Nash stable of game* (A, A)*.*

Proof. There is a similar proof in [83] for a modified claim. Here we connect the two. First of all, observe that if $(\mathbf{r}, \mathbf{r})$ is not Nash equilibrium for (A, A) game then there exists a j such that $r_j = 0$ and $(A\mathbf{r})_j > \mathbf{r}^\top A\mathbf{r}$. But $\frac{(A\mathbf{r})_j}{\mathbf{r}^\top A\mathbf{r}} > 1$ is an eigenvalue of $J^\mathbf{r}$.

Additionally, since $\mathbf{r}$ is stable, using Theorem 3.4 we have that $\mathbf{r}$ is a local maximum of $\pi(\mathbf{x}) = \mathbf{x}^\top A\mathbf{x}$, say in a neighborhood $\|\mathbf{x} - \mathbf{r}\| < \delta$. Let $\mathbf{y}$ be a vector with support subset of the support of $\mathbf{r}$ such that $\sum_i y_i = 0$. Firstly we rescale it w.l.o.g

so that $\|\mathbf{y}'\| < \delta$ and by setting $\mathbf{z} = \mathbf{y}' + \mathbf{r}$ we have that

$$\mathbf{z}^\top A \mathbf{z} = \mathbf{y}'^\top A \mathbf{y}' + \mathbf{r}^\top A \mathbf{r} + 2\mathbf{y}'^\top A \mathbf{r}.$$

But $\mathbf{y}'^\top A \mathbf{r} = 0$ since $(A\mathbf{r})_i = (A\mathbf{r})_j$ for all i, j s.t $r_i, r_j > 0$, $\sum_i y_i' = 0$, $\mathbf{y}'$ has support subset of the support of $\mathbf{r}$. Therefore $\mathbf{y}'^\top A \mathbf{y}' + \mathbf{r}^\top A \mathbf{r} = \mathbf{z}^\top A \mathbf{z} \leq \mathbf{r}^\top A \mathbf{r}$, thus $\mathbf{y}'^\top A \mathbf{y}' \leq 0$. Hence proved using Lemma 3.7. $\qquad\square$

Since stable fixed points always exist, so do Nash stable strategies (Lemma 3.8). Next we map strict Nash stable strategies to asymptotically stable fixed points, as the negative definiteness and strict symmetric Nash of the former implies strict local optima, and the next lemma follows.

Lemma 3.9 (Strict Nash stable implies asymptotically stable [83] § 9.2.5)**.** *Every strict Nash stable is asymptotically stable.*

Proof. The proof can be found in [83]. The sufficient conditions for a fixed point to be asymptotically stable in the proof are exactly the assumptions for a fixed point to be strict Nash stable. $\qquad\square$

The above two lemmas show that strict Nash stable $\subseteq$ asymptotically stable (by definition) $\subseteq$ stable (by definition) $\subseteq$ Nash stable. Further, by Theorem 1.2 and the definition of linearly stable fixed points we know that stable $\subseteq$ linearly stable. What remains is the relation between Nash stable and linearly stable. The next lemma answers this.

Lemma 3.10 (Nash stable equivalent with linearly stable). *Strategy* $\mathbf{r}$ *is Nash stable iff it is a linearly stable fixed point.*

Proof. Let t be the removed strategy (variable x_t) to create $J^{\mathbf{r}}$ (with $r_t > 0$). For every i such that $r_i = 0$ we have that $J_{ii}^{\mathbf{r}} = \frac{(A\mathbf{r})_i}{\mathbf{r}^\top A \mathbf{r}}$ and $J_{ij}^{\mathbf{r}} = 0$ for all $j \neq i$. Hence the corresponding eigenvalues of $J^{\mathbf{r}}$ of the rows i that do not belong in the support of $\mathbf{r}$

(i-th row has all zeros except the diagonal entry $J_{ii}^{\mathbf{r}} = \frac{(A\mathbf{r})_i}{\mathbf{r}^\top A \mathbf{r}}$) are $\frac{(A\mathbf{r})_i}{\mathbf{r}^\top A \mathbf{r}} > 0$ which are less than or equal to 1 iff $(\mathbf{r}, \mathbf{r})$ is a NE of the game (A, A).

Let $\mathbb{J}^{\mathbf{r}}$ be the submatrix of $J^{\mathbf{r}}$ by removing all columns/rows $j \notin SP(\mathbf{r})$. Let A' be the submatrix of A by removing all removing all columns/rows $j \notin SP(\mathbf{r})$. It suffices to prove that $T(A, \mathbf{r})$ is negative semi-definite iff $\mathbb{J}^{\mathbf{r}}$ has eigenvalues with absolute value at most 1.

Let $k = |SP(\mathbf{r})|$ and the $k \times k$ matrix L with $L_{ij} = r_i \frac{A_{ij}}{\mathbf{r}^\top A \mathbf{r}}$ and $i, j \in SP(\mathbf{r})$. Observe that L is stochastic and also symmetrizes to $L'_{ij} = \sqrt{r_i r_j} \frac{A_{ij}}{\mathbf{r}^\top A \mathbf{r}}$, i.e., L, L' have the same eigenvalues. Therefore L has an eigenvalue 1 and the rest eigenvalues are real between $(-1, 1)$ and also A' has eigenvalues with the same signs as L'.

Finally, we show that $det(L - \lambda I_k) = (1 - \lambda) \times det(\mathbb{J}'^{\mathbf{r}} - \lambda I_{k-1})$ with $\mathbb{J}'^{\mathbf{r}} = \mathbb{J}^{\mathbf{r}} - \mathbb{J}^{\mathbf{r}} - I_{k-1}$, namely L has the same eigenvalues as $\mathbb{J}'^{\mathbf{r}}$ plus eigenvalue 1. It is true for a square matrix that by row/column to another row/column, the determinant stays invariant. We consider $L - \lambda I_k$ and we do the following: We subtract the t-th column from every other column and on the resulting matrix, we add every row to the t-th row. The resulting matrix R has the property that $det(R) = (1 - \lambda) \times det(\mathbb{J}'^{\mathbf{r}} - \lambda I_{k-1})$ and also $det(R) = det(L - \lambda I_k)$.

From above we get that if $\mathbb{J}^{\mathbf{r}}$ has eigenvalues with absolute value at most 1, then $\mathbb{J}^{\mathbf{r}} - I_{k-1}$ has eigenvalues in $[-2, 0]$ (we know that are real from the fact that L is symmetrizes to L'), hence L' has eigenvalue 1 and the rest eigenvalues are in $[-2, 0]$ (since L is stochastic, the rest eigenvalues lie in $(-1, 0]$). Therefore A' has positive inertia 1 (see Sylvester's law of inertia) and the one direction For the converse, $T(A, \mathbf{r})$ being negative semi-definite implies A' has positive inertia 1, thus L' and so L have one eigenvalue positive (which is 1) and the rest non-positive (lie in $(-1, 0]$ since L is stochastic). Thus $\mathbb{J}^{\mathbf{r}} - I_{k-1}$ has eigenvalues in $(-1, 0]$ and therefore $\mathbb{J}^{\mathbf{r}}$ has eigenvalues in $(0, 1]$ (i.e., with absolute value at most 1). $\square$

Using Theorems 3.4 and 3.6, and Lemmas 3.8, 3.9 and 3.10 we get the following

characterization among all the notions of stability that we have discussed so far. We also remind you that asymptotically stable $\subseteq \mathcal{L} \subseteq$ linearly stable.

Theorem 3.11 (Relations between stability notions). *Given a symmetric matrix A, we have*

$$\text{Strict Nash stable} \subseteq \text{Asymptotically stable} \subseteq \mathcal{L} \subseteq \text{linearly stable} = \text{Nash stable}$$

$$\cap |$$

$$\text{stable} \subseteq \text{linearly stable} = \text{Nash stable}$$

As stated before, generically (random fitness matrix) we have hyperbolic fixed points and all the previous notions coincide. Given a fitness (positive) matrix A, let $\mathbf{x}$ be a limit point of dynamics f governed by (20) If it is not pure, *i.e.,* $|SP(\mathbf{x})| > 1$ then at least two alleles survive among the population, and we say the population is diverse in the limit.

3.6 Survival of diversity

Definition 12 (Survival of diversity). *We say that* diversity survives *in the limit if there exists* $\mathbf{x} \in \mathcal{L}$ *such that* $\mathbf{x}$ *is not pure (is mixed), and* diversity survives surely *if no* $\mathbf{x} \in \mathcal{L}$ *is pure.*

We provide sufficient conditions for two extreme cases of fitness matrix for the survival of diversity, where diversity always survives and where diversity disappears regardless of the starting population. Using this characterization we analyze the chances of survival of diversity when fitness matrix and starting populations are picked uniformly at random from atomless distributions.

Since $\mathcal{L} \subseteq$ Nash stable = linearly stable (Theorem 3.11), there has to be at least one mixed Nash (or linearly) stable strategy for diversity to survive (see Definition 12). Next we give a definition that captures the homozygote/heterozygote advantage and a lemma which uses it to identify instances that lack mixed Nash stable strategies.

Definition 13 (Dominating/dominated diagonal entries). *Diagonal entry* A_{ii} *is called* dominated *if and only if* $\exists j$, *such that* $A_{ij} > A_{ii}$. *And it is called* dominating *if and only if* $A_{ii} > A_{ij}$ *for all* $j \neq i$.

Next lemma characterizes instances that lack mixed Nash stable.

Lemma 3.12 (Dominating diagonal implies no mixed stable fixed points). *If all diagonal entries of A are dominating then there are no mixed linearly stable fixed points.*

Proof. Let $\mathbf{r}$ be a fixed point and w.l.o.g strategy 1 is in its support and assume that $J^{\mathbf{r}}$ is the projected Jacobian at $\mathbf{r}$ by removing strategy 1 (let $k \times k$ be its size). $J^{\mathbf{r}}$ has diagonal entries $1 + r_i \frac{A_{ii} - A_{i1}}{\mathbf{r}^\top A \mathbf{r}}$. Hence $tr(J^{\mathbf{r}}) = k + \sum_i r_i \frac{(A_{ii} - A_{i1})}{\mathbf{r}^\top A \mathbf{r}} > k$, as $A_{ii} > A_{ij}, \forall i \neq j$. Therefore there exists an eigenvalue with absolute value greater than 1 if $k > 0$. $\qquad\square$

The next theorem follows using Theorem 3.6 and Lemma 3.12 above. Informally, it states that if every diagonal entry of A is dominating then almost surely the dynamics converge to pure fixed points.

Theorem 3.13 (Homozygous advantage inhibitor of diversity). *If every diagonal entry of A is dominating then the set of initial conditions in Δ_n so that the dynamics (20) converges to mixed fixed points has measure zero, i.e., diversity dies almost surely.*

Next we show sure survival of diversity when diagonals are dominated.

Lemma 3.14. *Let $\mathbf{r}$ be a fixed point of f with $r_t = 1$. If A_{tt} is dominated, then $\mathbf{r}$ is linearly unstable.*

Proof. The equations of the projected Jacobian $J^{\mathbf{r}}$ at $\mathbf{r}$ are:

$J^{\mathbf{r}}_{i,i} = \frac{(A\mathbf{r})_i}{\mathbf{r}^\top A\mathbf{r}} + \mathbf{r}_i \frac{A_{ii} - A_{it}}{(\mathbf{r}^\top A\mathbf{r})} = \frac{A_{it}}{A_{tt}}$ and $J^{\mathbf{r}}_{i,j} = \mathbf{r}_i \frac{A_{ij} - A_{it}}{\mathbf{r}^\top A\mathbf{r}} = 0$. The eigenvalues of $J^{\mathbf{r}}$ are $\frac{A_{it}}{A_{tt}}$ for all $i \neq t$. By assumption, there exists a t' such that $A_{t't} > A_{tt}$ and hence $J^{\mathbf{r}}$ will have $\frac{A_{t't}}{A_{tt}} > 1$ as an eigenvalue. $\qquad\square$

If all pure fixed points that are linearly unstable, then all linearly stable fixed points are mixed, and thus the next theorem follows using Theorem 3.11 and Lemma 3.14.

Theorem 3.15 (Heterozygote advantage implies diversity). *If every diagonal of A is dominated then no $\mathbf{x} \in \mathcal{L}$ is pure, i.e., diversity survives almost surely.*

The following lemma shows that when the entries of a fitness matrix are picked uniformly independently from an atomless distribution, there is a positive probability (bounded away from zero for all n) so that every diagonal in A is dominated. This essentially means that generically, diversity survives with positive probability, bounded away from zero, where the randomness is taken with respect to both the payoff matrix and initial conditions.

Lemma 3.16 (Heterozygote advantage with constant probability). *Let entries of A be chosen i.i.d from an atomless distribution. The probability that all diagonals of A are dominated is at least $\frac{1}{3} - o(1)$.*

Proof. Let E_i be the event that A_{ii} is *dominating*. We get that:

$$\mathbb{P}[E_i] = \frac{1}{n}.$$

Also for $n \geq 6$ we have that

$$\mathbb{P}[E_i \cap E_j \cap E_k] \leq \frac{1}{(n-3)^3}$$

for $i \neq j \neq k \neq i$. To prove this let D_i correspond to the events $A_{ii} > A_{it}$ for all $t \neq i, j, k$ (in same way the definition of D_j, D_k). Clearly D_i, D_j, D_k are independent and thus $\mathbb{P}[D_i \cap D_j \cap D_k] = \frac{1}{(n-3)^3}$. Since $E_i \cap E_j \cap E_k \subset D_i \cap D_j \cap D_k$ the inequality follows.

Finally by counting argument (count all the favor permutations) we get that

$$\mathbb{P}\left[E_i \cap E_j\right] \geq \frac{2[\sum_{k=0}^{n-2}(2n-3-k)!\frac{(n-2)!}{(n-2-k)!}]}{(2n-1)!} = \frac{2}{n(n-1)}\sum_{k=0}^{n-2}\prod_{i=0}^{k+1}\frac{n-i}{2n-i-1}$$

for $i \neq j$. For $l = o(n)$, for example $l = \log n$ and using the fact that $\frac{n-i}{2n-i-1}$ is decreasing with respect to i we get that

$$\sum_{k=0}^{n-2}\prod_{i=0}^{k+1}\frac{n-i}{2n-i-1} \geq \sum_{k=0}^{l}\prod_{i=0}^{k+1}\frac{n-i}{2n-i-1}$$

$$\geq \sum_{k=0}^{l}\left(\frac{n-k-1}{2n-k-2}\right)^{k+2}$$

$$\geq \sum_{k=0}^{l}\left(\frac{n-l-1}{2n-l-2}\right)^{k+2}$$

$$= \left(\frac{n-l-1}{2n-l-2}\right)^{2}\left(\frac{1-(\frac{n-l-1}{2n-l-2})^{l+1}}{1-\frac{n-l-1}{2n-l-2}}\right) = \frac{1}{2} - o(1).$$

Therefore (inclusion-exclusion) we have that

$$\mathbb{P}\left[\cup E_i\right] \leq \sum_{i}\mathbb{P}\left[E_i\right] - \sum_{i<j}\mathbb{P}\left[E_i \cap E_j\right] + \sum_{i<j<k}\mathbb{P}\left[E_i \cap E_j \cap E_k\right],$$

thus

$$\mathbb{P}\left[\cap E_i^c\right] \geq \frac{1}{2} - o(1) - \frac{n(n-1)(n-2)}{6(n-3)^3} = \frac{1}{3} - o(1),$$

which is bounded away from zero. $\qquad\square$

The next theorem follows using Theorem 3.15 and Lemma 3.16.

Theorem 3.17 (Diversity survives with constant probability). *Assume that the fitness matrix has entries picked independently from an atomless distribution then with significantly high probability, at least $\frac{1}{3} - o(1)$, diversity will survive surely.*

Remark 5 (Typical instance). *Observe that letting X_i be the indicator random variable that A_{ii} is dominating and $X = \sum_i X_i$ we get that $E[X] = \sum_i E[X_i] = \sum_i \mathbb{P}[E_i] = n \times \frac{1}{n} = 1$ so in expectation we will have one dominating element. Also*

from the above proof of Lemma 3.16 we get that $E[X^2] = \sum_i E[X_i] + 2 \sum_{i<j} E[X_i X_j] = 1 + n(n-1)\mathbb{P}[E_i \cap E_j] \approx 2 - o(1)$ *(namely* $Var[X] \approx 1 - o(1)$*) so by Chebyshev's inequality* $\mathbb{P}[|X - 1| > k]$ *is* $O(\frac{1}{k^2})$.

3.7 NP-hardness results

Positive chance of survival of phenotypic (allele) diversity in the limit under the evolutionary pressure of selection (Definition 12), implies existence of a mixed linearly stable fixed point (Theorem 3.6). This notion encompasses all the other notions of stability (Theorem 3.11), and may contain points that are not attracting. Whereas, strict Nash stable and asymptotically stable are attracting. Here we show that checking if there exists a mixed stable profile, for any of the five notions of stability (Definitions 2, 3, 4 and 11), may not be easy. In particular, we show that the problem of checking if there exists a mixed profile that satisfies any of the stability conditions is NP-hard. In order to obtain hardness for checking survival of diversity as a result, in other words checking if set $\mathcal{L}$ has a mixed strategy, we design a unifying reduction.

Our reduction also gives NP-hardness for checking if a given pure strategy is played with non-zero probability (subset) at these. In other words, it is NP-hard to check if a particular allele is going to survive in the limit under the evolution. Finally we extend all the results to the typical class of matrices, where exactly one diagonal entry is dominating (see Definition 13 and Remark 5 in Section 3.6). All the reductions are from **k-Clique**, a well known NP-complete problem [34].

Definition 14 (k-Clique). *Given an undirected graph* $G = (V, E)$, *with* V *vertices and* E *edges, and integer* $0 < k < |V| - 1 = n - 1$, *decide if* G *has a clique of size* k.

Properties of G. Given a simple graph $G = (V, E)$ if we create a new graph $\bar{G}$ by adding a vertex u and connecting it to all the vertices $v \in V$, then it is easy to see that graph G has a clique of size k if and only if $\bar{G}$ has a clique of size $k + 1$. Therefore, w.l.o.g we can assume that there exists a vertex in G which is connected

to all the other vertices. Further, if $n = |V|$, then for us such a vertex is the n-th vertex. By abuse of notation we will use E an adjacency matrix of $\bar{G}$ too, $E_{ij} = 1$ if edge (i, j) present in $\bar{G}$ else it is zero.

3.7.1 Hardness for checking stability

In this section we show NP-hardness (completeness for some) results for decision versions on (strict) Nash stable strategies and (asymptotically) stable fixed points. Given graph $G = (V, E)$ and integer $k < n$, we construct the following symmetric $2n \times 2n$ matrix A, where E' is modification of E where off-diagonal zeros are replaced with $-h$ where $h > 2n^2 + 5$.

$$\forall i \leq j, \ A_{ij} = A_{ji} = \begin{cases} E'_{ij} & \text{if } i, j \leq n \\ k - 1 & \text{if } |i - j| = n \\ h & \text{if } i, j > n \text{ and } i = j, \text{ where } h > 2n^2 + 5 \\ -\epsilon & \text{otherwise, where } 0 < \epsilon \leq \frac{1}{10n^3}. \end{cases} \tag{24}$$

A is a symmetric but is not non-negative. Next lemma maps k-clique to mixed strategy that is also strict Nash stable fixed point. Note that such a fixed point satisfies all other stability notions as well, and hence implies existence of mixed limit point in $\mathcal{L}$.

Lemma 3.18 (Existence of clique implies strict Nash stable). *If there exists a clique of size at least k in graph G, then the game (A, A) has a mixed strategy $\mathbf{p}$ that is strict Nash stable.*

Proof. Let vertex set $C \subset V$ forms a clique of size k in graph G. Construct a maximal clique containing C, by adding vertices that are connected to all the vertices in the current clique. Let the corresponding vertex set be $S \subset V$ ($C \subset S$), and let $m = |S| \geq k$. W.l.o.g assume that $S = \{v_1, \ldots, v_m\}$. Now we construct a strategy profile $\mathbf{p} \in \Delta_{2n}$ and show that it is a strict Nash stable of game (A, A), with

$$p_i = \begin{cases} \frac{1}{m} & 1 \leq i \leq m \\ 0 & m+1 \leq i \leq 2n \end{cases}$$

Claim 3.19. $\mathbf{p}$ *is a strict SNE of game* (A, A).

Proof. To prove the claim we need to show that $(A\mathbf{p})_i > (A\mathbf{p})_j$, $\forall i \in [m], \forall j \notin [m]$, and $(A\mathbf{p})_i = (A\mathbf{p})_j$, $\forall i, j \in [m]$. Since S forms a clique in graph G, and by construction of A, the payoff from i-th pure strategy against $\mathbf{p}$ is

$$(A\mathbf{p})_i = \begin{cases} \sum_{r \leq m} \frac{1}{m} = \frac{m-1}{m}, & \forall i \in [m] \\ \sum_{r \leq m, E_{ir}=1} \frac{1}{m} - \sum_{r \leq m, E_{ir}=0} h < \frac{m-1}{m}, & \forall m < i \leq n \ (\because \ \exists r \leq m, E_{ir} = 0) \\ \frac{k-1}{m} - \epsilon(1 - \frac{1}{m}) < \frac{k-1}{m} \leq \frac{m-1}{m} & \forall n < i \leq 2n \ (\because m \geq k \text{ and } k < n-1). \end{cases}$$

Thus the claim follows. $\qquad \square$

Next consider the corresponding transformed matrix $B = T(A, [m])$ as defined in (23). Since $A_{ij} = 1 \ \forall i, j \in [m], i \neq j$ and $A_{ii} = 0$, $\forall i \in [m]$, we have

$$\forall i, j < m, \ B_{ij} = A_{ij} + A_{mm} - A_{im} - A_{mj} \ = -1 \text{ if } i \neq j,$$
$$= -2 \text{ if } i = j.$$

Claim 3.20. B *is negative definite.*

Proof. It is easy to check that B has all strictly negative eigenvalues. $\mathbf{w}^1 = \mathbf{1}_{m-1}$ is an eigenvector with eigenvalue $-m$, and $\forall 1 < i < m$, vector $\mathbf{w}^i$, where $w^i_1 = 1$ and $w^i_i = -1$, is an eigenvector with eigenvalue -1. Further, $\mathbf{w}^1, \ldots, \mathbf{w}^{m-1}$ are linearly independent. $\qquad \square$

Thus by Definition 11, $\mathbf{p}$ is a strict Nash stable for game (A, A) . $\qquad \square$

Since strict Nash stable is contained in all other sets, the above lemma implies existence of mixed strategy for all of them if there is a clique in G. Next we want to show the converse for all notions of stability. That is if mixed strategy exists for any notion of the five notions of stability then there is a clique of size at least k in

the graph G. Since each of the five stability implies Nash stability, it suffices to map mixed Nash stable strategy to clique of size k. For this, and reductions that follow, we use the following property due to negative semi-definiteness of Nash stability.

Lemma 3.21. *Given a fixed point $\mathbf{x}$, if $T(A, \mathbf{x})$ is negative semi-definite, then $\forall i \in SP(\mathbf{x}), A_{ii} \leq 2A_{ij}, \forall j \neq i \in SP(\mathbf{x})$. Moreover if $\mathbf{x}$ is a mixed Nash stable then it has in its support at most one strategy t with A_{tt} is dominating.*

Proof. A negative semi-definite matrix has the property that all the diagonal elements are non-positive. Observe that from definition of $T(A, \mathbf{r})$, we can choose any strategy to be removed that is in $SP(\mathbf{r})$, hence we choose i and we look at entry $B_{jj} = A_{ii} + A_{jj} - 2A_{ij}$ with $j \in SP(\mathbf{r}), j \neq i$ which must be non-positive since $T(A, \mathbf{r})$ is negative semi-definite. Hence $A_{ii} \leq A_{ii} + A_{jj} \leq 2A_{ij}$. Finally, if A_{ii}, A_{jj} are both dominating then $A_{ii} + A_{jj} > A_{ij} + A_{ji} = 2A_{ij}$ which is contradiction since $A_{ii} + A_{jj} - 2A_{ij} \leq 0$. □

Nash stable also implies symmetric Nash equilibrium. Next lemma maps (special) symmetric NE to k-clique.

Lemma 3.22. *Let $\mathbf{p}$ be a symmetric NE of game (A, A). If $SP(\mathbf{p}) \subset [n]$ and $|SP(\mathbf{p})| > 1$, then there exists a clique of size k in graph G.*

Proof. Let's define $\mathrm{SSP}(\mathbf{p}) = \{i \mid p_i > \frac{1}{n^2}\}$. We first show $|\mathrm{SSP}(\mathbf{p})| \geq k$.

Claim 3.23. $|\mathrm{SSP}(\mathbf{p})| \geq k$.

Proof. Note that $\sum_{i \in SP(\mathbf{p}) \setminus \mathrm{SSP}(\mathbf{p})} p_i \leq n\frac{1}{n^2} \leq \frac{1}{n}$. Therefore, $\sum_{i \in \mathrm{SSP}(\mathbf{p})} p_i \geq 1 - \frac{1}{n}$. Suppose $|\mathrm{SSP}(\mathbf{p})| < k$ by contradiction. Then $\exists r \in \mathrm{SSP}(\mathbf{p})$ such that $p_r \geq \frac{1 - \frac{1}{n}}{k-1} = \frac{n-1}{n(k-1)}$. Now consider the payoff from strategy $n + r$, which is

$$(A\mathbf{p})_{n+r} = (k-1)p_r - \epsilon(1 - p_r) \geq 1 - \frac{1}{n} - \epsilon.$$

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On the other hand we have

$$(A\mathbf{p})_r \leq 1 - p_r \leq 1 - \frac{n-1}{n(k-1)}.$$

Therefore,

$$(A\mathbf{p})_{n+r} - (A\mathbf{p})_r \geq 1 - \frac{1}{n} - \epsilon - 1 + \frac{n-1}{n(k-1)} \geq \frac{n-k}{n(k-1)} - \frac{1}{10n^3} > 0.$$

A contradiction to $\mathbf{p}$ being symmetric NE. □

Let's define $S = \{v_i \mid i \in \mathrm{SSP}(\mathbf{p})\}$. In order to prove the lemma, it suffices to show the vertex set S forms a clique in the graph G since $|S| = |\mathrm{SSP}(\mathbf{p})| \geq k$.

Claim 3.24. *The vertex set S forms a clique in the graph G.*

Proof. It suffices to show $\forall i, j \in \mathrm{SSP}(\mathbf{p})$ where $i \neq j$ we have $A_{ij} = 1$. Suppose not then $\exists i', j' \in \mathrm{SSP}(\mathbf{p})$ s.t. $i' \neq j'$ and $A_{i'j'} \neq 1$. We get $A_{i'j'} = -h$ by definition of A. Therefore, $(A\mathbf{p})_{j'} \leq -hp_{i'} + 1 \leq -1$ because $p_{i'} \geq \frac{1}{n^2}$ and $h \geq 2n^2$. On the other hand, we have $\forall i \notin [n]$, $(A\mathbf{p})_i \geq -\epsilon > -1$ by definition of A so we get a contradiction to $\mathbf{p}$ being symmetric NE. □

The proof is completed. □

We obtain the next lemma essentially using Lemmas 3.21 and 3.22.

Lemma 3.25. *If game (A, A) has a mixed Nash stable strategy, then graph G has a clique of size k.*

Proof. Let $\mathbf{p}$ be a Nash stable strategy of game (A, A), then by definition $\mathbf{p}$ is a SNE and matrix $B = T(A, \mathbf{p})$ is negative semi-definite. The latter implies $SP(\mathbf{p}) \subset [n]$ using Lemma 3.21, since for $i \notin [n]$ $A_{ii} = h > 2k > 2A_{ij}, \forall j \neq i$. Applying Lemma 3.22 with this fact together with the $\mathbf{p}$ being an SNE and $|SP(\mathbf{p})| > 1$ implies G has a clique of size k. □

We mention the following, which is necessary for the main theorem of this section.

Lemma 3.26. *Let A be a symmetric matrix, and $B = A + c$ for a $c \in \mathbb{R}$, then the set of (strict) Nash stable strategies of B are identical to that of A.*

Proof. For equivalence of (strict) Nash stable points, the set of (strict) symmetric NE are same for games (A, A) and (B, B), and matrix $T(A, \mathbf{x}) = T(B, \mathbf{x}), \forall \mathbf{x} \in \Delta_n$. ☐

The next theorem follows using Theorem 3.11, Lemmas 3.18 and 3.25, and the property observed in Lemma 3.26. Since there is no polynomial-time checkable condition for (asymptotically) stable fixed points[7] its containment in NP is not clear, while for (strict) Nash stable strategies containment in NP follows from the Definition 11.

Theorem 3.27 (**Main hardness result**). *Given a symmetric matrix A, checking if (i) game (A, A) has a mixed (strict) Nash stable (or linearly stable) strategy is NP-complete. (ii) dynamics f (20) has a mixed (asymptotically) stable fixed point is NP-hard. Even if A is a positive matrix.*

Note that since adding a constant to A does not change its strict Nash stable and Nash stable strategies (see Lemma 3.26), and since these two sandwiches all other stability notions, the second part of the above theorem follows.

As we note in Remark 5, matrix with i.i.d entries from any atomless distribution has in expectation exactly one row with dominating diagonal (see Definition 13). One could ask does the problem become easier for this typical case. We answer negatively by extending all the NP-hardness results to this case as well, where matrix A has exactly one row whose diagonal entry dominates all other entries of the row. See Section 3.7.2 for details, and thus the next theorem follows.

Theorem 3.28. *Given a symmetric matrix A, checking if (i) game (A, A) has a mixed (strict) Nash stable (or linearly stable) strategy is NP-complete. (ii) dynamics*

---

[7]These are same as (strict) local optima of function $\pi(\mathbf{x}) = \mathbf{x}^\top A \mathbf{x}$, and checking if a given $\mathbf{p}$ is a local optima can be inconclusive if hessian at $\mathbf{p}$ is (negative) semi-definite.

(20) applied on A has a mixed (asymptotically) stable fixed point is NP-hard. Even if A is strictly positive, or has exactly one row with dominating diagonal.

3.7.2 Hardness when single dominating diagonal

A symmetric matrix, when picked uniformly at random, has in expectation exactly one row with dominating diagonal (see Remark 5). One could ask does the problem become easier for this typical case. We answer negatively by extending all the NP-hardness results of Theorem 3.27 to this case as well, where matrix A has exactly one row whose diagonal entry dominates all other entries of the row, *i.e.,* $\exists i : A_{ii} > A_{ij}, \ \forall j \neq i$.

Consider the following modification of matrix A from (24), where we add an extra row and column. Matrix M is of dimension $(2n+1) \times (2n+1)$, described pictorially in Figure 5. Recall that $h > 2n^2 + 5$ and k is the given integer.

$$
\begin{aligned}
&M_{ij} = A_{ij} && \text{if } i, j \leq 2n \\
&M_{(2n+1)i} = M_{i(2n+1)} = 0 && \text{if } i \leq n \\
&M_{(2n+1)i} = M_{i(2n+1)} = h + \epsilon && \text{if } n < i \leq 2n, \text{ where } 0 < \epsilon < 1 \\
&M_{(2n+1)(2n+1)} = 3h
\end{aligned}
\tag{25}
$$

Clearly M has exactly one row/column with dominating diagonal, namely $(2n+1)$. The strategy constructed in Lemma 3.18 is still strict Nash stable in game (M, M). This is because their support is a subset of $[n]$, implying the extra strategy giving zero payoff which is strictly less than the expected payoff. Thus, we get the following:

Lemma 3.29. *If graph G has a clique of size k, then game (M, M) has a mixed strategy that is strict Nash stable where A is from (24).*

Next we show the converse. Nash stable strategies are super set of other three notion of stability (Theorem 3.11), so it suffices to map Nash stable to a k-clique. Further, if $\mathbf{p}$ is Nash stable then $T(M, \mathbf{p})$ is negative semi-definite (by definition). Using this property together with the lemmas from previous sections, we show the next lemma.
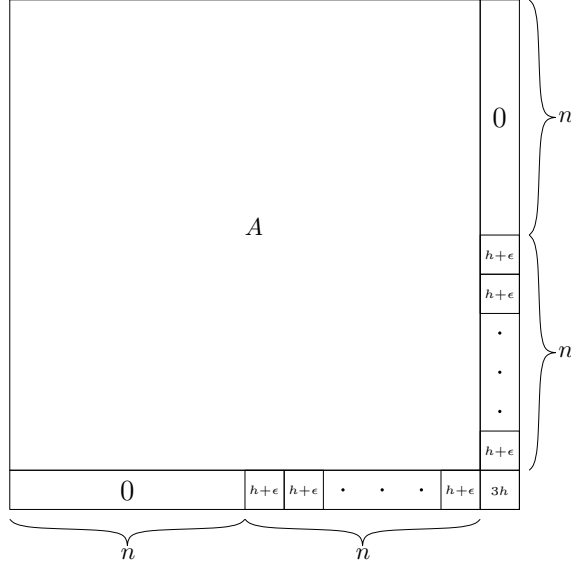
Figure 5: Matrix M as defined in (25)

Lemma 3.30. *Graph G has a clique of size k, if there is a mixed Nash stable strategy in (M, M).*

Proof. Let $\mathbf{q}$ be the Nash stable strategy, then it is a symmetric NE of game (M, M), $T(M, \mathbf{q})$ is negative semi-definite, and $|SP(\mathbf{q})| > 1$. Using Lemma 3.21 we have $SP(\mathbf{q}) \subseteq [n]$, as for $i = 2n + 1$, $M_{ii} = 3h > 2M_{ij}$, $\forall j \neq i$ implying $2n + 1 \notin SP(\mathbf{q})$, and $\forall n < i \leq 2n$, $M_{ii} = h > 2k > 2A_{ij}$, $\forall j \in SP(\mathbf{q})$. Thus for $2n$-dimensional vector $\mathbf{p}$, where $p_i = q_i, i \leq 2n$, we have $T(A, \mathbf{p}) = T(M, \mathbf{q})$ and $\mathbf{p}$ is a symmetric NE of game (A, A). Thus, stability property of $\mathbf{q}$ on matrix M carries forward to corresponding stability of $\mathbf{p}$ on matrix A. Rest follows using Lemma 3.25. $\square$

The next theorem follows using Theorem 3.11, Lemmas 3.26, 3.29, and 3.30. Containment in NP follows using the Definition 11.

Theorem 3.31. *Given a symmetric matrix M such that exactly one row/column in M has a dominating diagonal,*

- *it is NP-complete to check if game (M, M) has a mixed Nash stable (or linearly stable) strategy.*

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- *it is NP-complete to check if game (M, M) has a mixed strict Nash stable.*

- *it is NP-hard to check if dynamics (20) applied on M has a mixed stable fixed point.*

- *it is NP-hard to check if dynamics (20) applied on M has a mixed asymptotically stable fixed point.*

even if M is a assumed to be positive.

Strict positivity of the matrix in the above theorem follows using the fact that Nash stable and strict Nash stable strategies do not change when a constant is added to the matrix (Lemma 3.26).

3.7.3 Hardness for subset

Another natural question to ask is whether a particular allele is going to survive with positive probability in the limit, for a given fitness matrix. We show that this may not be easy either, by proving hardness for checking if there exists a stable strategy $\mathbf{p}$ such that $i \in SP(\mathbf{p})$ for a given i. In general, given a subset S of pure strategies it is hard to check if $\exists$ a stable profile $\mathbf{p}$ such that S is a subset of $SP(\mathbf{p})$.

Theorem 3.32. *Given a $d \times d$ symmetric matrix M and a subset $S \subset [d]$,*

- *it is NP-complete to check if game (M, M) has a Nash stable (or linearly stable) strategy $\mathbf{p}$ s.t. $S \subset SP(\mathbf{p})$.*

- *it is NP-complete to check if game (M, M) has a strict Nash stable strategy $\mathbf{p}$ s.t. $S \subset SP(\mathbf{p})$.*

- *it is NP-hard to check if dynamics (20) applied on M has a stable fixed point $\mathbf{p}$ s.t. $S \subset SP(\mathbf{p})$.*

- *it is NP-hard to check if dynamics (20) applied on M has a asymptotically stable fixed point $\mathbf{p}$ s.t. $S \subset SP(\mathbf{p})$.*

even if $|S| = 1$, or if M is a assumed to be positive or with exactly one row with dominating diagonal.

Proof. The reduction is again from k-clique. Our constructions of (24) and (25) works as is, and the target set is $S = \{n\}$.

Recall that vertex $v_n \in V$ is connected to every other vertex in G, and therefore is part of every maximal clique. Thus the construction of strategy $\mathbf{p}$ in Lemmas 3.18 and 3.29 will have $p_n > 0$, and therefore if k-clique exist then $S \subset SP(\mathbf{p})$.

For the converse consider a Nash stable strategy $\mathbf{p}$ with $\{n\} \subset SP(\mathbf{p})$. By definition it is a symmetric NE, and therefore $SP(\mathbf{p}) \neq \{n\}$ as in all cases row n has dominated diagonal, *i.e.,* $A_{nn} = 0 < k - \delta = A_{n,2n}$. Thus, $\mathbf{p}$ is a mixed profile, and then by applying Lemmas 3.25 and 3.30, for the respective cases we get that graph G has a k-clique. Thus proof follows using Theorem 3.11 and Lemma 3.26. □

3.7.4 Diversity and hardness

Finally we state the hardness result in terms of survival of phenotypic diversity in the limiting population of diploid organism with single locus. For this case, as we discussed before, the evolutionary process has been studied extensively [92, 82, 83], and that it is governed by dynamics f of (20) has been established. Here A is a symmetric fitness matrix; A_{ij} is the fitness of an organism with alleles i and j in the locus of two chromosomes. Thus, for a given A the question of deciding "If phenotypic diversity will survive with positive probability?" translates to "If dynamics f converges to a mixed fixed point with positive probability?". We wish to show NP-hardness for this question.

Theorem 3.6 establishes that all, except for zero-measure, of starting distributions f converges to linearly stable fixed points. From this we can conclude that "Yes" answer to the above question implies existence of a mixed linearly stable fixed point. However the converse may not hold. In other words, "No" answer does not imply

non-existence of mixed linearly stable fixed points. Although, in that case we can conclude non-existence of mixed strict Nash stable strategy (Theorem 3.11). Thus, none of the above reductions seem to directly give NP-hardness for our question.

At this point, the fact that same reduction (of Section 3.7.1) gives NP-hardness for all four notions of stability, and in particular for strict Nash stable as well as linearly stable (Nash stable) fixed points come to our rescue. In particular, for the matrix A of (24) non-existence of mixed limit point in $\mathcal{L}$ (points where f converges with positive probability) implies non-existence of strict Nash stable strategy, which in turn imply non-existence of mixed linearly stable fixed point (Theorem 3.11). If not, then graph G will have k-clique (Lemma 3.25 and Theorem 3.11), which in turn implies existence of a mixed strict Nash stable strategy (Lemma 3.18). Therefore, we can conclude that mixed linearly stable fixed point exist if and only if f converges to a mixed fixed point with positive probability and thus the next theorem follows.

Theorem 3.33. *Given a fitness matrix A for a diploid organism with single locus, it is NP-hard to decide if, under evolution, diversity will survive (by converging to a specific mixed equilibrium with positive probability) when starting allele frequencies are picked i.i.d from uniform distribution. Also, deciding if a given allele will survive is NP-hard.*

Remark 6. *As noted in Section 1.4.1, coordination games are very special and they always have a pure Nash equilibrium which is easy to find; NE computation in general game is PPAD-complete [36]. Thus, it is natural to wonder if decision versions on coordination games are also easy to answer.*

In the process of obtaining the above hardness results, we stumbled upon NP-hardness for checking if a symmetric coordination game has a NE (not necessarily symmetric) where each player randomizes among at least k strategies. Again the reduction is from k-clique. Thus, it seems highly probable that other decision version on (symmetric) coordination games are also NP-complete.

3.8   Conclusion and remarks

The results of this chapter appear in [86] and it is joint work with Ruta Mehta, Georgios Piliouras and Sadra Yazdanbod. We establish complexity theoretic hardness results implying that even in the textbook case of single locus (gene) diploid models, predicting whether diversity survives or not given its fitness landscape is algorithmically intractable. Our hardness results are structurally robust along several dimensions, *e.g.,* choice of parameter distribution, different definitions of stability/persistence, restriction to typical subclasses of fitness landscapes. Technically, our results exploit connections between game theory, nonlinear dynamical systems, and complexity theory and establish hardness results for predicting the evolution of a deterministic variant of the well known multiplicative weights update algorithm in symmetric coordination games; finding one Nash equilibrium is easy in these games. Finally, we complement our results by establishing that under randomly chosen fitness landscapes diversity survives with significant probability.

A future direction of this work would be to analyze the diploid dynamics for multiple genes (loci). As the number of genes increases, the dynamics becomes more complicated and is hard to perform stability analysis and characterize (partially) the unstable fixed points. Another question could be to find out on average and in worst case, how many steps discrete replicator needs to reach an ϵ-neighborhood of a fixed point (we address the last question in Chapter 4).

CHAPTER IV

MUTATION AND SURVIVAL IN DYNAMIC ENVIRONMENTS

4.1   Introduction

A new, potent approach to studying evolution was initiated by Valiant [134], namely viewing it through the lens of computation. This viewpoint has already started yielding concrete insights by translating qualitative hypotheses in biological systems to provable computational properties of Markov chains and other dynamical systems (see [135, 136, 79, 23, 87] and Chapters 2, 3, 5 of this thesis). We build on this direction whilst focusing on the challenge of evolving environments. As discussed in Chapter 2, building on the work of Nagylaki [92], Chastain *et al.* [23] showed that natural selection under sexual reproduction in haploid species (see Section A.1 for terms used in biology) can be interpreted as the Multiplicative Weight Update Algorithm (MWUA) which we call discrete replicator dynamics, in coordination games played among genes. Theorem 2.9 (main) of Chapter 2 argues that under mild conditions on the fitness matrix, replicator dynamics converges with probability one to pure fixed points under random initial conditions[1] (the biological interpretation is that diversity disappears in the limit). Two important ingredients in this result are the lack of mutations and the fact that the fitness matrix remains fixed.

In this chapter we address two important questions in the case of sexual reproduction: *the role of mutation*, especially in the *presence of changes to the environment*, *i.e.,* fitness matrix. In the case of asexual reproduction, the change of environment was studied by Wolf *et al.* [139]. They modeled a changing environment via a Markov

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[1]Any prior measure absolutely continuous with respect to Lebesgue satisfies the statement.

chain and described a model in which in the absence of mutation, the population goes extinct, but in the presence of mutation, the population survives with positive probability. The question arises *whether this is enough to safeguard against extinction in a changing environment, or is mutation still needed.*

Following Chapter 2, we consider a haploid organism with two genes. Each gene can be viewed as a player in a game and the alleles of each gene represent strategies of that player. Once an allele is decided for each gene, an individual is defined, and its fitness is the payoff to each of the players, *i.e.,* both players have the same payoff matrix, and therefore it is a coordination/partnership game. We model the change of environments as in [139], via a Markov chain. Each state of the Markov chain represents an environment and has its own fitness matrix.

Our contribution. We show under the model described above, where mutations are captured through a standard model appeared in [61], the following theorems:

Informal Theorem 1 (Mutation and survival). For a class of Markov chains (satisfying mild conditions), a haploid species under *sexual evolution*[2] without mutation dies out with probability one (see Theorem 4.11). In contrast, under sexual evolution with mutation the probability of long term survival is strictly positive (see Theorem 4.15).

For each gene, if we think of its allele frequencies in a given population as defining a mixed strategy, then after reproduction, the frequencies change as per discrete replicator dynamics, as in Chapter 2. Furthermore, in the presence of mutation [61], every allele mutates to another allele of the corresponding gene in a small fraction of offsprings. As it turns out, in every generation, the population size (of the species) changes by a multiplicative factor of the current expected payoff (mean fitness). Hence, in order to prove Theorems 4.11, 4.15, we need to analyze replicator

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[2]We refer to 'evolution by natural selection under sexual reproduction' by sexual evolution for brevity.

dynamics (and its variant which captures mutations) in a time-evolving coordination game whose matrix is changing as per a Markov chain. The idea behind Theorem 4.11 is as follows: It is known that MWUA converges, in the limit, to a pure equilibrium in coordination games, as discussed in Chapter 2. This implies that in a static environment, in the limit the population will be rendered monomorphic. Showing such a convergence in a stochastically changing environment is not straightforward. We first show that such an equilibrium can be reached fast enough in a static environment. We then appeal to the Borel-Cantelli theorem to argue that with probability one, the Markov chain will visit infinitely often and remain sufficiently long in one environment at some point and hence the population will eventually become monomorphic. An assumption in our theorem is that for each individual, there are bad environments, *i.e.,* one in which it will go extinct. Eventually the monomorphic population will reach such an unfavorable environment and will die out. Although mutations seem to hurt mean population fitness in the short run in static environments, they are critical for survival in dynamic environments, as shown in Theorem 4.15; it is proved as follows. The random exploration done by mutations and aided by the selection process, which rapidly boosts the frequency of alleles with good mean fitness, helps the population to survive. Essentially we couple the random variable capturing population size with a biased random walk, with a slight bias towards increase. The result then follows using a well-known lemma on biased random walks.

Polynomial time convergence in static environment. For such a reasoning to be applicable we need a fast convergence result, which does not hold in the worst case, since by choosing initial conditions sufficiently close to the stable manifold of an unstable equilibrium, we are bound to spend super-polynomial time near such unstable states. To circumvent this we take a typical approach of introducing a small noise into the dynamics [108, 70, 58], and provide the first, to our knowledge, polynomial convergence bound for noisy MWUA in coordination games; this result is

of independent interest. We note that MWUA captures frequency changes of alleles in case of infinite population, and the small noise can also be thought of as sampling error due to finiteness of the population. In the following theorem, dependence on all identified system parameters is necessary (see discussion in Section 4.8).

Informal Theorem 2 (Speed of convergence). In static environments under small random noise ($||.||_\infty = \delta$), sexual evolution (without mutation) converges with probability $1 - \epsilon$ to a monomorphic fixed point in time $O\left(\frac{n \log \frac{n}{\epsilon}}{\gamma^4 \delta^6}\right)$, where n is the number of alleles, and γ the minimum fitness difference between two genotypes (see Theorem 4.9).

Robustness to mutations. Finally we show that the convergence of discrete replicator dynamics (without mutation) in static environments (see Chapter 2) can be extended to the case where mutations are also present. The former result critically hinges on the fact that mean fitness strictly increases under MWUA in coordination games, and thereby acts as a potential function. This is no more the case. However, using an inequality due to Baum and Eagon [14] we manage to obtain a new potential function which is the product of mean fitness and a term capturing diversity of the allele distribution. The latter term is essentially the product of allele frequencies.

Informal Theorem 3 (Convergence with mutations). In static environments, sexual evolution with mutation converges, for any level of mutation. Specifically, if we are not at equilibrium, at the next time generation at least one of mean population fitness or product of allele frequencies will increase.

Besides adding computational insights to biologically inspired themes, which to some extent may never be fully settled, we believe that our work is of interest even from a purely computational perspective. The nonlinear dynamical systems arising from these models are gradient-like systems of non-convex optimization problems. Their importance and the need to develop a theoretical understanding beyond worst

case analysis has been pinpointed as a key challenge for numerous computational disciplines, *e.g.*, from [7]:

> *"Many procedures in statistics, machine learning and nature at large – Bayesian inference, deep learning, protein folding – successfully solve non-convex problems ... Can we develop a theory to resolve this mismatch between reality and the predictions of worst-case analysis?"*

Our theorems and techniques share this flavor. Theorem 1 expresses time-average efficiency guarantees for gradient-like heuristics in the case of time-evolving optimization problems. Theorem 2 argues about speedup effects by adding noise to escape out of saddle points, whereas Theorem 3 is a step towards arguing about robustness to implementation details. We make this methodological similarities more precise by pointing them out in more detail in Section 4.2.
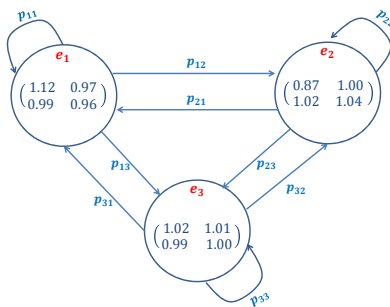
Figure 6: An example of a Markov chain model of fitness landscape evolution.

4.2 Related work

In the last few years we have witnessed a rapid cascade of theoretical results on the intersection of computer science and evolution (see discussion and references in Sections 2.1, 2.2 and Chapter 3). It is also possible to introduce connections between satisfiability and evolution [79]. The error threshold is the rate of errors in genetic mixing above which genetic information disappears [44]. Vishnoi [136] shows existence of such sharp thresholds. Moreover, in Chapter 5 we shed light on the speed of asexual

evolution (see also [137]). Finally, in [39] Dixit *et al.* present finite population models for asexual haploid evolution that closely track the standard infinite population model of Eigen [43] (see Section 5.7.2). Wolf, Vazirani, and Arkin [139] analyze models of mutation and survival of diversity also for asexual populations but the dynamical systems in this case are linear and the involved methodologies are rather different.

Introducing noise in non-linear dynamics has been shown to be able to simplify the analysis of nonlinear dynamical systems by "destroying" Turing-completeness of classes of dynamical systems and thus making the system's long-term behavior computationally predictable [20]. Those techniques focus on establishing invariant measures for the systems of interest and computing their statistical characteristics. In our case, our unperturbed dynamical systems have exponentially many saddle points and numerous stable fixed points and species survival is critically dependent on the amount of time that trajectories spend in the vicinity of these points thus much stronger topological characterizations are necessary. Adding noise to game theoretic dynamics [70, 2, 26] to speed up convergence to approximate equilibria in potential games is a commonly used approach in algorithmic game theory, however, the respective proof techniques and notions of approximation are typically sensitive to the underlying dynamic, the nature of noise added as well as the details of the class of games.

In the last year there has been a stream of work on understanding how gradient (and more generally gradient-like) systems escape out of the saddle fixed points fast [58, 74]. This is critically important for a number of computer science applications, including speeding up the training of deep learning networks. The approach pursued by these papers is similar to our work, including past papers in the line of TCS and biology/game theory literature [70] and Chapter 2 of this thesis. For example, in Chapter 2 it has been established that in non-convex optimization settings gradient-like systems (*e.g.,* variants of Multiplicative Weights Updates Algorithm) converge

for all but a zero measure of initial conditions to local minima of the fitness landscape (instead of saddle points even in the presence of exponentially many saddle points). Moreover, as shown in [70] noisy dynamics diverge fast from the set of saddle points whose Jacobian has eigenvalues with large positive real parts. Similar techniques and arguments can be applied to argue generic convergence to local minima of numerous other dynamics (including noisy/deterministic versions of gradient dynamics). Finally, in Chapter 7 we argue that gradient dynamics converge to local minima with probability one in non-convex optimization problems even in the presence of continuums of saddle points, answering an open question in [74]. We similarly hope that techniques developed here about fast and robust convergence can also be extended to other classes of gradient(-like) dynamics in non-convex optimization settings.

Finite population evolutionary models over time evolving fitness landscapes are typically studied via simulations (*e.g.,* [77] and references therein). These models have also inspired evolutionary models of computation, *e.g.,* genetic algorithms, whose study under dynamic fitness environments is a well established area with many applications (*e.g.,* [141] and references therein) but with little theoretical understanding and even theoretical papers on the subject typically rely on combinations of analytical and experimental results [19].

4.3 Preliminaries

4.3.1 Discrete replicator dynamics with mutation - A combinatorial interpretation

For a haploid species[3] (one with single set of chromosomes, unlike diploids such as humans who have chromosome pairs) with two genes (coordinates), let S_1 and S_2 be the set of possible alleles (types) for the first and second gene respectively. Then, an individual of such a species can be represented by an ordered pair $(i, j) \in S_1 \times S_2$. Let W_{ij} be the fitness of such an individual capturing its ability to reproduce during

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[3]See Section A.1 in the appendix for a short discussion of all relevant biological terms.

a mating. Thus, fitness landscape of such a species can be represented by matrix W of dimension $n \times n$, where we assume that $n = |S_1| = |S_2|$.

Sexual Model without mutation. In every generation, each individual (i, j) mates with another individual (i', j') picked uniformly at random from the population (can pick itself). The offspring can have any of the four possible combinations, namely $(i, j), (i, j'), (i', j), (i', j')$, with equal probability. Let X_i be a random variable that denotes the proportion of the population with allele i in the first coordinate, and similarly Y_j be the frequency of the population with allele j in the second coordinate. After one generation, the expected number of offsprings with allele i in first coordinate is proportional to $X_i \cdot X_i \cdot (W\mathbf{Y})_i + 2\frac{1}{2}(1 - X_i)X_i \cdot (W\mathbf{Y})_i = X_i(W\mathbf{Y})_i$ (X_i^2 stands for the probability both individuals have allele i in the first coordinate - which the offspring will inherit - and $2\frac{1}{2}(1 - X_i)X_i$ stands for the probability that exactly one of the individuals has allele i in the first coordinate and the offspring will inherit). Similarly the expected number of offsprings with allele j for the second coordinate is $Y_j(W^\top \mathbf{X})_j$. Hence, if $\mathbf{X}', \mathbf{Y}'$ denote the frequencies of the alleles in the population in the next generation (random variables)

$$E[X_i'|\mathbf{X}, \mathbf{Y}] = \frac{X_i(W\mathbf{Y})_i}{\mathbf{X}^\top W \mathbf{Y}} \text{ and } E[Y_j'|\mathbf{X}, \mathbf{Y}] = \frac{Y_j(W^\top \mathbf{X})_j}{\mathbf{X}^\top W \mathbf{Y}}.$$

We are interested in analyzing a *deterministic* version of the equations above, which essentially captures an infinite population model. Thus if frequencies at time t are denoted by $(\mathbf{x}(t), \mathbf{y}(t))$, they obey the following dynamics governed by the function $g : \Delta \to \Delta$, where $\Delta = \Delta_n \times \Delta_n$:

$$\text{Let } (\mathbf{x}(t+1), \mathbf{y}(t+1)) = g(\mathbf{x}(t), \mathbf{y}(t)), \text{ where } \begin{array}{l} \forall i \in S_1, \ x_i(t+1) = x_i(t)\frac{(W\mathbf{y}(t))_i}{\mathbf{x}^\top(t)W\mathbf{y}(t)} \\ \forall j \in S_2, \ y_j(t+1) = y_j(t)\frac{(W^\top \mathbf{x}(t))_j}{\mathbf{x}^\top(t)W\mathbf{y}(t)}. \end{array}$$
$$(26)$$

It is easy to see that g is well-defined when W is a positive matrix. This is the dynamics for haploids as it appeared in Chapter 2, Section 2.4.1. Chastain *et al.* [23]

gave a game theoretic interpretation of deterministic Equations (26). It can be seen as a repeated two player coordination game (each gene is a player), the possible alleles for a gene are its pure strategies and both players play according to dynamics (26). A modification of these dynamics has also appeared in models of grammar acquisition [101]. The difference between the Equations (26) and those (13) in Chapter 2 (on game $(W, W^\top)$) is that matrix W is square here. Furthermore, we have shown in Chapter 2 that dynamics with Equations (26) converges point-wise to a pure fixed point, *i.e.,* where exactly one coordinate is non-zero in both $\mathbf{x}$ and $\mathbf{y}$, for all but measure zero of initial conditions in Δ, when W has distinct entries.

Sexual Model with mutation. Next we extend the dynamics of (26) to incorporate mutation. The mutation model which appears in Hofbauer's book [61], is a two step process. The first step is governed by (26), and after that in each individual, and for each of its gene, corresponding allele, say k, mutates to another allele of the same gene, say k', with probability $\tau > 0$ for all $k' \neq k$. After a simple calculation (see Section 4.3.2 below for calculations) the resulting dynamics turns out to be as follows, where f is a $\Delta \to \Delta$ function:

$$\text{Let } (\mathbf{x}', \mathbf{y}') = f(\mathbf{x}, \mathbf{y}), \text{ then } \begin{array}{rcl} x_i' & = & (1 - n\tau)x_i \frac{(W\mathbf{y})_i}{\mathbf{x}^\top W \mathbf{y}} + \tau, \ \forall i \in S_1 \\ y_j' & = & (1 - n\tau)y_j \frac{(\mathbf{x}^\top W)_j}{\mathbf{x}^\top W \mathbf{y}} + \tau, \ \forall j \in S_2. \end{array} \tag{27}$$

4.3.2   Calculations for mutation

Let $(\hat{\mathbf{x}}, \hat{\mathbf{y}}) = g(\mathbf{x}, \mathbf{y})$. If in every generation, allele $i \in S_1$ mutates to allele $k \in S_1$ with probability μ_{ik}, where $\sum_k \mu_{ik} = 1$, $\forall i$, then the final proportion (after reproduction, mutation) of allele $i \in S_1$ in the population will be

$$x_i' = \sum_{k \in S_1} \mu_{ki} \hat{x}_k.$$

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Similarly, if $j \in S_2$ mutates to $k \in S_2$ with probability δ_{jk}, then proportion of allele $j \in S_2$ will be

$$y_j' = \sum_{k \in S_2} \delta_{ki} \hat{y}_k.$$

If mutation happens after every selection (mating), then we get the following dynamics with update rule $f' : \Delta \to \Delta$ governing the evolution (update rule contains selection+mutation).

Let $(\mathbf{x}', \mathbf{y}') = f'(\mathbf{x}, \mathbf{y})$, then
$$\begin{aligned} x_i' &= \sum_{k \in S_1} \mu_{ki} x_k \frac{(W\mathbf{y})_k}{\mathbf{x}^\top W \mathbf{y}}, \ \forall i \in S_1, \\ y_j' &= \sum_{k \in S_2} \delta_{kj} y_k \frac{(\mathbf{x}^\top W)_k}{\mathbf{x}^\top W \mathbf{y}}, \ \forall j \le S_2. \end{aligned} \tag{28}$$

Suppose $\forall k$, $\forall i \neq k$ and $\forall j \neq k$, we have $\mu_{ik} = \delta_{jk} = \tau$, where $\tau \le \frac{1}{n}$. Since $\sum_k \mu_{ik} = \sum_k \delta_{jk} = 1$, we have $\mu_{ii} = \delta_{jj} = 1 - (n-1)\tau = 1 + \tau - n\tau$. Hence

$$\begin{aligned} x_i' &= \sum_{k \in S_1} \mu_{ki} x_k \frac{(W\mathbf{y})_k}{\mathbf{x}^\top W \mathbf{y}} \\ &= (1 + \tau - n\tau) x_i \frac{(W\mathbf{y})_i}{\mathbf{x}^\top W \mathbf{y}} + \tau \sum_{k \neq i} x_k \frac{(W\mathbf{y})_k}{\mathbf{x}^\top W \mathbf{y}} \\ &= (1 - n\tau) x_i \frac{(W\mathbf{y})_i}{\mathbf{x}^\top W \mathbf{y}} + \tau \sum_k x_k \frac{(W\mathbf{y})_k}{\mathbf{x}^\top W \mathbf{y}} \\ &= (1 - n\tau) x_i \frac{(W\mathbf{y})_i}{\mathbf{x}^\top W \mathbf{y}} + \tau. \end{aligned}$$

The same is true for vector $\mathbf{y}'$. The dynamics of (28) where $\mu_{ik} = \delta_{ik} = \tau$ for all $k \neq i$ simplifies to the Equations (27) as appear in the preliminaries.

4.3.3 Our model

In section we will analyze a noisy version of (26), (27). Essentially we add small random noise to non-zero coordinates of $(\mathbf{x}(t), \mathbf{y}(t))$ [4].

Definition 15. *Given $\mathbf{z} \in \Delta$ and a small $0 < \delta$ (δ is $o_n(\tau)$), define $\Delta(\mathbf{z}, \delta)$ to be a set of vectors $\{\mathbf{z} + \delta \in \Delta \mid \mathrm{supp}(\delta) = \mathrm{supp}(\mathbf{z}); \ \delta_i \in \{-\delta, +\delta\}, \ \forall i\}$.* [5]

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[4] This is different from diffusion approximation, noise helps to avoid saddle points essentially.

[5] *In case the size of the support of $\mathbf{z}$ is odd, there will be a zero entry in δ, so $|\mathrm{supp}(\delta)| = |\mathrm{supp}(\mathbf{z})| - 1$.*

Note that if $\mathbf{z}$ is pure (has support size one), then δ is all zero vector[6]. Define noisy versions of both g from (26) and f from (27) as follows: Given $(\mathbf{x}(t), \mathbf{y}(t))$ pick $\delta_{\mathbf{x}} \in \Delta(\mathbf{x}(t), \delta)$ and $\delta_{\mathbf{y}} \in \Delta(\mathbf{y}(t), \delta)$ uniformly at random. Set with probability half $\delta_{\mathbf{x}}$ to zero, and with the other half set $\delta_{\mathbf{y}}$ to zero. Then redefine dynamics g of (26) as follows:

$$(\mathbf{x}(t+1), \mathbf{y}(t+1)) = g_{\delta}(\mathbf{x}(t), \mathbf{y}(t)) = g(\mathbf{x}(t), \mathbf{y}(t)) + (\delta_{\mathbf{x}}, \delta_{\mathbf{y}}). \tag{29}$$

And redefine dynamics f of (28) capturing sexual evolution with mutation as follows.

$$(\mathbf{x}(t+1), \mathbf{y}(t+1)) = f_{\delta}(\mathbf{x}(t), \mathbf{y}(t)) = f(\mathbf{x}(t), \mathbf{y}(t)) + (\delta_{\mathbf{x}}, \delta_{\mathbf{y}}). \tag{30}$$

Furthermore, we will have that if any x_i, y_j goes below δ, we set it to zero. This is crucial for our theorems because otherwise the dynamics with Equations (26) and (27) (or even (29) and (30)) can converge to a fixed point at $t \to \infty$, but never reach a point in a finite amount of time. This is true in the main result of Chapter 2, the dynamics converge almost surely to pure fixed points as $t \to \infty$ but do not reach fixation in a finite time. So x_i, y_j reaches fixation (set it to zero) if $x_i, y_j < \delta$. We need to re-normalize after this step.

$$\forall i \in S_1, \text{ if } x_i(t) < \delta \text{ then set } x_i(t) = 0. \text{ Re-normalize } \mathbf{x}(t).$$
$$\forall j \in S_1, \text{ if } y_j(t) < \delta \text{ then set } y_j(t) = 0. \text{ Re-normalize } \mathbf{y}(t). \tag{31}$$

Definition 16 (Negligible vector). *We call a vector* $\mathbf{v}$ *negligible if there exists an* i *s.t* $v_i < \delta$.

Tracking population size. Suppose the size of the initial population is N^0, and let population at time t be N^t. In every time period N^t gets multiplied by average fitness of the current population, namely $\mathbf{x}(t)^{\top} W(t) \mathbf{y}(t)$, where $(\mathbf{x}(t), \mathbf{y}(t))$ denote the frequencies of alleles at generation t and $W(t)$ the matrix fitness/environment at

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[6]There are no sampling errors in monomorphic population

time (see discussion below about changing of environments).

Let average fitness $\Phi^t = \mathbf{x}(t)^\top W(t)\mathbf{y}(t)$ then $\mathbb{E}[N^{t+1}|\mathbf{x}(t), \mathbf{y}(t), N^t] = N^t \Phi^{t+1}$. (32)

We will consider $N^{t+1} = N^t \Phi^{t+1}$ (see also [118]). Based on the value of N^t, we give the definition of survival and extinction.

Definition 17 (**Survival - extinction**). *We say the population* goes extinct *if for initial population size* N^0, *there exists a time t so that $N^t < 1$. On the other hand, we say that population* survives *if for all times $t \in \mathbb{N}$ we have that $N^t \geq 1$.*

Model of environment change. Following the work of Wolf *et al.* [139], we consider a Markov chain based model of changing environment. Let $\mathcal{E}$ be the set of different possible environments, and W^e be the fitness matrix in environment $e \in \mathcal{E}$. E denotes the set of (e, e') pairs if there is a non-zero probability $p_{e,e'} \in (0,1)$ to go from environment e to e'. See Figure 6 for an example. For a parameter $p < 1$ we assume that $\sum_{e':(e,e')\in E} p_{e,e'} \leq p$, $\forall e \in \mathcal{E}$. That is, after every generation of the dynamics (29) or (30), the environment changes to one of its neighboring environment with probability at most $p < 1$, and remains unchanged with probability at least $(1 - p)$. The graph formed by edges in $\mathcal{E}$ is assumed to be connected, thus the resulting Markov chain eventually will stabilize to a stationary distribution π_e (is ergodic).

Even though fitness matrices W^e can be arbitrary, it is generally assumed that W^e has distinct positive entries (as in [24], and also Chapter 2). Furthermore, no individual can survive all the environments on average. Mathematically, if π_e is the stationary distribution of this Markov chain then, $\forall i, j$, $\prod_{e\in\mathcal{E}}(W_{ij}^e)^{\pi_e} < 1$.

Furthermore, we assume that every environment has alleles of good type as well as bad type. An allele i of good type has uniform fitness (*i.e.*, $\frac{\sum_j W_{ij}}{n}$) of at least $(1 + \beta)$ for some $\beta > 0$, and alleles of bad type are dominated by a good type allele

point-wise[7]. Finally, the number of bad alleles are $o(n)$ (sublinear in n). Let the set of bad alleles for genes $i = 1, 2$ in environment e be denoted by B_i^e.

Putting all of the above together, the Markov chain for environment change is defined by set $\mathcal{E}$ of environments and its adjacency graph, fitness matrices $W^e, \forall e \in \mathcal{E}$, probability $1 - p$ with which dynamics remains in current environment, sets $B_i^e \subset S_i$, $i = 1, 2$ of bad alleles in environment e, and $\beta > 0$ to lower-bound average fitness of good type alleles. See also Section 4.8.2 for discussion on the assumptions where we claim that most of them are necessary for our theorems. In the next sections we will analyze the dynamics with Equations (29), (30) in terms of convergence and population size for fixed and dynamic environments.

Symbol	Interpretation
W^e	fitness matrix at environment e
$W(t), W^{e(t)}$	fitness matrix at time t
γ^e	minimum difference between entries in fitness matrix W^e
$\mathbf{x}, \mathbf{y}$	frequencies of (alleles) strategies
δ	noise/perturbation
Φ	potential/average fitness $\mathbf{x}^\top W \mathbf{y}$
β	If allele i is of good type in environment e then it satisfies $\frac{\sum_j W_{ij}^e}{n} \geq 1 + \beta$
τ	probability that an individual with allele k mutates to k' (of the same gene)

Table 1: List of parameters

4.4   *Overview of proofs*

The dynamical systems that we analyze, namely (29) and (30), under the evolving environment model of Section 4.3.3 are (stochastically perturbed) nonlinear replicator-like dynamical systems whose parameters evolve according to a (possibly slow mixing) Markov chain. We reduce the analysis of this complex setting to a series of smaller, modular arguments that combine as set-pieces to produce our main theorems.

Convergence rate for evolution without mutation in static environment. Our starting point is Chapter 2 where it was shown that in the case of noise-free sexual

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[7]Think of bad type alleles akin to a terminal genetic illness. Such assumptions are typical in the biological literature (*e.g.,* [77]).

dynamics governed by (26) the average population fitness increases in each step and the system converges to equilibria, and moreover that for almost all initial conditions the resulting fixed point corresponds to a monomorphic population (pure/not mixed equilibrium). Conceptually, the first step in our analysis tries to capitalize on this stronger characterization by showing that convergence to such states happens fast. This is critical because while there are only linearly many pure equilibria, there are (generically) exponentially many isolated, mixed ones [24], which are impossible to meaningfully characterize. By establishing the predictive power of pure states, we radically reduce our uncertainty about system behavior and produce a building block for future arguments.

Without noise we cannot hope to prove fast convergence to pure states since by choosing initial conditions sufficiently close to the stable manifold of an unstable equilibrium, we are bound to spend super-polynomial time near such unstable states. In finite population models, however, the system state (proportions of different alleles) is always subject to small stochastic shocks (akin to sampling errors). These small shocks suffice to argue fast convergence by combining an inductive argument and a potential/Lyapunov function argument.

To bound the convergence time to a pure fixed point starting at an arbitrary mixed strategy (maybe with full support), it suffices to bound the time it takes to reduce the size of the support by one, because once a strategy x_i becomes zero it remains zero under (29), *i.e.,* an extinct allele can never come back in absence of mutations (and then use induction). For the inductive step, we need two non trivial arguments. First we need a lower bound on the rate of increase of the mean population fitness when the dynamics is not at approximate fixed points[8], shown in Lemma 4.1. This requires a quantitative strengthening of potential/(nonlinear dynamical system) arguments of Chapter 2. Secondly, we show that the noise suffices to escape fast

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[8]We call these states α-close points.

(with high probability) from the influence of fixed points that are not monomorphic (these are like saddle points). This requires a combination of stochastic techniques including origin returning random walks, Azuma type inequalities for submartingales, and arguing about the increase in expected mean fitness $\mathbf{x}(t)^\top W(t)\mathbf{y}(t)$ in a few steps (Lemmas 4.4-4.8), where $\mathbf{x}$ and $\mathbf{y}$ capture allele frequencies at time step t. As a result we show polynomial time convergence of (29) to pure equilibrium under static environment in Theorem 4.9. This result may be of independent interest since fast convergence of nonlinear dynamics to equilibrium is not typical [88].

Survival, extinction under dynamic environments. As described in Section 4.3.3, we consider a Markov chain based model of environmental changes, where after every selection step, the fitness matrix changes with probability at most p. Suppose the starting population size is $N^0 > 0$ and let N^t denote the size at time t then in every step N^t gets multiplied by the mean fitness $\mathbf{x}(t)^\top W(t)\mathbf{y}(t)$ of the current population (see (32)). We say that population goes extinct if for some t, $N^t < 1$, and it survives if $N^t \geq 1$, for all t.

We assume that there do not exist "all-weather" phenotypes. We encode this by having the monomorphic population of any genotype decrease when matched to an environment chosen according to the stationary distribution of the Markov chain.[9] In other words, an allele may be both "good" and "bad" as environment changes, sometimes leading to growth, and other times to decrease in population.

Case a) sexual evolution without mutation. If the population becomes monomorphic then this single phenotype can not survive in all environments, and will eventually wither as its population will be in exponential decline once the Markov chain

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[9]If, for any genotype, the population increased in expectation over the randomly chosen environment, then once monomorphic population consisting of only such a genotype is reached, the population would blow up exponentially (and forever) as soon as the Markov chain reached its mixing time.

mixes. The question is whether monomorphism is achieved under changing environment; the above analysis is not applicable directly as the fitness matrix is not fixed any more. Our first theorem (Theorem 4.9) upper bounds the amount of time T needed to "wait" in a single environment so as the probability of convergence to a monomorphic state is at least some constant (*e.g.,* $\frac{1}{2}$). Breaking up the time history in consecutive chunks of size T and applying Borel-Cantelli theorem implies that the population will become monomorphic with probability one (Theorem 4.11). This is the strongest possible result without explicit knowledge of the specifics of the Markov chain (*e.g.,* mixing time).

Case b) sexual evolution with mutation. As described in Section 4.3.1, we consider a well-established model of mutation [61], where after every selection step, each allele mutates with probability τ. The resulting dynamics is governed by (27), and we analyze its noisy counterpart (30). This ensures that in each period the proportion of every allele is at least τ. We show that this helps the population to survive.

Unlike the no mutation case of Chapter 2, the average fitness $\mathbf{x}(t)^\top W \mathbf{y}(t)$ is no more increasing in every step, even in absence of noise. Instead we derive another potential function that is a combination of average fitness and entropy. Due to mutations forcing exploration, natural selection weeds out the bad alleles fast (Lemma 4.12). Thus there may be initial decrease in fitness, however the decrease is upper bounded. Furthermore, we show that the fitness is bound to increase significantly within a short time horizon due to increase in population of good alleles (Lemma 4.13). Since population size gets multiplied by average fitness in each iteration, this defines a biased random walk on logarithm of the population size. Using upper and lower bounds on decrease and increase respectively, we show that the probability of extinction stochastically dominates a simpler to analyze random variable pertaining to biased random walks on the real line (Lemma 4.14). Thus, the probability of long

term survival is strictly positive (Theorem 4.15). This completes the proof of informal Theorem 1.

Deterministic convergence despite mutation in static environments: Finally, as an independent result for the case of noise free dynamics (infinite population) with mutation governed by (27), we show convergence to fixed points in the limit, by defining a novel potential function which is the product of mean fitness $\mathbf{x}^\top W \mathbf{y}$ and a term capturing diversity of the allele distribution (Theorem 4.16). The latter term is essentially the product of allele frequencies ($\prod_i x_i \prod_i y_i$). Such convergence results are not typical in dynamical systems literature [88], and therefore this potential function may be useful to understand limit points of this and similar dynamics (the continuous time analogue can be found here [61]). One way to interpret this result is a homotopy method for computing equilibria in coordination games, where the algorithm always converges to fixed points, and as mutation goes to zero the stable fixed points correspond to the pure Nash equilibria [24].

4.5 Rate of convergence: dynamics without mutation in fixed environments

In this section we show a polynomial bound on the convergence time of dynamics (29), governing sexual evolution under natural selection with noise, in a static environment. In addition, we show that the fixed points reached by the dynamics are pure. Consider a fixed environment e and we use W to denote its fitness matrix W^e. It is known that average fitness $\mathbf{x}^\top W \mathbf{y}$ increases under the non-noisy counterpart (26). In the next lemma we obtain a lower bound on this increase.

Lemma 4.1. *Let* $(\hat{\mathbf{x}}, \hat{\mathbf{y}}) = g(\mathbf{x}, \mathbf{y})$ *where* $(\mathbf{x}, \mathbf{y}) \in \Delta$ *and g is from equation (26). Then,*

$$\hat{\mathbf{x}}^\top W \hat{\mathbf{y}} - \mathbf{x}^\top W \mathbf{y} \geq C \left(\sum_i x_i \left((W\mathbf{y})_i - \mathbf{x}^\top W \mathbf{y} \right)^2 + \sum_i y_i \left((W^\top \mathbf{x})_i - \mathbf{x}^\top W \mathbf{y} \right)^2 \right),$$

for $C = \frac{3}{8 \cdot \max_{i,j} W_{ij}}$.

Proof. From the definition of g (equation 26) we get,

$$2 \left(\hat{\mathbf{x}}^\top W \hat{\mathbf{y}} \right) \left(\mathbf{x}^\top W \mathbf{y} \right)^2 = 2 \sum_{ij} W_{ij} \hat{x}_i \hat{y}_j \left(\mathbf{x}^\top W \mathbf{y} \right)^2$$

$$=2 \sum_{ij} W_{ij} x_i y_j \frac{(W\mathbf{y})_i}{\mathbf{x}^\top W \mathbf{y}} \frac{(W^\top \mathbf{x})_j}{\mathbf{x}^\top W \mathbf{y}} \left(\mathbf{x}^\top W \mathbf{y} \right)^2 = 2 \sum_{i,j} W_{ij} x_i y_j (W\mathbf{y})_i (W^\top \mathbf{x})_j$$

$$=\sum_{i,j,k} W_{ij} W_{ik} x_i y_j y_k (W^\top \mathbf{x})_j + \sum_{i,j,k} W_{ij} W_{jk}^\top x_i x_k y_j (W\mathbf{y})_i$$

$$=\sum_{i,j,k} W_{ij} W_{ik} x_i y_j y_k \frac{1}{2}((W^\top \mathbf{x})_j + (W^\top \mathbf{x})_k) + \sum_{i,j,k} W_{ij} W_{kj} x_i x_k y_j \frac{1}{2}((W\mathbf{y})_i + (W\mathbf{y})_k)$$

$$\geq \sum_{i,j,k} W_{ij} W_{ik} x_i y_j y_k \sqrt{(W^\top \mathbf{x})_j (W^\top \mathbf{x})_k} + \sum_{i,j,k} W_{ij} W_{kj} x_i x_k y_j \sqrt{(W\mathbf{y})_i (W\mathbf{y})_k}$$

$$=\sum_{i} x_i \left(\sum_j y_j W_{ij} \sqrt{(W^\top \mathbf{x})_j} \right)^2 + \sum_{j} y_j \left(\sum_i x_i W_{ij} \sqrt{(W\mathbf{y})_i} \right)^2$$

$$\geq \left(\sum_{i,j} x_i y_j W_{ij} \sqrt{(W^\top \mathbf{x})_j} \right)^2 + \left(\sum_{j,i} y_j x_i W_{ij} \sqrt{(W\mathbf{y})_i} \right)^2 \quad \text{by convexity of } f(z) = z^2$$

$$=\left(\sum_j y_j (W^\top \mathbf{x})_j^{3/2} \right)^2 + \left(\sum_i x_i (W\mathbf{y})_i^{3/2} \right)^2. \tag{0}$$

Let ξ be a random variable that takes value $(W\mathbf{y})_i$ with probability x_i. Then $\mathbb{E}[\xi] = \mathbf{x}^\top W \mathbf{y}$, $\mathbb{V}[\xi] = \sum_i x_i ((W\mathbf{y})_i - \mathbf{x}^\top W \mathbf{y})^2$ and ξ takes values in the interval $[0, \mu]$ with $\mu = \max_{ij} W_{ij}$. Consider the function $f(z) = z^{3/2}$ on the interval $[0, \mu]$ and observe that $f''(z) \geq \frac{3}{4} \frac{1}{\sqrt{\mu}}$ on $[0, \mu]$ since $\mu \geq \mathbf{p}^\top W \mathbf{q} \geq 0$ for all $(\mathbf{p}, \mathbf{q}) \in \Delta$. Observe also that $f(\mathbb{E}[\xi]) = (\mathbf{x}^\top W \mathbf{y})^{3/2}$ and $\mathbb{E}[f(\xi)] = \sum_i x_i (W\mathbf{y})_i^{3/2}$.

Claim 4.2. $\mathbb{E}[f(\xi)] \geq f(\mathbb{E}[\xi]) + \frac{A}{2} \mathbb{V}[\xi]$, *where* $A = \frac{3}{4\sqrt{\mu}}$.

Proof. By Taylor expansion we get that (we expand with respect to the expectation of ξ, namely $\mathbb{E}[\xi]$)

$$f(z) \geq f(\mathbb{E}[\xi]) + f'(\mathbb{E}[\xi])(z - \mathbb{E}[\xi]) + \frac{A}{2}(z - \mathbb{E}[\xi])^2$$

and hence we have that:

$$f(z) \geq f(\mathbb{E}[\xi]) + f'(\mathbb{E}[\xi])(z - \mathbb{E}[\xi]) + \frac{A}{2}(z - \mathbb{E}[\xi])^2 \overset{\text{taking expectation}}{\Longrightarrow}$$

$$\mathbb{E}[f(\xi)] \geq \mathbb{E}[f(\mathbb{E}[\xi])] + f'(\mathbb{E}[\xi])(\mathbb{E}[\xi] - \mathbb{E}[\xi]) + \frac{A}{2}\mathbb{V}[\xi]$$

$$= f(\mathbb{E}[\xi]) + \frac{A}{2}\mathbb{V}[\xi].$$

$\square$

Using the above claim it follows that:

$$\sum_i x_i(W\mathbf{y})_i^{3/2} \geq (\mathbf{x}^\top W\mathbf{y})^{3/2} + \frac{3}{8\sqrt{\mu}}\sum_i x_i((W\mathbf{y})_i - \mathbf{x}^\top W\mathbf{y})^2.$$

Squaring both sides and omitting one square from the r.h.s we get

$$\left(\sum_i x_i(W\mathbf{y})_i^{3/2}\right)^2 \geq (\mathbf{x}^\top W\mathbf{y})^3 + \frac{3}{4\sqrt{\mu}}(\mathbf{x}^\top W\mathbf{y})^{3/2}\sum_i x_i((W\mathbf{y})_i - \mathbf{x}^\top W\mathbf{y})^2. \quad (33)$$

We do the same by setting ξ to be $(W^\top\mathbf{x})_i$ with probability y_i and using similar argument we get

$$\left(\sum_i y_i(W^\top\mathbf{x})_i^{3/2}\right)^2 \geq (\mathbf{x}^\top W\mathbf{y})^3 + \frac{3}{4\sqrt{\mu}}(\mathbf{x}^\top W\mathbf{y})^{3/2}\sum_i y_i((W^\top\mathbf{x})_i - \mathbf{x}^\top W\mathbf{y})^2. \quad (34)$$

Therefore it follows that

$$2(\hat{\mathbf{x}}^\top W\hat{\mathbf{y}})(\mathbf{x}^\top W\mathbf{y})^2 \geq \left(\sum_j y_j(W^\top\mathbf{x})_j^{3/2}\right)^2 + \left(\sum_i x_i(W\mathbf{y})_i^{3/2}\right)^2 \quad \text{by inequality (0)}$$

$$\overset{33+34}{\geq} 2(\mathbf{x}^\top W\mathbf{y})^3 + \frac{3}{4\sqrt{\mu}}(\mathbf{x}^\top W\mathbf{y})^{3/2}\times$$

$$\times\left(\sum_i x_i\left((W\mathbf{y})_i - \mathbf{x}^\top W\mathbf{y}\right)^2 + \sum_i y_i\left((W^\top\mathbf{x})_i - \mathbf{x}^\top W\mathbf{y}\right)^2\right).$$

Finally we divide both sides by $2(\mathbf{x}^\top W\mathbf{y})^2$ and we get that

$$(\hat{\mathbf{x}}^\top W\hat{\mathbf{y}}) \geq (\mathbf{x}^\top W\mathbf{y}) + \frac{3}{8\sqrt{\mu(\mathbf{x}^\top W\mathbf{y})}}\times$$

$$\times\left(\sum_i x_i\left((W\mathbf{y})_i - \mathbf{x}^\top W\mathbf{y}\right)^2 + \sum_i y_i\left((W^\top\mathbf{x})_i - \mathbf{x}^\top W\mathbf{y}\right)^2\right)$$

$$\geq (\mathbf{x}^\top W\mathbf{y}) + \frac{3}{8\mu}\left(\sum_i x_i\left((W\mathbf{y})_i - \mathbf{x}^\top W\mathbf{y}\right)^2 + \sum_i y_i\left((W^\top\mathbf{x})_i - \mathbf{x}^\top W\mathbf{y}\right)^2\right),$$

with $\frac{3}{8\sqrt{\mu\Phi(\mathbf{x},\mathbf{y})}} \geq \frac{3}{8\mu}$ since $\mu \geq \mathbf{x}^\top W\mathbf{y}$. This inequality and the proof techniques can be seen as a generalization of an inequality and proof techniques in [83]. $\qquad\square$

For the rest of the section, C denotes $\frac{3}{8 \cdot W_{\max}}$ where $W_{\max} = \max_{ij} W_{ij}$ and $W_{\min} = \min_{ij} W_{ij}$. Note that the lower bound obtained in Lemma 4.1 is strictly positive unless $(\mathbf{x},\mathbf{y})$ is a fixed point of (26). This gives an alternate proof of the fact that, under dynamics (26), average fitness is a potential function, *i.e.,* increases in every step. On the other hand, the lower bound can be arbitrarily small at some points, and therefore it does not suffice to bound the convergence time. Next, we define points where this lower-bound is relatively small.

Definition 18 (α-close). *We call a point $(\mathbf{x},\mathbf{y})$ α-close for an $\alpha > 0$, if for all $\mathbf{x}',\mathbf{y}' \in \Delta$ such that $\operatorname{supp}(\mathbf{x}') \subseteq \operatorname{supp}(\mathbf{x})$ and $\operatorname{supp}(\mathbf{y}') \subseteq \operatorname{supp}(\mathbf{y})$ we have $|\mathbf{x}^\top W\mathbf{y} - \mathbf{x}'^\top W\mathbf{y}| \leq \alpha$ and $|\mathbf{x}^\top W\mathbf{y} - \mathbf{x}^\top W\mathbf{y}'| \leq \alpha$.*

α-close points, are a specific class of *"approximate" stationary points*, where the progress in average fitness is not significant (see Figure 8, the big circles contain these points). From now on, think α as a small parameter that will be determined in the end of this section. If a given point $(\mathbf{x},\mathbf{y})$ is not α-close and not *negligible* (see Definition 16) then using Lemma 4.1 it follows that the increase in potential is at least $C\delta\alpha^2$. Formally:

Corollary 4.3 (Not α-close, negligible implies good progress in dynamics). *If $(\mathbf{x},\mathbf{y}) \in \Delta$ is neither α-close nor negligible, and $(\hat{\mathbf{x}},\hat{\mathbf{y}}) = g(\mathbf{x},\mathbf{y})$, then*

$$\hat{\mathbf{x}}^\top W\hat{\mathbf{y}} \geq \mathbf{x}^\top W\mathbf{y} + C\delta\alpha^2.$$

Proof. Since the vector $(\mathbf{x},\mathbf{y})$ is neither α-close nor negligible, it follows that there exists an index i such that $|(W\mathbf{y})_i - \mathbf{x}^\top W\mathbf{y}| > \alpha$ and $x_i \geq \delta$ and hence $x_i((W\mathbf{y})_i - \mathbf{x}^\top W\mathbf{y})^2 > \delta\alpha^2$, or $|(W^\top\mathbf{x})_i - \mathbf{x}^\top W\mathbf{y}| > \alpha$ and $y_i \geq \delta$ and hence $y_i((W^\top\mathbf{x})_i - \mathbf{x}^\top W\mathbf{y})^2 > \delta\alpha^2$. Therefore in Lemma 4.1, the r.h.s is at least $C\delta\alpha^2$ and thus we get that $\hat{\mathbf{x}}^\top W\hat{\mathbf{y}} - \mathbf{x}^\top W\mathbf{y} \geq C\delta\alpha^2$. $\qquad\square$

In the analysis above we considered non-noisy dynamics governed by (26). Our goal is to analyze finite population dynamics, which introduces noise and the resulting dynamics is (29). This changes how the fitness increases/decreases. The next lemma shows that in expectation the average fitness remains unchanged after the introduction of noise.

Lemma 4.4 (Noise is zero in expectation). *Let $\delta = (\delta_{\mathbf{x}}, \delta_{\mathbf{y}})$ be the noise vector. It holds that $\mathbb{E}_\delta[(\mathbf{x} + \delta_{\mathbf{x}})^\top W(\mathbf{y} + \delta_{\mathbf{y}})] = \mathbf{x}^\top W \mathbf{y}$.*

Proof. Vectors $(\delta_{\mathbf{x}}, \delta_{\mathbf{y}}), (-\delta_{\mathbf{x}}, \delta_{\mathbf{y}}), (\delta_{\mathbf{x}}, -\delta_{\mathbf{y}}), (-\delta_{\mathbf{x}}, -\delta_{\mathbf{y}})$ appear with the same probability, and observe that

$$(\mathbf{x} + \delta_{\mathbf{x}})^\top W(\mathbf{y} + \delta_{\mathbf{y}}) + (\mathbf{x} - \delta_{\mathbf{x}})^\top W(\mathbf{y} + \delta_{\mathbf{y}})$$
$$+ (\mathbf{x} + \delta_{\mathbf{x}})^\top W(\mathbf{y} - \delta_{\mathbf{y}}) + (\mathbf{x} - \delta_{\mathbf{x}})^\top W(\mathbf{y} - \delta_{\mathbf{y}})$$
$$= 4\mathbf{x}^\top W \mathbf{y},$$

and the claim follows. $\qquad\square$

Next, we show how random noise can help the dynamic escape from a polytope of α-close points. We first analyze how adding noise may help increase fitness with high enough probability. A simple application of Catalan numbers shows that:

Lemma 4.5. *The probability of a (unbiased) random walk on the integers that consist of $2m$ steps of unit length, beginning at the origin and ending at the origin, that never becomes negative is $\frac{1}{m+1}$.*

We define $\gamma = \min_{(i,j) \neq (i',j')} |W_{ij} - W_{i'j'}|$. The following lemma is essentially a corollary of Lemma 4.5.

Lemma 4.6. *Let $\delta_{\mathbf{y}}$ be a random noise with support size m. For all i in the support of $\mathbf{x}$ we have that $(W\delta_{\mathbf{y}})_i \geq \frac{\gamma \delta m}{2}$ with probability at least $\frac{1}{1+m/2}$ (same is true for $\delta_{\mathbf{x}}$ and $\mathbf{y}$).*

Proof. Assume w.l.o.g that we have $W_{i1} \geq W_{i2} \geq ...$ (otherwise we permute them so that are in decreasing order). Consider the case where the signs are revealed one at a time, in the order of indices of the sorted row. The probability that $+$ signs dominate $-$ signs through the process is $\frac{1}{m/2+1}$ (ballot theorem/Catalan numbers) (see 4.5). It is clear that when the $+$ signs dominate the $-$ signs then

$$(W\delta_{\mathbf{y}})_i = \sum_j^m W_{ij}\delta_j \quad \geq \quad \sum_{j=1}^{m/2}(W_{i(2j-1)} - W_{i(2j)})\delta \quad \geq \quad \gamma\delta\frac{m}{2}.$$

$\square$

We will also need the following theorem due to Azuma [41] on submartingales.

Theorem 4.7 (Azuma inequality [41]). . *Suppose* $\{X_k, k = 0, 1, 2, ..., N\}$ *is a submartingale and also* $|X_k - X_{k-1}| < c$ *almost surely then for all positive integers* N *and all* $t > 0$ *we have that*

$$\mathbb{P}\left[X_N - X_0 \leq -t\right] \leq e^{-\frac{t^2}{2Nc^2}}$$

Towards our main goal of showing polynomial time convergence of the noisy dynamics (29) (shown in Theorem 4.9), we need to show that the fitness increases within a few iterations of the dynamic with high probability. It suffices to show that the average fitness under some transformation is a submartingale, and then the result will follow using Azuma's inequality.

Lemma 4.8 (Potential is a submartingale). *Let* Φ^t *be the random variable which corresponds to the average fitness at time t. Assume that for the time interval* $t = 0, ..., 2T$ *the trajectory* $(\mathbf{x}(t), \mathbf{y}(t))$ *has the same support. Let* $m = \max\{|\text{supp}(\mathbf{x}(t))|, |\text{supp}(\mathbf{y}(t))|\}$, *and the non-zero entries of* $(\mathbf{x}(t), \mathbf{y}(t))$ *be at least* δ. *If* $\frac{1}{(m+2)}(\frac{\gamma\delta m}{2} - 2\alpha)^2 \geq \delta\alpha^2$ *then we have that*

$$E[\Phi^{2t+2}|\Phi^{2t}, ..., \Phi^0] \geq \Phi^{2t} + C\delta\alpha^2.$$

In other words, the sequence $Z^t \equiv \Phi^{2t} - t \cdot C\delta\alpha^2$ *for* $t = 1, ..., T$ *is a submartingale and also* $|Z^{t+1} - Z^t| \leq W_{\max} - W_{\min}$.

Proof. First of all, since the average fitness is increasing in every generation (before adding noise) and by Lemma 4.4 we get that for all $t \in \{0, ..., 2T\}$

$$\mathbb{E}[\Phi^{t+1}|\Phi^t] \geq \Phi^t,$$

namely the average fitness is a submartingale (00).

Let $(\mathbf{x}^t, \mathbf{y}^t) := (\mathbf{x}(t), \mathbf{y}(t))$ be the frequency vector at time t which has average fitness $\Phi^t \equiv \Phi(\mathbf{x}^t, \mathbf{y}^t) = \mathbf{x}^{t\top} W \mathbf{y}^t$ (abusing notation we use $\Phi(\mathbf{x}, \mathbf{y})$ for function $\mathbf{x}^\top W \mathbf{y}$ and Φ^t for the value of average fitness at time t), also we denote $(\hat{\mathbf{x}}^t, \hat{\mathbf{y}}^t) = g(\mathbf{x}^t, \mathbf{y}^t)$ and recall that $(\mathbf{x}^{t+1}, \mathbf{y}^{t+1}) = (\hat{\mathbf{x}}^t + \delta_{\mathbf{x}}^t, \hat{\mathbf{y}}^t + \delta_{\mathbf{y}}^t)$. Assume that in the next generation $(\hat{\mathbf{x}}^{2t}, \hat{\mathbf{y}}^{2t}) = g(\mathbf{x}^{2t}, \mathbf{y}^{2t})$ the average fitness before the noise, namely $\hat{\mathbf{x}}^{2t\,T} W \hat{\mathbf{y}}^{2t}$ will be at least $\Phi^{2t} + C\delta\alpha^2$. Hence by Lemma 4.4 we get that $\mathbb{E}[\Phi^{2t+1}|\Phi^{2t}] = \hat{\mathbf{x}}^{2t\,T} W \hat{\mathbf{y}}^{2t} \geq \Phi^{2t} + C\delta\alpha^2$ (01). Therefore we have that

$$\begin{aligned}
\mathbb{E}[\Phi^{2t+2}|\Phi^{2t}] &= \mathbb{E}_{\delta^{2t+1}, \delta^{2t}}[(\hat{\mathbf{x}}^{2t+1} + \delta_{\mathbf{x}}^{2t+1})^\top W(\hat{\mathbf{y}}^{2t+1} + \delta_{\mathbf{y}}^{2t+1})|\Phi^{2t}] \\
&= \mathbb{E}_{\delta^{2t}}[(\hat{\mathbf{x}}^{2t+1})^\top W \hat{\mathbf{y}}^{2t+1}|\Phi^{2t}] \\
&\geq \mathbb{E}_{\delta^{2t}}[(\mathbf{x}^{2t+1})^\top W \mathbf{y}^{2t+1}|\Phi^{2t}] \\
&= \mathbb{E}[\Phi^{2t+1}|\Phi^{2t}] \\
&\geq \Phi^{2t} + C\delta\alpha^2,
\end{aligned}$$

where second inequality is Expression (01) and the first inequality comes from inequality 4.1 (since the r.h.s of inequality 4.1 is non-negative). The first, third equality comes from model definition and second equality comes from Lemma 4.4.

Assume now that in the next generation $(\hat{\mathbf{x}}^{2t}, \hat{\mathbf{y}}^{2t}) = g(\mathbf{x}^{2t}, \mathbf{y}^{2t})$ the average fitness before the noise, namely $\hat{\mathbf{x}}^{2t\,T} W \hat{\mathbf{y}}^{2t}$ will be less than $\Phi^{2t} + C\delta\alpha^2$. This means that the vector $(\mathbf{x}^{2t}, \mathbf{y}^{2t})$ is α-close by Corollary 4.3, so after adding the noise by the definition of α-close we get that $\hat{\mathbf{x}}^{2t\,T} W \hat{\mathbf{y}}^{2t} + \alpha \geq \Phi^{2t+1} \geq \hat{\mathbf{x}}^{2t\,T} W \hat{\mathbf{y}}^{2t} - \alpha$ (02). From Lemma 4.6 we will have with probability at least $\frac{1}{2} \frac{1}{m/2+1}$ that $(W \mathbf{y}^{2t+1})_i \geq (W \hat{\mathbf{y}}^{2t})_i + \frac{\gamma \delta m}{2}$ for all i in the support of vector $\mathbf{x}^t$ (we multiplied the probability by $\frac{1}{2}$ since you perturb

y with probability half) (03). The same argument works if we perturb **x**, so w.l.o.g we work with perturbed vector **y** which has support of size at least 2. Essentially by inequality 4.1 we get the following inequalities:

$$\mathbb{E}[\Phi^{2t+2}|\Phi^{2t}] = \mathbb{E}_{\delta^{2t+1},\delta^{2t}}[(\hat{\mathbf{x}}^{2t+1} + \delta_{\mathbf{x}}^{2t+1})^\top W(\hat{\mathbf{y}}^{2t+1} + \delta_{\mathbf{y}}^{2t+1})|\Phi^{2t}]$$

$$= \mathbb{E}_{\delta^{2t}}[(\hat{\mathbf{x}}^{2t+1})^\top W\hat{\mathbf{y}}^{2t+1}|\Phi^{2t}]$$

$$\overset{4.1}{\geq} \mathbb{E}_{\delta^{2t}}[(\mathbf{x}^{2t+1})^\top W\mathbf{y}^{2t+1}|\Phi^{2t}]+$$

$$+ C \cdot \mathbb{E}_{\delta^{2t}}\left[\sum_i x_i^{2t+1} \cdot \left((W\mathbf{y}^{2t+1})_i - (\mathbf{x}^{2t+1})^\top W\mathbf{y}^{2t+1}\right)^2 \middle| \Phi^{2t}\right]$$

$$\geq \Phi^{2t} + \frac{C}{m+2}\left(\frac{\gamma\delta m}{2} - 2\alpha\right)^2$$

$$\geq \Phi^{2t} + C\delta\alpha^2,$$

where last inequality comes from the assumption and second inequality comes from claim (00), (02), (03). Hence by induction we get that

$$\mathbb{E}[\Phi^{2t+2} - (t+1)\cdot C\delta\alpha^2|\Phi^{2t}] \geq \Phi^{2t} - t\cdot C\delta\alpha^2.$$

It is easy to see that $W_{\max} \geq \Phi^t \geq W_{\min}$ for all t. $\qquad\square$

Using all the above analysis and Azuma's inequality (Theorem 4.7), we establish our first main result on convergence time of the noisy dynamics governed by (29) for sexual evolution under natural selection and without mutation.

Theorem 4.9 (Main 2 - Speed of convergence). *For all conditions $(\mathbf{x}(0), \mathbf{y}(0)) \in \Delta$, the dynamics governed by (29) in an environment represented by fitness matrix W reaches a pure fixed point with probability $1 - \epsilon$ after $O\left(\frac{(W_{\max})^4 n \ln(\frac{2n}{\epsilon})}{\delta^6\gamma^4}\right)$ iterations.*

Proof. It suffices to show that support size of the **x** or **y** reduces by one in a bounded number of iterations with at least $1 - \frac{\epsilon}{2n}$ probability.

Using Lemma 4.8 we have that the random variable $\Phi^{2t} - t\cdot C\delta\alpha^2$ is a submartingale and since $W_{\min} \leq \Phi^t \leq W_{\max}$ we use Azuma's inequality 4.7 and we get that

$$\mathbb{P}\left[\Phi^{2t} - t\cdot C\delta\alpha^2 \leq \Phi^0 - \lambda\right] \leq e^{-\frac{\lambda^2}{2tW_{max}^2}},$$

hence for $\lambda = \sqrt{2tW_{max}^2 \ln(\frac{2n}{\epsilon})}$ we get that the average fitness after $2t$ steps will be at least $\Phi^0 - \sqrt{2tW_{max}^2 \ln(\frac{2n}{\epsilon})} + t \cdot C\delta\alpha^2$ with probability at least $1 - \frac{\epsilon}{2n}$. By setting $t \geq \frac{8W_{max}^2}{C^2\delta^2\alpha^4} \ln\left(\frac{2n}{\epsilon}\right)$ we have that the average fitness at time $2t$ will be greater than $W_{\max}$ with probability $1 - \frac{\epsilon}{2n}$, but since the potential is at most $W_{\max}$ for all vectors in the simplex, it follows that at some point the frequency vector become *negligible, i.e.,* a coordinate of $\mathbf{x}$ or $\mathbf{y}$ became less than δ. Hence, the probability that the support size decreased during the process is at least $1 - \frac{\epsilon}{2n}$.

By union bound (the initial support size is at most $2n$) we conclude that dynamics (29) reaches a pure fixed point with probability $1 - \epsilon$ after t iterations with $t = 2n\frac{8W_{max}^2}{C^2\delta^2\alpha^4} \ln\left(\frac{2n}{\epsilon}\right)$. Finally, for assumption $\frac{1}{(m+2)}(\frac{\gamma\delta m}{2} - 2\alpha)^2 \geq \delta\alpha^2$ used in Lemma 4.8 to hold for $2 \leq m \leq n$, we set α to be such that $\alpha \leq \frac{\gamma\delta}{4}$ where we have $\frac{4(m-1)^2}{(m+2)} \geq 1 > \delta$. Using such an α it follows that dynamics (29) reaches a pure fixed point with probability $1 - \epsilon$ after $\frac{2^{18}}{9} \times \frac{nW_{\max}^4}{\delta^6\gamma^4} \ln\left(\frac{2n}{\epsilon}\right)$ iterations. $\qquad\square$

4.6   Changing environment: survival or extinction?

In this section we analyze how evolutionary pressures under changing environment may lead to survival/extinction depending on the underlying mutation level. Motivated from Wolf *et al.* work [139], we use Markov chain based model to capture the changing environment, where every state captures a particular environment (see Section 4.3.3 for details).

4.6.1   Extinction without mutation

We show that the population goes extinct with probability one, if the evolution is governed by (29), *i.e.,* natural selection *without* mutations under sexual reproduction. The proof of this result critically relies on polynomial-time convergence to monomorphic population shown in Theorem 4.9 in case of fixed environment.

As discussed in Section 4.3.3, we have assume that the Markov chain is such that

no individual can be fit to survive in all environments. Formally,

$$\forall i, j, \quad \prod_{e \in \mathcal{E}} (W_{ij}^e)^{\pi_e} < 1. \tag{35}$$

Thus, if we can show convergence to monomorphic population under evolving environments as well then the extinction is guaranteed using (35) and the fact that population size N^t gets multiplied by current average fitness (see (32)). However, showing convergence in stochastically changing environment is tricky because environment can change in any step with some probability and then the argument described in the previous section breaks down. To circumvent this we will make use of Borel-Cantelli theorem where we say that *an event happens* if environment remains unchanged for a large but fixed number of steps.

Theorem 4.10 (Second Borel-Cantelli [50]**).** *Let $E_1, E_2, ...$ be a sequence of events. If the events E_n are independent and the sum of the probabilities of the E_n diverges to infinity, then the probability that infinitely many of them occur is 1.*

Using the above theorem with appropriate event definition, we prove the first part of Theorem 1 stated in introduction.

Theorem 4.11 (Main 1a - Extinction without mutation). *Regardless of the initial distributions $(\mathbf{x}(0), \mathbf{y}(0)) \in \Delta$, the population goes extinct with probability one under dynamics governed by (29), capturing sexual evolution without mutation under natural selection.*

Proof. Let T^e be the number of iterations the dynamics (29) need to reach a pure fixed point with probability $\frac{1}{2}$. Theorem 4.9 implies $T^e = O\left(\frac{nW_{\max}^{e^4}}{\delta^6 \gamma^{e^4}} \ln 4n\right)$. Let $T = \max_e T^e$. We consider the time intervals $1, ..., T, T+1, ..., 2T, ...$ which are multiples of T. The probability that Markov chain will remain at a specific environment e in the time interval $kT+1, ..., (k+1)T$ is $\rho_k = (1-p)^T$. We define the sequence of events $E_1, E_2, ...$, where E_i corresponds to the fact that the chain remains in the same

environment from time $(i-1)T+1, ..., iT$. It is clear that E_i's are independent and also $\sum_{i=1}^{\infty} \mathbb{P}[E_i] = \sum_{i=1}^{\infty} \rho_i = \infty$. From Borel-Cantelli Theorem 4.10 it follows that E_i's happen infinitely often with probability 1. When E_i happens there is a time interval of length T that the chain remains in the same environment and therefore with probability $\frac{1}{2}$ the dynamics will reach a pure fixed point. After E_i happen for k times, the probability to reach a pure fixed point is at least $1 - \frac{1}{2^k}$. Hence with probability one (letting $k \to \infty$), the dynamics (29) will reach a pure fixed point.

To finish the proof, let T_{pure} be a random variable that captures the time when a pure fixed point, say (i, j), is reached. The population will have size at most $N^0 V^{T_{pure}}$ where $V = \max_e W_{\max}^e$. Under the assumption on the entries (see inequality (35)) it follows that at any time T' sufficiently large we get that the population at time $T' + T_{pure}$ will be roughly at most

$$N^0 V^{T_{pure}} \prod_e (W_{ij}^e)^{T'\pi_e} = N^0 V^{T_{pure}} \left(\prod_e (W_{ij}^e)^{\pi_e} \right)^{T'}.$$

By choosing $T' \geq \frac{\ln(N^0 V^{T_{pure}})}{-\ln\left((W_{ij}^e)^{\pi_e}\right)}$ (and also satisfying that is much greater than the mixing time) it follows that $N^{T'+T_{pure}} < 1$ and hence the population dies. So, the population goes extinct with probability one in the dynamics without mutation. $\square$

4.6.2 Survival with mutation

In this section we consider evolutionary dynamics governed by (30) capturing sexual evolution *with* mutation under natural selection. Contrary to the case where there are no mutations we show that population survives with positive probability. Furthermore, this result turns out to be robust in the sense that it holds even when every environment has some (few) very bad type alleles. Also, the result is independent of the starting distribution of the population.

The main intuition behind proving this result is that, as for the mutation model in [61], every allele is carried by at least τ fraction of the population in every generation. Therefore even if a "good" allele becomes "bad" as the environment changes, as far

as the new environment has a few fit alleles, there will be some individuals carrying those who will then procreate fast, spreading their alleles further and leading to overall survival. However, unlike in the no mutation case (see Chapter 2), average fitness is no more a potential function even for non-noisy dynamics, *i.e.*, it may decrease, and therefore showing such an improvement is tricky.

First we show that if some small amount of time is spent in an environment then the frequencies of the bad alleles become small and their effect is negligible. Recall the assumption on good/bad type alleles (Section 4.3.3). Formally, let B_i^e be the set of bad type alleles for $i = 1, 2$ in environment e,

$$
\begin{aligned}
\forall i \in S_1 \setminus B_1^e, \ \frac{\sum_j W_{ij}^e}{n} \geq 1 + \beta, \quad &\text{and} \quad \forall i \in S_1 \setminus B_1^e, \forall k \in B_1^e, W_{ij}^e \geq W_{kj}^e, \ \forall j \\
\forall j \in S_2 \setminus B_2^e, \ \frac{\sum_i W_{ij}^e}{n} \geq 1 + \beta, \quad &\text{and} \quad \forall j \in S_2 \setminus B_2^e, \forall k \in B_2^e, W_{ij}^e \geq W_{ik}^e, \ \forall i
\end{aligned}
\tag{36}
$$

Lemma 4.12 (Frequencies of bad alleles become small). *Suppose that the environment e is static for time at least $t \geq \frac{\ln(2n)}{n\tau}$. For any $(\mathbf{x}(0), \mathbf{y}(0)) \in \Delta$, we have that $\sum_{i \in B_1^e} x_i(t) + \sum_{j \in B_2^e} y_j(t) \leq \frac{2(|B_1^e| + |B_2^e|)}{n} = \frac{2|B^e|}{n}$ with $B^e = B_1^e \cup B_2^e$.*

Proof. Consider one step of the dynamics that starts at $(\mathbf{x}, \mathbf{y})$ and has frequency vector $(\tilde{\mathbf{x}}, \tilde{\mathbf{y}})$ in the next step before adding the noise. Let $i*$ be the bad allele that has the greatest fitness at it, namely $(W^e\mathbf{y})_{i*} \geq (W^e\mathbf{y})_i$ for all $i \in B_1^e$. It holds that

$$
\begin{aligned}
\sum_{i \in B_1^e} \tilde{x}_i &= (1 - n\tau) \sum_{i \in B_1^e} x_i \frac{(W^e\mathbf{y})_i}{\mathbf{x}^\top W^e \mathbf{y}} + \tau |B_1^e| \\
&= (1 - n\tau) \frac{\sum_{i \in B_1^e} x_i (W^e\mathbf{y})_i}{\sum_{i \in G_1 \setminus B_1^e} x_i (W^e\mathbf{y})_i + \sum_{i \in B_1^e} x_i (W^e\mathbf{y})_i} + \tau |B_1^e| \\
&\leq (1 - n\tau) \frac{\sum_{i \in B_1^e} x_i (W^e\mathbf{y})_{i*}}{\sum_{i \in G_1 \setminus B_1^e} x_i (W^e\mathbf{y})_i + \sum_{i \in B_1^e} x_i (W^e\mathbf{y})_{i*}} + \tau |B_1^e| \qquad (*) \\
&\leq (1 - n\tau) \frac{\sum_{i \in B_1^e} x_i (W^e\mathbf{y})_{i*}}{\sum_{i \in G_1 \setminus B_1^e} x_i (W^e\mathbf{y})_{i*} + \sum_{i \in B_1^e} x_i (W^e\mathbf{y})_{i*}} + \tau |B_1^e| \\
&= (1 - n\tau) \frac{(W^e\mathbf{y})_{i*} \sum_{i \in B_1^e} x_i}{(W^e\mathbf{y})_{i*} \sum_i x_i} + \tau |B_1^e| \\
&= (1 - n\tau) \sum_{i \in B_1^e} x_i + \tau |B_1^e|,
\end{aligned}
$$

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where inequality (*) is true because if $\frac{a}{b} < 1$ then $\frac{a}{b} < \frac{a+c}{b+c}$ for all a, b, c positive. Hence after we add noise δ with $||\delta||_\infty = \delta$, the resulting vector $(\mathbf{x}', \mathbf{y}')$ (which is the next generation frequency vector) will satisfy $\sum_{i \in B_1^e} x_i' \leq (1-n\tau) \sum_{i \in B_1^e} x_i + \tau |B_1^e| + \delta |B_1^e|$. By setting $S_t = \sum_{i \in B_1^e} x_i(t)$ it follows that $S_{t+1} \leq (1-n\tau)S_t + (\tau + \delta)|B_1^e|$ and also $S_0 \leq$ 1. Therefore $S_t \leq (\tau + \delta)|B_1^e| \frac{1-(1-n\tau)^t}{n\tau} + (1-n\tau)^t$. By choosing $t = -\frac{\ln(2n)}{\ln(1-n\tau)} \approx \frac{\ln(2n)}{n\tau}$ it follows that $\sum_{i \in B_1^e} x_i(t) \leq \frac{(1+o(1))|B_1^e| + 1/2}{n} \leq \frac{2|B_1^e|}{n}$ where we used the assumption that $\delta = o_n(\tau)$. The same argument holds for B_2^e. $\qquad\square$

Using the fact that number of individuals with bad type alleles decreases very fast, established in Lemma 4.12, we can prove that within an environment while there may be decrease in average fitness initially, this decrease is lower bounded. Moreover, it will later increase fast enough so that the initial decrease is compensated.

Lemma 4.13 (**Phase transition on the size of population**). *Suppose that the environment e is static for time t and also $\tau \leq \frac{\beta}{16n}$, $|B^e| \ll n\beta$ then there exists a threshold time T_{thr} such that for any given initial distributions of the alleles $(\mathbf{x}(0), \mathbf{y}(0)) \in \Delta$, if $t < T_{thr}$ then the population size will experience a loss factor of at most $\frac{1}{d}$, otherwise it will experience a gain factor of at least d for some $d > 1$, where $T_{thr} = \frac{6\ln(2n)}{n\tau\beta W_{\min}}$ and $W_{\min} = \min_e W_{\min}^e$.*

Proof. By Lemma 4.12 after $\frac{\ln(2n)}{n\tau}$ generations it follows that

$$\sum_{i \in B_1^e} x_i(t) + \sum_{j \in B_2^e} y_j(t) \leq \frac{2|B^e|}{n}. \tag{37}$$

We consider the average fitness function $\mathbf{x}^\top W^e \mathbf{y}$ which is not increasing (as has already been mentioned). Let $\tau = \tau \cdot (1, ..., 1)^\top$, $(\tilde{\mathbf{x}}, \tilde{\mathbf{y}}) = f(\mathbf{x}, \mathbf{y})$ and $(\hat{\mathbf{x}}, \hat{\mathbf{y}}) = g(\mathbf{x}, \mathbf{y})$ with fitness matrix W^e and also denote by $(\mathbf{x}', \mathbf{y}')$ the resulting vector after noise δ is added. It is easy to observe that

$$\tilde{\mathbf{x}}^\top W^e \tilde{\mathbf{y}} = (1-n\tau)^2 \hat{\mathbf{x}}^\top W^e \hat{\mathbf{y}} + (1-n\tau)\hat{\mathbf{x}}^\top W^e \tau + (1-n\tau)\tau^\top W^e \hat{\mathbf{y}} + \tau^\top W^e \tau$$

and also that

$$\mathbf{x'}^\top W^e \mathbf{y'} \geq \tilde{x}^\top W^e \tilde{y} - 2n\delta W^e_{\max} \geq \tilde{x}^\top W^e \tilde{y} \left(1 - O\left(2n\delta \frac{W_{max}}{W_{min}}\right)\right) = (1 - o_{n\tau}(1))\tilde{x}^\top W \tilde{y},$$

where $W_{\max} = \max_e W^e_{\max}$. Under the assumption 36 we have the following upper bounds:

- $\hat{\mathbf{x}}^\top W^e \tau \geq (1+\beta)n\tau \left(1 - \frac{2|B^e_1|}{n}\right)$ and $\hat{\tau}^\top W^e \hat{\mathbf{y}} \geq (1+\beta)n\tau \left(1 - \frac{2|B^e_2|}{n}\right)$.

- $\tau^\top W^e \tau \geq (n\tau)^2(1+\beta)\left(1 - \frac{|B^e|}{n}\right) \geq (1+\beta)\left(1 - \frac{2|B^e|}{n}\right)^2 n^2\tau^2$.

First assume that $\mathbf{x}^\top W^e \mathbf{y} \leq 1 + \frac{\beta}{2}$. We get the following system of inequalities:

$$\frac{\mathbf{x'}^\top W^e \mathbf{y'}}{\mathbf{x}^\top W^e \mathbf{y}} \geq (1 - o_{n\tau}(1))\frac{\tilde{\mathbf{x}}^\top W^e \tilde{\mathbf{y}}}{\mathbf{x}^\top W^e \mathbf{y}}$$

$$\geq (1 - o_{n\tau}(1))\left((1 - n\tau)^2 \frac{\hat{\mathbf{x}}^\top W^e \hat{\mathbf{y}}}{\mathbf{x}^\top W^e \mathbf{y}} + 2(1 - n\tau)n\tau \left(1 - \frac{2|B^e|}{n}\right)\frac{(1+\beta)}{\mathbf{x}^\top W^e \mathbf{y}} + \right.$$

$$\left. + \frac{(1+\beta)}{\mathbf{x}^\top W^e \mathbf{y}}\left(1 - \frac{2|B^e|}{n}\right)^2 n^2\tau^2\right)$$

$$\geq (1 - o_{n\tau}(1))\left((1 - n\tau)^2 + 2(1 - n\tau)n\tau \left(1 - \frac{2|B^e|}{n}\right)\left(1 + \frac{\beta}{2+\beta}\right) + \right.$$

$$\left. + \left(1 + \frac{\beta}{2+\beta}\right)\left(1 - \frac{2|B^e|}{n}\right)^2 n^2\tau^2\right)$$

$$\geq (1 - o_{n\tau}(1))\left(1 + n\tau\left(\frac{2\beta}{2+\beta} - \frac{6|B^e|}{n} - \frac{2\beta}{2+\beta}n\tau\right)\right)$$

$$\geq 1 + n\tau\left(\frac{\beta}{2+\beta}\right).$$

Second inequality comes from the fact that $\hat{\mathbf{x}}^\top W^e \hat{\mathbf{y}} \geq \mathbf{x}^\top W^e \mathbf{y}$ (the average fitness is increasing for the no mutation setting) and also since $\mathbf{x}^\top W^e \mathbf{y} \leq 1 + \frac{\beta}{2}$. The third and the fourth inequality use the fact that $|B^e| \ll n\beta$ and $\tau \leq \frac{\beta}{16n}$. Therefore, the fitness increases in the next generation for the mutation setting as long as the current fitness $\mathbf{x}^\top W^e \mathbf{y} \leq 1 + \frac{\beta}{2}$ with a factor of $1 + n\tau\frac{\beta}{2+\beta}$ (i). Hence the time we need to reach the value of 1 for the average fitness is $\frac{2\ln\frac{1}{h}}{n\tau\frac{\beta}{2+\beta}}$ which is dominated by $t_1 = \frac{\ln(2n)}{n\tau}$. Therefore the total loss factor is at most $\frac{1}{d} = h^{t_1}$, namely $d = \left(\frac{1}{h}\right)^{t_1}$. Let t_2 be the time for the

average fitness to reach $1+\frac{\beta}{4}$ (as long as it has already reached 1), thus $t_2 = \frac{2}{n\tau}$ which is dominated by t_1. By similar argument, let's now assume that $\mathbf{x}^\top W^e \mathbf{y} \geq 1+\frac{\beta}{2}$ then

$$\frac{\mathbf{x}'^\top W^e \mathbf{y}'}{\mathbf{x}^\top W^e \mathbf{y}} \geq (1 - o_{n\tau}(1)) \left(\frac{\tilde{\mathbf{x}}^\top W^e \tilde{\mathbf{y}}}{\mathbf{x}^\top W^e \mathbf{y}} \right)$$

$$\geq (1 - o_{n\tau}(1)) \left((1 - n\tau)^2 \frac{\hat{\mathbf{x}}^\top W^e \hat{\mathbf{y}}}{\mathbf{x}^\top W^e \mathbf{y}} + 2(1 - n\tau)n\tau \left(1 - \frac{2|B^e|}{n} \right) \frac{(1+\beta)}{\mathbf{x}^\top W^e \mathbf{y}} + \right.$$

$$\left. + \frac{(1+\beta)}{\mathbf{x}^\top W^e \mathbf{y}} \left(1 - \frac{2|B^e|}{n} \right)^2 n^2\tau^2 \right)$$

$$\geq 1 - 2n\tau.$$

Hence $\mathbf{x}'^\top W^e \mathbf{y}' \geq (1 - 2n\tau)(1 + \frac{\beta}{2})$, namely $\mathbf{x}'^\top W^e \mathbf{y}' \geq 1 + \frac{\beta}{4}$ (ii) for $\tau < \frac{\beta}{16n}$. Therefore as long as the fitness surpasses $1+\frac{\beta}{4}$, it never goes below $1+\frac{\beta}{4}$ (conditioned on the fact you remain at the same environment). This is true from claims (i), (ii). When the fitness is at most $1 + \frac{\beta}{2}$, it increases in the next generation and when it is greater than $1 + \frac{\beta}{2}$, it remains at least $1 + \frac{\beta}{4}$ in the next generation. To finish the proof we compute the times. The time t_3 to have a total gain factor of at least d, will be such that $(1 + \frac{\beta}{4})^{t_3} = \frac{1}{h^{t_1}}$. Hence $t_3 = t_1 \frac{2 \ln \frac{1}{h}}{\beta}$. By setting $T_{thr} = \frac{6 \ln(2n)}{n\tau\beta W_{\min}} > \frac{6 \ln \frac{1}{h} \ln(2n)}{n\tau\beta} > 3t_3 > t_1 + t_2 + t_3$ the proof finishes. □

To show the second part of Theorem 1 (main result), we will couple the random variable corresponding to the number of individuals at every iteration with a biased random walk on the real line. This can be done since in Lemma 4.13 we established that the decrease and increase in average fitness is upper and lower bounded, respectively. We will apply the following lemma about the biased random walks.

Lemma 4.14 (Biased random walk). *Assume we perform a random walk on the real line, starting from point $k \in \mathbb{N}$ and going right (+1) with probability $q > \frac{1}{2}$ and left (-1) with probability $1 - q$. The probability that we will eventually reach 0 is $\left(\frac{1-q}{q} \right)^k$.*

Using Lemma 4.13 together with the biased random walk Lemma 4.14, we show our next result on survival of population under mutation in the following theorem.

Theorem 4.15 (Main 1b - Mutation implies survival). *If $p < \frac{1}{2T_{thr}}$ where $T_{thr} = \frac{6\ln(2n)}{n\tau\beta W_{\min}}$ then the probability of survival is at least $1 - \left(\frac{pT_{thr}}{1-pT_{thr}}\right)^{c\ln N^0}$ for some c independent of N^0, $c = \left(\frac{n\tau W_{\min}}{\ln(2n)}\right)$.*

Proof. The probability that the chain remains at a specific environment for least T_{thr} iterations is $(1-p)^{T_{thr}} > 1 - pT_{thr}$ (from the moment it enters the environment until it departs) and hence the probability that the chain stays at an environment for time less that T_{thr} is at most pT_{thr}. Let $N^t = N^0 \prod_{j=1}^{t} \mathbf{x}(j)^{\top} W^{e(j)} \mathbf{y}(j)$ (see (32) where here $e(j)$ corresponds to the environment at time j) the number of individuals at time t and Z^i be the position of the biased random walk at time i as defined in Lemma 4.14 with $q = 1 - pT_{thr}$ and assume that $Z^0 = \lfloor \log_d N^0 \rfloor$ (d is from lemma 4.13). Let $t_1, t_2, ...$ be the sequence of times where there is a change of environment (with $t_0 = 0$) and consider the trivial coupling where when the chain changes environment then a move is made on the real line. If the chain remained in the environment for time less than T_{thr} then the walk goes left, otherwise it goes right. It is clear by Lemma 4.13 that random variable $\log_d N^{t_i}$ dominates Z^i. Hence, the probability that the population survives is at least the probability that Z^i never reaches zero ($Z^i > 0$ for all $i \in \mathbb{N}$). By Lemma 4.14 this is at most $\left(\frac{pT_{thr}}{1-pT_{thr}}\right)^{\lfloor \log_d N^0 \rfloor}$ and thus the probability of survival is at least $1 - \left(\frac{pT_{thr}}{1-pT_{thr}}\right)^{c\ln N^0}$ where $c = \left(\frac{n\tau W_{\min}}{\ln(2n)}\right)$ depends on n, τ and fitness matrices W^e (the minimum $W_{\min} = \min_e W_{\min}^e$, and also from Lemma 4.13 we have that $\ln d \approx \frac{\ln 2n}{W_{\min}n\tau}$). $\qquad\square$

4.7 Convergence of discrete replicator dynamics with mutation in fixed environments

In this section we extend the convergence result 2.9 of Chapter 2 for dynamics (26) in static environment to dynamics governed by (28) where mutations are also present. The former result critically hinges on the fact that mean fitness strictly increases unless the system is at a fixed point, and thereby acts as a potential function. Despite

the fact that this is no longer the case when mutations are introduced, we manage to show that the system still converges and follows an intuitively clear behavior. Namely, in every step of the dynamic, either the average fitness $\mathbf{x}^\top W\mathbf{y}$ or the product of the proportions of all different alleles $\prod_i x_i \prod_i y_i$ (or both) will increase. This latter quantity is, a measure of how mixed/diverse the population is. To argue this we apply inequality 1.1 due to Baum and Eagon and we establish a potential function P for the dynamics governed by (28), capturing sexual evolution with mutation. This will imply convergence for the dynamics. Note that feasible values of τ are in $[0, \frac{1}{n}]$, since τ represents fraction of allele i mutating to allele i' of the same gene implying $n\tau \leq 1$.

Theorem 4.16 (Main 3 - Convergence with mutations). *Given a static environment W, dynamics governed by (28) with mutation parameter $\tau \leq \frac{1}{n}$ has a potential function $P(\mathbf{x}, \mathbf{y}) = (\mathbf{x}^\top W\mathbf{y})^{1-n\tau} \prod_i x_i^\tau \prod_i y_i^\tau$ that strictly increases unless an equilibrium (fixed point) is reached. Thus, the system converges to equilibria, in the limit. Equilibria are exactly the set of points $(\mathbf{p}^*, \mathbf{q}^*)$ that satisfy for all $i, i' \in S_1$, $j, j' \in S_2$:*

$$\frac{(W\mathbf{q}^*)_i}{1 - \frac{\tau}{p_i^*}} = \frac{(W\mathbf{q}^*)_{i'}}{1 - \frac{\tau}{p_{i'}^*}} = \frac{\mathbf{p}^{*T}W\mathbf{q}^*}{1 - n\tau} = \frac{(W^\top\mathbf{p}^*)_j}{1 - \frac{\tau}{q_j^*}} = \frac{(W^\top\mathbf{p}^*)_{j'}}{1 - \frac{\tau}{q_{j'}^*}}.$$

Proof. We first prove the results for rational τ; let $\tau = \kappa/\lambda$. We use the Theorem 1.1. Let

$$L(\mathbf{x}, \mathbf{y}) = (\mathbf{x}^\top W\mathbf{y})^{\lambda - m\kappa} \prod_i x_i^\kappa \prod_i y_i^\kappa.$$

Then

$$x_i \frac{\partial L}{\partial x_i} = 2\kappa L + \frac{2x_i(W\mathbf{y})_i(\lambda - m\kappa)L}{\mathbf{x}^\top W\mathbf{y}}.$$

It follows that

$$\begin{aligned}
\frac{x_i \frac{\partial L}{\partial x_i}}{\sum_i x_i \frac{\partial L}{\partial x_i}} &= \frac{2\kappa L + \frac{2x_i(W\mathbf{y})_i(\lambda - m\kappa)L}{\mathbf{x}^\top W\mathbf{y}}}{2m\kappa L + 2(\lambda - m\kappa)L} \\
&= \frac{2\kappa L}{2\lambda L} + \frac{2L(\lambda - m\kappa)x_i(W\mathbf{y})_i}{2\lambda L\mathbf{x}^\top W\mathbf{y}} \\
&= (1 - n\tau)x_i \frac{(W\mathbf{y})_i}{\mathbf{x}^\top W\mathbf{y}} + \tau,
\end{aligned}$$

where the first equality comes from the fact that $\sum_{i=1}^{n} x_i(W\mathbf{y})_i = \mathbf{x}^\top W\mathbf{y}$. The same is true for $y_i \frac{\partial L}{\partial y_i}$. Since L is a homogeneous polynomial of degree 2λ, from Theorem 1.1 we get that L is strictly increasing along the trajectories, namely

$$L(f(\mathbf{x}, \mathbf{y})) > L(\mathbf{x}, \mathbf{y}),$$

unless $(\mathbf{x}, \mathbf{y})$ is a fixed point (f is the update rule of the dynamics, see also (27)). So $P(\mathbf{x}, \mathbf{y}) = L^{1/\kappa}(\mathbf{x}, \mathbf{y})$ is a potential function for the dynamics. To prove the result for irrational τ, we just have to see that the proof of [14] holds for all homogeneous polynomials with degree d, even irrational.

To finish the proof let $\Omega \subset \Delta$ be the set of limit points of an orbit $\mathbf{z}(t) = (\mathbf{x}(t), \mathbf{y}(t))$ (frequencies at time t for $t \in \mathbb{N}$). $P(\mathbf{z}(t))$ is increasing with respect to time t by above and so, because P is bounded on Δ, $P(\mathbf{z}(t))$ converges as $t \to \infty$ to $P^* = \sup_t\{P(\mathbf{z}(t))\}$. By continuity of P we get that $P(\mathbf{v}) = \lim_{t\to\infty} P(\mathbf{z}(t)) = P^*$ for all $\mathbf{v} \in \Omega$. So P is constant on Ω. Also $\mathbf{v}(t) = \lim_{k\to\infty} \mathbf{z}(t_k + t)$ as $k \to \infty$ for some sequence of times $\{t_i\}$ and so $\mathbf{v}(t)$ lies in Ω, i.e., Ω is invariant. Thus, if $\mathbf{v} \equiv \mathbf{v}(0) \in \Omega$ the orbit $\mathbf{v}(t)$ lies in Ω and so $P(\mathbf{v}(t)) = P^*$ on the orbit. But P is strictly increasing except on equilibrium orbits and so Ω consists entirely of fixed points. $\qquad\square$

As a consequence of the above theorem we get the following:

Corollary 4.17. *Along every nontrivial trajectory of dynamics governed by (28) at least one of average fitness $\mathbf{x}^\top W\mathbf{y}$ or product of allele frequencies $\prod_i x_i \prod_i y_i$ strictly increases at each step.*

4.8   Discussion on the assumptions and examples

In this section, we discuss why our assumptions are necessary and their significance.

4.8.1   On the parameters

The effective range of δ is $o\left(\frac{1}{n}\right)$, where $||\delta||_\infty = \delta$, whereas for γ is $O\left(\frac{1}{n^2}\right)$. For example, if we consider the entries of fitness matrices W^e to be uniform from interval

$(1 - \sigma, 1 + \sigma)$ for some positive $\sigma > 0$ then γ is of $\Theta(\frac{1}{n^2})$ order. If the entries of the matrix are constants (in weak selection scenario they lie in the interval $(1 - \sigma, 1 + \sigma)$) then the convergence time of dynamics (29) is polynomial with respect to n (size of fitness matrices W^e is $n \times n$). We note that the main result of Chapter 2 for dynamics (26) has been derived under the assumption that the entries of the fitness matrix are all distinct. It is proven that this assumption is necessary by giving examples where the dynamic doesn't converge to pure fixed points if the fitness matrix has some entries that are equal (the trivial example is when W has all entries equal, then every frequency vector in Δ is a fixed point). This is an indication that γ is needed to analyse the running time and is not artificial. The noise vector δ has coordinates $\pm\delta$, so it is uniformly chosen from hypercube, but there is no dependence on the current frequency vector (δ is independent of current $(\mathbf{x}, \mathbf{y})$). Finally, β should be thought of as a small constant number (like in weak selection) independent of n, and τ to be $O(\frac{1}{n})$ ($1 - n\tau \geq 0$ must hold so that the dynamics with mutation are meaningful and from Lemma 4.13, it must hold that $\tau \leq \frac{\beta}{16n}$).

4.8.2 On the environments

We analyze a finite population model where N^t is the population size at time t. It is natural to define survival if $N^t \geq 1$ for all $t \in \mathbb{N}$ (number of people is at least 1 at all times) and extinction if $N^t < 1$ for some t (if the number of people is less than one at some point then the population goes extinct). As described in preliminaries, $N^t = N^{t-1} \cdot \Phi^t$ where $\Phi^t = x(t)^\top W^{e(t)} y(t)$ is the average fitness at time t and $W^{e(t)}$ is the fitness matrix of environment $e(t)$ (at time t).

Fix a fitness matrix W (*i.e.*, fix an environment). If $W_{ij} > 1 + \epsilon$ for all (i, j) then $\mathbf{x}^\top W \mathbf{y} \geq 1$ for all $(\mathbf{x}, \mathbf{y}) \in \Delta$ and thus the number of individuals is increasing along the generations by a factor of $1 + \epsilon$ (the population survives). On the other hand, if $W_{ij} < 1 - \epsilon$ for all (i, j) then $\mathbf{x}^\top W \mathbf{y} < 1 - \epsilon$ for all $(\mathbf{x}, \mathbf{y}) \in \Delta$, so it is clear that

the number of individuals is decreasing with a factor of $1 - \epsilon$ (thus population goes extinct). So either extreme makes the problem irrelevant.

Finally, it is natural to assume that complete diversity should favor survival, *i.e.,* if the population is uniform along the alleles/types then the population size must not decrease in the next generation. Therefore, we assume that the average fitness under uniform frequencies is $\geq 1 + \beta$ (for all but few number of bad alleles that can be seen as deleterious). The alleles that are good should dominate entry-wise the bad alleles. Example Figure 7 shows that this assumption is necessary. In Figure 7, $\tau = 0.03$ and $W^e = \begin{pmatrix} 0.99 & 0.37 \\ 0.56 & 2.09 \end{pmatrix}$. If we start from any vector $(\mathbf{x}, \mathbf{y})$ in the shaded area, the dynamics converges to the stable fixed point B. The average fitness $\mathbf{x}^\top W \mathbf{y}$ at B is less than the maximum at the corner which is $W^e_{1,1} = 0.99 < 1$. So if the size of population is Q when entering e, after t generations on the environment e, the population size will be at most $Q \cdot 0.99^t$ (which decreases exponentially). In that case Theorem 4.15 does not hold, even if $\frac{0.99 + 0.37 + 0.56 + 2.09}{4} = 1.0025 > 1$ and $\beta = 0.0025$ (qualitatively we would have the same picture for any $\tau \in [0, 0.03]$ and W^e).

The assumption defined in (35) is necessary as well for the following reason: Assume there is a combination of alleles (i, j) so that $\prod_e (W^e_{ij})^{\pi_e} \geq 1$ (**). In that case we can have one of the environments so that $x_i = 1, y_j = 1$ is a stable fixed point and hence there are initial frequencies so that the dynamics (29) converge to it. After that, it is easy to argue that this monomorphic population survives on average because of (**), so the probability of survival in that case is non zero.

4.8.3 Explanation of figure 6

Figure 6 on the title page shows the adjacency graph of a Markov chain. There are 3 environments with fitness matrices, say $W^{e_1}, W^{e_2}, W^{e_3}$, and the entries of every matrix are distinct. Take $p_{ii} = 1 - p$ and $p_{ij} = \frac{p}{2}$ so that the stationary distribution is $(1/3, 1/3, 1/3)$. Observe that $W^{e_1}_{1,1} \cdot W^{e_2}_{1,1} \cdot W^{e_3}_{1,1} = 1.12 \cdot 1.02 \cdot 0.87 < 0.994 < 1$. The

same is true for entries (1,2),(2,1),(2,2). So the assumption defined in (35) is satisfied.

Moreover, observe that if we choose $\beta = 0.005$ and hence $\tau = \frac{0.005}{32}$ it follows that the assumptions defined in (36) are satisfied (also the bad alleles are dominated entry-wise by the good alleles). Hence, in case of no mutation, from theorem 4.11 the population dies out with probability 1 for all initial population sizes N^0 and all initial frequency vectors in Δ. In case of mutation, and for sufficiently large initial population size N^0, for all initial frequency vectors in Δ the probability of survival is positive (Theorem 4.15).

4.9 Figures

To draw the phase portrait of a discrete time system $f : \Delta \to \Delta$, we draw vector $f(\mathbf{x}) - \mathbf{x}$ at point $\mathbf{x}$.
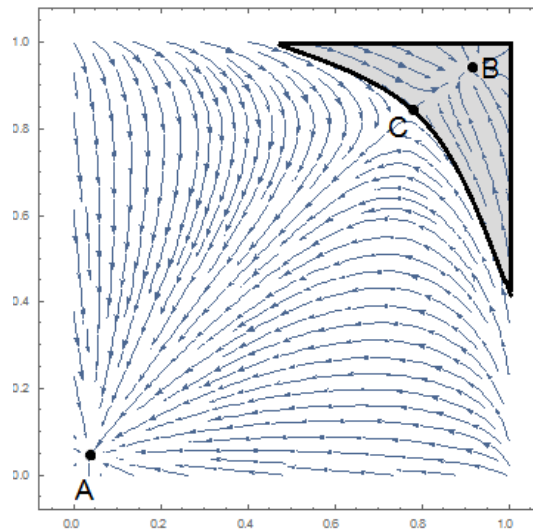
Figure 7: Example where population goes extinct in environment e for some initial frequency vectors $(\mathbf{x}, \mathbf{y})$ that are close to stable point B (inside the shaded area). Mutation probability is $\tau = 0.03$ and the fitness matrix of environment e is $W_{1,1}^e = 0.99, W_{2,2}^e = 2.09, W_{1,2}^e = 0.37, W_{2,1}^e = 0.56$.
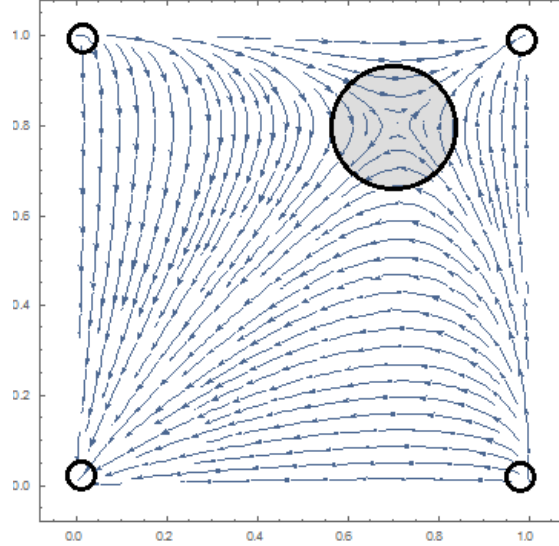
Figure 8: Example of dynamics without mutation in specific environment $W_{1,1}^e = 0.99, W_{2,2}^e = 2.09, W_{1,2}^e = 0.37, W_{2,1}^e = 0.56$. The circles qualitatively show all the points that slow down the increase in the average fitness $\mathbf{x}^\top W^e \mathbf{y}$, *i.e.,* α-close points or negligible.

4.10   Conclusion and remarks

The results of this chapter appear in [85] and it is joint work with Ruta Mehta, Georgios Piliouras, Prasad Tetali and Vijay Vazirani. In this chapter we show various aspects of discrete replicator-like/MWUA dynamics and show three results: Two for dynamics with fixed parameters, and one where the parameters evolve over time as per a Markov chain. Theorem 4.9 establishes that a noisy version of discrete replicator dynamics converges *polynomially fast* to pure fixed points in coordination games. Due to the connections established by Chastain *et al.* [23], this implies that evolution under sexual reproduction in haploids converges fast to a monomorphic population if the environment is static (fitness/payoff matrix is fixed). Introducing mutations to this model, as in [61], augments the replicator dynamics, and our second result shows convergence for this augmented replicator in coordination games. The proof is via a novel potential function, which is a combination of mean payoff and entropy, which

may be of independent interest.

Finally, for the replicator dynamics with noise, capturing finite populations, we show that assuming some mild conditions, the population size will eventually become zero with probability one (extinction) under (standard) replicator, while under augmented replicator (with mutations) it will never whither out (survival) with a non-trivial probability.

A host of novel questions arise from this model and there is space for future work:

- For the fast convergence result (first result above), we assumed that the random noise δ lies in a subset of hypercube of length δ, *i.e.*, every entry δ_i is ± 1 times magnitude δ and $\sum_i \delta_i = 0$. Can the result be generalized for a different class of random noise, where the noise also depends on the distribution of the alleles at every step and or population size?

- The second result talks about convergence to fixed points, which happens at the limit (time $t \to \infty$). Therefore, an interesting question would be to settle the speed of convergence. Additionally, for the no mutations case, the result 2.9 shows that all the stable fixed points are pure. It would be interesting to perform stability analysis for the *replicator with mutations* as well.

- Mutation can be modeled in an alternative way, where an individual can mutate to a completely new allele that is not part of some in advance fixed set of alleles. This is equivalent to adding a strategy to the coordination game. It will be interesting to define and analyze dynamics where mutation is modeled in such a way. Finally, what happens if environment changes are not completely independent but are instead affected by population size?

CHAPTER V

EVOLUTIONARY MARKOV CHAINS

5.1 Introduction

We start this chapter by a motivating example. Given a total number of N red and blue balls we have the following process:

- (*Reproduction* step): From the N balls, each red ball is replaced by $a_r \in \mathbb{Z}_+$ new red balls and each blue ball is replaced by $a_B \in \mathbb{Z}_+$ new blue balls.

- (*Selection* step): N of these offsprings are randomly selected with replacement.

- (*Mutation* step): Each of N balls from the previous step flips color with probability μ and keeps the same color with probability $1 - \mu$.

The stochastic process above is a Markov chain with state space all the $(x, y) \in \mathbb{N}^2$ with $x + y = N$, *i.e.,* it has $N + 1$ states. As long as $\mu > 0$, it is easy to see that the Markov chain is ergodic and it converges to a unique stationary distribution. The main question is how fast it converges, and as discussed in the section 1.3 this is captured by the mixing time. The mixing time of a Markov chain, t_{mix}, is defined to be the smallest time t such that for all $x \in \Omega$, the distribution of the Markov chain starting at x after t-time steps is within an ℓ_1-distance of $1/4$ of the steady state.[1]

In this chapter we will give some generic theorems about bounding the mixing time of Markov chains that have the same flavor as the above process, which we call *evolutionary* Markov chains. These processes arise in the context of evolution and have also been used to model a wide variety of social, economical and cultural

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[1]Recall that if one is willing to pay an additional factor of $\log 1/\epsilon$, one can bring down the error from $1/4$ to ϵ for any $\epsilon > 0$; see [75].

phenomena, see [100]. Typically, in such Markov chains, each state consists of a population of size N where each individual is of one of m *types*. Thus, the state space Ω has size $\binom{N+m-1}{m-1}$, and it is huge even for constant m.[2] At a very high level, in each iteration, the different types in the current generation reproduce according to some fitness function f, the reproduction could be *asexual* or *sexual* and have *mutations* that transform one type into another. This gives rise to an intermediate population that is subjected to the force of *selection*; a sample of size N is selected giving us the new generation. The specific way in which the reproduction, mutation and selection steps happen determine the transition matrix of the corresponding Markov chain.

Most questions in evolution reduce to understanding the statistical properties of the steady state of an evolutionary Markov chain and how it changes with its parameters. However, in general, there seems to be no way to compute the desired statistical properties other than to sample from (close to) the steady state distribution by running the Markov chain for sufficiently long [39]. The examples we examine in Section 5.7 have the property that the underlying Markov chains are ergodic but not reversible and we do not know a another way to compute or approximate the stationary distribution, apart from running the chain. Apart from dictating the computational feasibility of sampling procedures, the mixing time also gives us the number of generations required to reach the steady state; an important consideration for validating evolutionary models [133, 39].

5.1.1 Evolutionary Markov chains

It is convenient to think of each state of an evolutionary Markov chain as a vector which captures the fraction of each type in the current population. Thus, each state is

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[2]For example, even when $m = 40$ and the population is of size $10,000$, the number of states is more than 2^{300}, *i.e.,* more than the number of atoms in the universe!

a $1/N$-integral point (each coordinate is a multiple of $1/N$) in the m-dimensional probability simplex Δ_m,[3] and we can think of the state space $\Omega \subseteq \Delta_m$. We are also given a (fitness) function $f : \Delta_m \mapsto \Delta_m$. If $\mathbf{X}^{(t)}$ is the current state of the chain, inspired by the Wright-Fisher model, the state at $t+1$ is obtained by sampling N times independently from the distribution $f(\mathbf{X}^{(t)})$. In other words, $\mathbf{X}^{(t+1)} \sim \frac{1}{N}\mathrm{Mult}(N, f(\mathbf{X}^{(t)}))$ (multiplied by renormalization factor $1/N$ so that $\mathbf{X}^{(t+1)} \in \Delta_m$), where $\mathrm{Mult}(n, \mathbf{p})$ denotes the multinomial distribution with parameters $(n, \mathbf{p} := (p_1, ..., p_m))$. We will say that this evolutionary Markov chain is *a stochastic evolution guided by f*. It is not hard to see that it holds

$$f(\mathbf{X}^{(t)}) := \mathbb{E}\left[\mathbf{X}^{(t+1)}|\mathbf{X}^{(t)}\right], \tag{38}$$

where the expectation is over one step of the chain. This quantity is called the *expected motion* of the chain at $\mathbf{X}^{(t)}$. Notice that $\mathbf{x}_{k+1} = f(\mathbf{x}_k)$ is a discrete dynamical system in the simplex. *What can the expected motion of a Markov chain tell us about the mixing time of a Markov chain?* Of course, for general Markov chains we do not expect a very interesting answer, but since we get N samples i.i.d to compute the next state, additional structure is imposed to the equation (38) (*e.g.,* we have concentration around the expectation due to Chernoff bounds, see Theorem 5.5).

Our contribution. Our key contribution is to connect the mixing time of an evolutionary Markov chain with the geometry of the corresponding dynamical system it induces (its expected motion). More formally, we prove the following mixing time bounds which depend on the *structure of the limit sets* of the expected motion:

- One unique fixed point which is stable[4] – the mixing time is $O(\log N)$, see Theorem 5.7

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[3]Recall that the probability simplex Δ_m is $\{p \in \mathbb{R}^m : p_i \geq 0 \; \forall i, \; \sum_i p_i = 1\}$.

[4]Abusing the definition, when we say stable in this chapter, we mean that the spectral radius of the Jacobian at the fixed point is less than one. Moreover by unstable, we mean that the Jacobian has spectral radius greater than one.

(a) One stable fixed point $\Rightarrow$ fast mixing

(b) 3 stable fixed points $\Rightarrow$ slow mixing
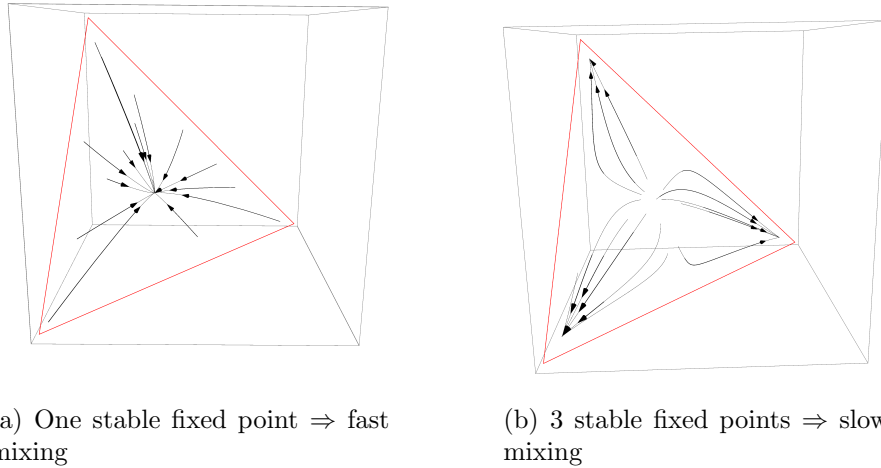
Figure 9: One/multiple stable fixed points.

- One stable fixed point and multiple unstable fixed points – the mixing time is $O(\log N)$, see Theorem 5.8.

- Multiple stable fixed points – the mixing time is $e^{\Omega(N)}$, see Theorem 5.9.

- Periodic orbits – the mixing time is $e^{\Omega(N)}$, see Theorem 5.10.

Roughly, this is achieved by using the geometry of the dynamical system around the fixed points (for the first two theorems we construct a *contractive coupling*).

Moreover we provide two applications in Section 5.7. Theorem 5.7 enables us to establish rapid mixing for evolutionary Markov chains which capture the evolution of species (RSM or Eigen's dynamics [43]) where reproduction is *asexual* (see Theorem 5.11). Finally, combining Theorems 5.7, 5.9 we are able to show a phase transition result in a model which captures how children acquire grammar [101, 71] and which can be interpreted as a process in which the species reproduce is *sexual* (see Theorem 5.12). While we describe these models later, we note that, as one changes the parameters of the model, the limit sets of the expected motion can exhibit the kind of complex behavior mentioned above and a finer understanding of how they influence the mixing time is desired.

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5.2 Related Work

There have been glimpses in the probability literature that connections between Markov chains and dynamical systems might be useful, see [109, 15, 140, 81, 55, 80] and references therein. We study the connection between dynamical systems and the mixing time of Markov chains formally in this chapter. Technically, our results strengthen the connection between Markov chains/stochastic processes and dynamical systems. We focus on a class of Markov chains called evolutionary and inspired by the Wright-Fisher model in population genetics.

The motivating example (as an infinite population dynamics) which also appears in Section 5.7.1 and belongs to the class of Markov chains we focus on, was proposed in the pioneering work of Eigen and co-authors [43, 45]. Importantly, this particular dynamical system has found use in modeling rapidly evolving viral populations (such as HIV), which in turn has guided drug and vaccine design strategies. As a result, these dynamics are well-studied; see [39, 135, 137] for an in depth discussion.

However, even in the simplest of stochastic evolutionary models there has been a lack of rigorous mixing time bounds for the full range of evolutionary parameters; see [42, 49, 47] for results under restricted assumptions. Our Theorems give rigorous bounds for mixing times under minimal assumptions.

5.3 Preliminaries and formal statement of results

5.3.1 Important Definitions and Tools

In preparation for formally stating our results, we first discuss some definitions and technical tools that will be used later on. We then formally state our main theorems in Section 5.3.2 and our applications in Section 5.7. We start this section by defining formally the class of evolutionary Markov chains we focus on for the rest of this chapter.

Definition 19 (Stochastic evolution Markov chains). *Given an $f : \Delta_m \to \Delta_m$*

which is twice differentiable in the relative interior of Δ_m with bounded second deriva-tive and a population parameter N, we define a Markov chain called the stochastic evolution guided by f as follows. The state at time t is a probability vector $\mathbf{X}^{(t)} \in \Delta_m$. The state $\mathbf{X}^{(t+1)}$ is then obtained in the following manner. Define $\mathbf{Y}^{(t)} = f(\mathbf{X}^{(t)})$. Ob-tain N independent samples from the probability distribution $\mathbf{Y}^{(t)}$, and denote by $\mathbf{Z}^{(t)}$ the resulting counting vector over $[m]$. Then

$$\mathbf{X}^{(t+1)} := \frac{1}{N}\mathbf{Z}^{(t)} \quad \text{and therefore } \mathbb{E}[\mathbf{X}^{(t+1)}|\mathbf{X}^{(t)}] = f(\mathbf{X}^{(t)}).$$

We call f the expected motion *of the stochastic evolution.*

Operators and norms. The following theorem, stated here only in the special case of the $1 \to 1$ norm, relates the spectral radius with other matrix norms.

Theorem 5.1 (Gelfand's formula, specialized to the $1 \to 1$ norm). *For any square matrix M, we have*

$$\text{sp}\,(M) = \lim_{l \to \infty} \left\| M^l \right\|_1^{1/l}.$$

Theorem 5.2 (Taylor's theorems, truncated). *Let $f : \mathbb{R}^m \to \mathbb{R}^m$ be a twice differentiable function, and let $J(\mathbf{z})$ denote the Jacobian of f at $\mathbf{z}$. Let $\mathbf{x}, \mathbf{y} \in \mathbb{R}^m$ be two points, and suppose there exists a positive constant B such that at every point on the line segment joining $\mathbf{x}$ to $\mathbf{y}$, the Hessians of each of the m co-ordinates f_i of f have operator norm at most $2B$. Then, there exists a $\mathbf{v} \in \mathbb{R}^m$ such that*

$$f(\mathbf{x}) = f(\mathbf{y}) + J(\mathbf{y})(\mathbf{x} - \mathbf{y}) + \mathbf{v},$$

and $|v_i| \leq B \left\| \mathbf{x} - \mathbf{y} \right\|_2^2$ for each $i \in [m]$.

Theorem 5.3 (Taylor's theorem, first order remainder). *Let $f : \mathbb{R}^m \to \mathbb{R}$ be differentiable and $\mathbf{x}, \mathbf{y} \in \mathbb{R}^m$. Then there exists some ξ in the line segment from $\mathbf{x}$ to $\mathbf{y}$ such that $f(\mathbf{y}) = f(\mathbf{x}) + \nabla f(\xi)(\mathbf{y} - \mathbf{x})$.*

Remark 7 (**On the zero eigenvalue of Jacobian of** $f : \Delta_m \to \Delta_m$). *Since* $f : \Delta_m \to \Delta_m$ *and hence* $\sum_i f_i(\mathbf{x}) = 1$ *for all* $\mathbf{x} \in \Delta_m$, *if we define* $h_i(\mathbf{x}) = \frac{f_i(\mathbf{x})}{\sum_i f_i(\mathbf{x})}$ *so that* $h(\mathbf{x}) = f(\mathbf{x})$ *for all* $\mathbf{x} \in \Delta_m$, *we get that* $\sum_i \frac{\partial h_i(\mathbf{x})}{\partial x_j} = 0$ *for all* $j \in [m]$. *This means without loss of generality we can assume that the Jacobian* $J(\mathbf{x})$ *of* f *has* $\mathbf{1}^\top$ *(the all-ones vector) as a left eigenvector with eigenvalue 0.*

The definition below quantifies the instability of a fixed point as is standard in the literature. Essentially, an α unstable fixed point is repelling in any direction.

Definition 20 (α-**unstable fixed point**). *Let* $\mathbf{z}$ *be a fixed point of a dynamical system* f. *The point* $\mathbf{z}$ *is called* α-unstable *if* $|\lambda_{\min}(J(\mathbf{z}))| > \alpha > 1$ *where* $\lambda_{\min}$ *corresponds to the minimum eigenvalue of the Jacobian of* f *at the fixed point* $\mathbf{z}$, *excluding the eigenvalue 0 that corresponds to the left eigenvector* $\mathbf{1}^\top$.

Also we need to define what a stable periodic orbit is, since we use it in Theorem 5.10. Let $C = \{\mathbf{x}_1, \ldots, \mathbf{x}_k\}$ be a periodic orbit of size k. We call C a *stable* periodic orbit (we also use the terminology *stable limit cycle*) if $\mathrm{sp}\left(J_{f^k}(\mathbf{x}_1)\right) < \rho < 1$, where $J_{f^k}(\mathbf{x}_1)$ denotes the Jacobian of function f^k at $\mathbf{x}_1$.

Couplings and mixing times. We revisit from Introduction some facts about couplings and mixing times, adjusted to the problem of this chapter. Let $\mathbf{p}, \mathbf{q} \in \Delta_m$ be two probability distributions on m objects. A *coupling* $\mathcal{C}$ of $\mathbf{p}$ and $\mathbf{q}$ is a distribution on ordered pairs in $[m] \times [m]$, such that its marginal distribution on the first coordinate is equal to $\mathbf{p}$ and that on the second coordinate is equal to $\mathbf{q}$. A simple, if trivial, example of a coupling is the joint distribution obtained by sampling the two coordinates independently, one from $\mathbf{p}$ and the other from $\mathbf{q}$.

Couplings allow a very useful dual characterization of the total variation distance, as stated in the following well known lemma (see also 1.4).

Lemma 5.4 (**Coupling lemma** [4]). *Let* $\mathbf{p}, \mathbf{q} \in \Delta_m$ *be two probability distributions*

on m objects. Then,

$$\|\mathbf{p} - \mathbf{q}\|_{\mathrm{TV}} = \frac{1}{2}\|\mathbf{p} - \mathbf{q}\|_1 = \min_{\mathcal{C}} \mathbb{P}_{(A,B)\sim\mathcal{C}}\left[A \neq B\right],$$

where the minimum is taken over all valid couplings $\mathcal{C}$ of $\mathbf{p}$ and $\mathbf{q}$.

Moreover, the coupling in the lemma can be explicitly described. We use this coupling extensively in our arguments, hence we record some of its properties here.

Definition 21 (Optimal coupling). *Let $\mathbf{p}, \mathbf{q} \in \Delta_m$ be two probability distributions on m objects. For each $i \in [m]$, let $s_i := \min(p_i, q_i)$, and $s := \sum_{i=1}^{m} s_i$. Sample U, V, W independently at random as follows:*

$$\mathbb{P}\left[U = i\right] = \frac{s_i}{s}, \; \mathbb{P}\left[V = i\right] = \frac{p_i - s_i}{1 - s}, \; \text{and} \; \mathbb{P}\left[W = i\right] = \frac{q_i - s_i}{1 - s}, \; \text{for all } i \in [m].$$

We then sample (independent of U, V, W) a Bernoulli random variable H with mean s. The sample (A, B) given by the coupling is (U, U) if $H = 1$ and (V, W) otherwise.

It is easy to verify that $A \sim \mathbf{p}$, $B \sim \mathbf{q}$ and $\mathbb{P}\left[A = B\right] = s = 1 - \|\mathbf{p} - \mathbf{q}\|_{\mathrm{TV}}$. Another easily verified but important property is that for any $i \in [m]$

$$\mathbb{P}\left[A = i, B \neq i\right] = \begin{cases} 0 & \text{if } p_i < q_i, \\ p_i - q_i & \text{if } p_i \geq q_i. \end{cases}$$

A standard technique for obtaining upper bounds on mixing times is to use the Coupling Lemma above. Suppose $S_1^{(t)}$ and $S_2^{(t)}$ are two evolutions of an ergodic chain M such that their evolutions are coupled according to some coupling $\mathcal{C}$. Let T be the stopping time such that $S_1^{(T)} = S_2^{(T)}$. Then, if it can be shown that $\mathbb{P}\left[T > t\right] \leq 1/e$ for every pair of starting states $(S_1^{(0)}, S_2^{(0)})$, then it follows that $t_{\mathrm{mix}} := t_{\mathrm{mix}}(1/e) \leq t$.

Concentration. We discuss some concentration results that are used extensively in our later arguments. We begin with standard Chernoff-Hoeffding type bounds.

Theorem 5.5 (Chernoff-Hoeffding bounds [41]**).** *Let* $Z_1, Z_2, \ldots, Z_N$ *be i.i.d Bernoulli random variables with mean* μ*. We then have*

1. *When* $0 < \delta \leq 1$,

$$\mathbb{P}\left[\left|\frac{1}{N}\sum_{i=1}^{N} Z_i - \mu\right| > \mu\delta\right] \leq 2\exp\left(-N\mu\delta^2/3\right).$$

2. *When* $\delta \geq 1$,

$$\mathbb{P}\left[\left|\frac{1}{N}\sum_{i=1}^{N} Z_i - \mu\right| > \mu\delta\right] \leq \exp\left(-N\mu\delta/3\right).$$

3. *For* $\epsilon > 0$,

$$\mathbb{P}\left[\left|\frac{1}{N}\sum_{i=1}^{N} Z_i - \mu\right| > \epsilon\right] \leq 2\exp\left(-2N\epsilon^2\right).$$

An important tool in our later development is the following lemma, which bounds additional "discrepancies" that can arise when one samples from two distribution $\mathbf{p}$ and $\mathbf{q}$ using an optimal coupling. The important feature for us is the fact that the additional discrepancy (denoted as $\mathbf{e}$ in the lemma) is bounded as a *fraction* of the "initial discrepancy" $\|\mathbf{p} - \mathbf{q}\|_1$. However, such relative bounds on the discrepancy are less likely to hold when the initial discrepancy itself is very small, and hence, there is a trade-off between the lower bound that needs to be imposed on the initial discrepancy $\|\mathbf{p} - \mathbf{q}\|_1$, and the desired probability with which the claimed relative bound on the additional discrepancy $\mathbf{e}$ is to hold. The lemma makes this delicate trade-off precise.

Lemma 5.6. *Let* $\mathbf{p}$ *and* $\mathbf{q}$ *be probability distributions on a universe of size* m*, so that* $\mathbf{p}, \mathbf{q} \in \Delta_m$*. Consider an optimal coupling of the two distributions, and let* $\mathbf{x}$ *and* $\mathbf{y}$ *be random frequency vectors with* m *co-ordinates (normalized to sum to 1) obtained by taking* N *independent samples from the coupled distributions, so that* $\mathbb{E}[\mathbf{x}] = \mathbf{p}$ *and* $\mathbb{E}[\mathbf{y}] = \mathbf{q}$*. Define the random error vector* $\mathbf{e}$ *as*

$$\mathbf{e} := (\mathbf{x} - \mathbf{y}) - (\mathbf{p} - \mathbf{q}).$$

Suppose $c > 1$ and t (possibly dependent upon N) are such that $\|\mathbf{p} - \mathbf{q}\|_1 \geq \frac{ctm}{N}$. We then have

$$\|\mathbf{e}\|_1 \leq \left(\frac{2}{\sqrt{c}}\right) \|\mathbf{p} - \mathbf{q}\|_1$$

with probability at least $1 - 2m \exp(-t/3)$.

Proof. The properties of the optimal coupling of the distributions $\mathbf{p}$ and $\mathbf{q}$ imply that since the N coupled samples are taken independently,

1. $|x_i - y_i| = \frac{1}{N} \sum_{j=1}^{N} R_j$, where R_j are i.i.d. Bernoulli random variables with mean $|p_i - q_i|$, and

2. $x_i - y_i$ has the same sign as $p_i - q_i$.

The second fact implies that $|e_i| = ||x_i - y_i| - |(p_i - q_i)||$. By applying the concentration bounds from 5.5 to the first fact, we then get (for any arbitrary $i \in [m]$)

$$\mathbb{P}\left[|e_i| > \sqrt{\frac{t}{N |p_i - q_i|}} \cdot |p_i - q_i|\right] \leq 2 \exp(-t/3), \text{ if } \frac{t}{N |p_i - q_i|} \leq 1, \text{ and}$$

$$\mathbb{P}\left[|e_i| > \frac{t}{N |p_i - q_i|} \cdot |p_i - q_i|\right] \leq \exp(-t/3), \text{ if } \frac{t}{N |p_i - q_i|} > 1.$$

One of the two bounds applies to every $i \in [m]$ (except those i for which $|p_i - q_i| = 0$, but in those cases, we have $|e_i| = 0$, so the bounds below will apply nonetheless). Thus, taking a union bound over all the indices, we see that with probability at least $1 - 2m \exp(-t/3)$, we have

$$\|\mathbf{e}\|_1 = \sum_{i=1}^{m} |e_i| \leq \sqrt{\frac{t}{N}} \sum_{i=1}^{m} \sqrt{|p_i - q_i|} + \frac{tm}{N}$$

$$\leq \sqrt{\frac{tm}{N}} \sqrt{\|\mathbf{p} - \mathbf{q}\|_1} + \frac{tm}{M} \tag{39}$$

$$\leq \left(\frac{1}{\sqrt{c}} + \frac{1}{c}\right) \|\mathbf{p} - \mathbf{q}\|_1. \tag{40}$$

Here, (39) uses Cauchy-Schwarz inequality to bound the first term while (40) uses the hypothesis in the lemma that $\frac{ctm}{N} \leq \|\mathbf{p} - \mathbf{q}\|_1$. The claim follows since $c > 1$. $\square$

For concreteness, in the rest of this chapter, we use t_{mix} to refer to $t_{\text{mix}}(1/e)$ (though any other constant smaller than $1/2$ could be chosen as well in place of $1/e$ without changing any of the claims).

5.3.2 Main theorems

We are now ready to state our main theorem. We begin by formally defining the conditions on the evolution function required by Theorem 5.7.

Definition 22 (Smooth contractive evolution). *A function $f : \Delta_m \to \Delta_m$ is said to be a (L, B, ρ) smooth contractive evolution if it has the following properties:*

Smoothness *f is twice differentiable in the interior of Δ_m. Further, the Jacobian J of f satisfies $\|J(x)\|_1 \leq L$ for every $\mathbf{x}$ in the interior of Δ_m, and the operator norms of the Hessians of its co-ordinates are uniformly bounded above by $2B$ at all points in the interior of Δ_m.*

Unique fixed point *f has a unique fixed point τ in Δ_m which lies in the interior of Δ_m.*

Contraction near the fixed point *At the fixed point τ, the Jacobian $J(\tau)$ of f satisfies*

$$\text{sp}\left(J(\tau)\right) < \rho < 1.$$

Convergence to fixed point *For every $\epsilon > 0$, there exists an ℓ such that for any $\mathbf{x} \in \Delta_m$,*

$$\left\|f^{\ell}(\mathbf{x}) - \tau\right\|_1 < \epsilon.$$

Remark 8. *Note that the last condition implies that $\|f^t(\mathbf{x}) - \tau\|_1 = O(\rho^t)$ in the light of the previous condition and the smoothness condition (see Lemma 5.18). Also, it is easy to see that the last two conditions imply the uniqueness of the fixed point, i.e., the second condition. However, the last condition on global convergence does not*

by itself imply the third condition on contraction near the fixed point. Consider, e.g.,
$g : [-1, 1] \to [-1, 1]$ *defined as* $g(x) = x - x^3$. *The unique fixed point of* g *in its domain is* 0, *and we have* $g'(0) = 1$, *so that the third condition is not satisfied. On the other hand, the last condition is satisfied, since for* $x \in [-1, 1]$ *satisfying* $|x| \geq \epsilon$, *we have* $|g(x)| \leq |x| (1 - \epsilon^2)$. *In order to construct a function* $f : [0, 1] \to [0, 1]$ *with the same properties, we note that the range of* g *is* $[-x_0, x_0]$ *where* $x_0 = 2/(3\sqrt{3})$, *and consider* $f : [0, 1] \to [0, 1]$ *defined as* $f(x) = x_0 + g(x - x_0)$. *Then, the unique fixed point of* f *in* $[0, 1]$ *is* x_0, $f'(x_0) = g'(0) = 1$, *the range of* f *is contained in* $[0, 2x_0] \subseteq [0, 1]$, *and* f *satisfies the fourth condition in the definition but does not satisfy the third condition.*

Given an f which is a smooth contractive evolution, and a population parameter N, our first result is the following:

Theorem 5.7 (Unique stable). *Let* f *be a* (L, B, ρ) *smooth contractive evolution. Then, the mixing time of the stochastic evolution guided by* f *is* $O(\log N)$.

Moreover, in the second theorem we allow f to have multiple unstable fixed points, but still a unique stable.

Theorem 5.8 (One stable/multiple unstable). *Let* $f : \Delta_m \to \Delta_m$ *be twice differentiable in the interior of* Δ_m *with bounded second derivative. Assume that* $f(\mathbf{x})$ *has a finite number of fixed points* $\mathbf{z}_0, \ldots, \mathbf{z}_l$ *in the interior, where* $\mathbf{z}_0$ *is a stable fixed point, i.e.,* $\mathrm{sp}\,(J(\mathbf{z}_0)) < \rho < 1$ *and* $\mathbf{z}_1, \ldots, \mathbf{z}_l$ *are* α-*unstable fixed points* $(\alpha > 1)$. *Furthermore, assume that* $\lim_{t \to \infty} f^t(\mathbf{x})$ *exists for all* $\mathbf{x} \in \Delta_m$. *Then, the stochastic evolution guided by* f *has mixing time* $O(\log N)$.

In the third result, we allow f to have multiple stable fixed points (in addition to any number of unstable fixed points). For this setting, we prove that the stochastic evolution guided by f has mixing time $e^{\Omega(N)}$. The phase transition result on model discussed in Section 5.7.3 relies crucially on Theorem 5.9.

Theorem 5.9 (Multiple stable). *Let $f : \Delta_m \to \Delta_m$ be continuously differentiable in the interior of Δ_m. Assume that $f(\mathbf{x})$ has at least two stable fixed points in the interior $\mathbf{z}_1, \ldots, \mathbf{z}_l$, i.e., $\mathrm{sp}\,(J(\mathbf{z}_i)) < \rho_i < 1$ for $i = 1, 2, \ldots, l$. Then, the stochastic evolution guided by f has mixing time $e^{\Omega(N)}$.*

Finally, we allow f to have a stable limit cycle. We prove that in this setting the stochastic evolution guided by f has mixing time $e^{\Omega(N)}$. This result seems important for evolutionary dynamics as periodic orbits often appear [112, 107].

Theorem 5.10 (Stable limit cycle). *Let $f : \Delta_m \to \Delta_m$ be continuously differentiable in the interior of Δ_m. Assume that $f(\mathbf{x})$ has a stable limit cycle with points $\mathbf{w}_1, \ldots, \mathbf{w}_s$ of size $s \geq 2$ in the sense that $\mathrm{sp}\,(\prod_{i=1}^{s} J(\mathbf{w}_{s-i+1})) < \rho < 1$. Then the stochastic evolution guided by f has mixing time $e^{\Omega(N)}$.*

We also provide two applications of the theorems above for two specific dynamics, discussed extensively in Section 5.7.

Theorem 5.11 (Rapid mixing for RSM model). *The mixing time of the RSM model is $O(\log N)$ for all matrices Q, A and values of m.*

Theorem 5.12 (Phase transition for grammar acquisition). *There is a critical value τ_c of the mutation parameter τ such that the mixing time of the grammar acquisition dynamics is: (i) $\exp(\Omega(N))$ for $0 < \tau < \tau_c$ and (ii) $O(\log N)$ for $\tau > \tau_c$ where N is the size of the population.*

5.4   Technical overview

5.4.1   Overview of Theorem 5.7

We analyze the mixing time of our stochastic process by studying the time required for evolutions started at two arbitrary starting states $\mathbf{X}^{(0)}$ and $\mathbf{Y}^{(0)}$ to collide. More precisely, let $\mathcal{C}$ be any Markovian coupling of two stochastic evolutions $\mathbf{X}$ and $\mathbf{Y}$, both guided by a smooth contractive evolution f, which are started at $\mathbf{X}^{(0)}$ and $\mathbf{Y}^{(0)}$.

Let T be the first (random) time such that $\mathbf{X}^{(T)} = \mathbf{Y}^{(T)}$. It is well known that if it can be shown that $\mathbb{P}\left[T > t\right] \leq 1/4$ for every pair of starting states $\mathbf{X}^{(0)}$ and $\mathbf{Y}^{(0)}$ then $t_{\mathrm{mix}}(1/4) \leq t$. We show that such a bound on $\mathbb{P}\left[T > t\right]$ holds if we couple the chains using the optimal coupling of two multinomial distributions (see Section 5.3 for a definition of this coupling).

Our starting point is the observation that the optimal coupling and the definition of the evolutions implies that for any time t,

$$\mathbb{E}\left[\left\|\mathbf{X}^{(t+1)} - \mathbf{Y}^{(t+1)}\right\|_1 \mid \mathbf{X}^{(t)}, \mathbf{Y}^{(t)}\right] = \left\|f(\mathbf{X}^{(t)}) - f(\mathbf{Y}^{(t)})\right\|_1. \tag{41}$$

Now, if f were *globally* contractive, so that the right hand side of (41) was always bounded above by $\rho' \left\|\mathbf{X}^{(t)} - \mathbf{Y}^{(t)}\right\|_1$ for some constant $\rho' < 1$, then we would get that the expected distance between the two copies of the chains contracts at a constant rate. Since the minimum possible positive ℓ_1 distance between two copies of the chain is $1/N$, this would have implied an $O(\log N)$ mixing time using standard arguments. However, such a global assumption on f, which is equivalent to requiring that the Jacobian J of f satisfies $\|J(\mathbf{x})\|_1 < 1$ for all $\mathbf{x} \in \Delta_m$, is far too strong. In particular, it is not satisfied by standard systems such as Eigen's dynamics discussed later in Section 5.7.1.

Nevertheless, these dynamics do satisfy a more local version of the above condition. That is, they have a unique fixed point τ to which they converge quickly, and *in the vicinity* of this fixed point, *some* form of contraction holds. These conditions motivate the "unique fixed point", "contraction near the fixed point", and the "convergence to fixed point" conditions in our definition of a smooth contractive evolution (22). However, crucially, the "contraction near the fixed point" condition, inspired from the definition of "asymptotically stable" fixed points in dynamical systems, is weaker than the stepwise contraction condition described in the last paragraph, even in the vicinity of the fixed point. As we shall see shortly, this weakening is essential for generalizing the earlier results of [137] to the $m > 2$ case, but comes at the cost of

making the analysis more challenging.

However, we first describe how the "convergence to fixed point" condition is used to argue that the chains come close to the fixed point in $O(\log N)$ time. This step of our argument is the only one technically quite similar to the development in [137]; our later arguments need to diverge widely from that paper. Although this step is essentially an iterated application of appropriate concentration results along with the fact that the "convergence to fixed point" condition implies that the deterministic evolution f comes close to the fixed point τ at an exponential rate, complications arise because f can amplify the effect of the random perturbations that arise at each step. In particular, if $L > 1$ is the maximum of $\|J(\mathbf{x})\|_1$ over Δ_m, then after ℓ steps, a random perturbation can become amplified by a factor of L^ℓ. As such, if ℓ is taken to be too large, these accumulated errors can swamp the progress made due to the fast convergence of the deterministic evolution to the fixed point. These considerations imply that the argument can only be used for $\ell = \ell_0 \log N$ steps for some small constant ℓ_0, and hence we are only able to get the chains within $\Theta(N^{-\gamma})$ distance of the fixed point, where $\gamma < 1/3$ is a small constant. In particular, the argument cannot be carried out all the way down to distance $O(1/N)$, which, if possible, would have been sufficient to show that the coupling time is small with high probability. Nevertheless, it does allow us to argue that both copies of the chain enter an $O(N^{-\gamma})$ neighborhood of the fixed point in $O(\log N)$ steps.

At this point, [137] showed that in the $m = 2$ case, one could take advantage of the contractive behavior near the fixed point to construct a coupling obeying (41) in which the right hand side was indeed contractive: in essence, this amounted to a proof that $\|J\|_1 < 1$ was indeed satisfied in the small $O(N^{-\gamma})$ neighborhood reached at the end of the last step. This allowed [137] to complete the proof using standard arguments, after some technicalities about ensuring that the chains remained for a sufficiently long time in the neighborhood of the fixed point had been taken care of.

The situation however changes completely in the $m > 2$ case. It is no longer possible to argue in general that $\|J(\mathbf{x})\|_1 < 1$ when $\mathbf{x}$ is in the vicinity of the fixed point, even when there is fast convergence to the fixed point. Instead, we have to work with a weaker condition (the "contraction to the fixed point" condition alluded to earlier) which only implies that there is a positive integer k, possibly larger than 1, such that in some vicinity of the fixed point, $\|J^k\|_1 < 1$. In the setting used by [137], k could be taken to be 1, and hence it could be argued via (41) that the distance between the two coupled copies of the chains contracts in each step. This argument however does not go through when only a kth power of J is guaranteed to be contractive while J itself could have $1 \to 1$ norm larger than 1. This inability to argue stepwise contraction is the major technical obstacle in our work when compared to the work of [137], and the source of all the new difficulties that arise in this more general setting.

As a first step toward getting around the difficulty of not having stepwise contraction, we prove 5.13, which shows that the eventual contraction after k steps can be used to ensure that the distance between two evolutions $\mathbf{x}^{(t)}$ and $\mathbf{y}^{(t)}$ close to the fixed point contracts by a factor $\rho^k < 1$ over an *epoch* of k steps (where k is as described in the last paragraph), even when the evolutions undergo arbitrary perturbations $\mathbf{u}^{(t)}$ and $\mathbf{v}^{(t)}$ at each step, *provided* that the difference $\mathbf{u}^{(t)} - \mathbf{v}^{(t)}$ between the two perturbations is small compared to the difference $\mathbf{x}^{(t-1)} - \mathbf{y}^{(t-1)}$ between the evolutions at the previous step. The last condition actually asks for a relative notion of smallness, *i.e.*, it requires that

$$\left\|\xi^{(t)}\right\|_1 := \left\|\mathbf{u}^{(t)} - \mathbf{v}^{(t)}\right\|_1 \leq \delta \left\|\mathbf{x}^{(t-1)} - \mathbf{y}^{(t-1)}\right\|_1, \tag{42}$$

where δ is a constant specified in the theorem. Note that the theorem is a statement about deterministic evolutions against possibly adversarial perturbations, and does *not* require $\mathbf{u}^{(t)}$ and $\mathbf{v}^{(t)}$ to be stochastic, but only that they follow the required conditions on the difference of the norm (in addition to the implied condition that

the evolution $\mathbf{x}^{(t)}$ and $\mathbf{y}^{(t)}$ remain close to the fixed point during the epoch).

Thus, in order to use 5.13 for showing that the distance $\left\|\mathbf{X}^{(t)} - \mathbf{Y}^{(t)}\right\|_1$ between the two coupled chains contracts after every k iterations of (41), we need to argue that the required condition on the perturbations in (42) holds with high probability over a given epoch during the coupled stochastic evolution of $\mathbf{X}^{(t)}$ and $\mathbf{Y}^{(t)}$. (In fact, we also need to argue that the two chains individually remain close to the fixed point, but this is easier to handle).

However, at this point, a complication arises from the fact that 5.13 requires the difference $\xi^{(t)}$ between the perturbations at time t to be bounded *relative* to the difference $\left\|\mathbf{X}^{(t-1)} - \mathbf{Y}^{(t-1)}\right\|_1$ at time $t-1$. In other words, the upper bounds required on the $\xi^{(t)}$ become more stringent as the two chains come closer to each other. This fact creates a trade-off between the probability with which the condition in (42) can be enforced in an epoch, and the required *lower* bound on the distance between the chains required during the epoch so as to ensure that probability (this trade-off is technically based on 5.6). To take a couple of concrete examples, when $\left\|\mathbf{X}^{(t)} - \mathbf{Y}^{(t)}\right\|_1$ is $\Omega(\log N/N)$ in an epoch, we can ensure that (42) remains valid with probability at least $1 - N^{-\Theta(1)}$ (see the discussion following 5.16), so that with high probability $\Omega(\log N)$ consecutive epochs admit a contraction allowing the distance between the chains to come down from $\Theta(N^{-\gamma})$ at the end of the first step to $\Theta(\log N/N)$ at the end of this set of epochs.

Ideally, we would have liked to continue this argument till the distance between the chains is $\Theta(1/N)$ and (due to the properties of the optimal coupling) they have a constant probability of colliding in a single step. However, due to the trade-off referred to earlier, when we know only that $\left\|\mathbf{X}^{(t)} - \mathbf{Y}^{(t)}\right\|_1$ is $\Omega(1/N)$ during the epoch, we can only guarantee the condition of (42) with probability $\Theta(1)$ (see the discussion following the proof of 5.16). Thus, we cannot claim directly that once the distance between the chains is $O(\log N/N)$, the next $\Omega(\log \log N)$ epochs will exhibit contraction in distance

leading the chain to come as close as $O(1/N)$ with a high enough positive probability. To get around this difficulty, we consider $O(\log \log N)$ epochs with successively weaker guaranteed upper bounds on $\left\|\mathbf{X}^{(t)} - \mathbf{Y}^{(t)}\right\|_1$. Although the weaker lower bounds on the distances lead in turn to weaker concentration results when 5.16 is applied, we show that this trade-off is such that we can choose these progressively decreasing guarantees so that after this set of epochs, the distance between the chains is $O(1/N)$ with probability that it is small but at least a *constant*. Since the previous steps, *i.e.,* those involving making both chains come within distance $O(N^{-\gamma})$ of the fixed point (for some small constant $\gamma < 1$), and then making sure that the distance between them drops to $O(\log N/N)$, take time $O(\log N)$ with probability $1 - o(1)$, we can conclude that under the optimal coupling, the collision or coupling time T satisfies

$$\mathbb{P}\left[T > O(\log N)\right] \le 1 - q, \tag{43}$$

for some small enough constant q, irrespective of the starting states $\mathbf{X}^{(0)}$ and $\mathbf{Y}^{(0)}$ (note that here we are also using the fact that once the chains are within distance $O(1/N)$, the optimal coupling has a constant probability of causing a collision in a single step). The lack of dependence on the starting states allows us to iterate (43) for $\Theta(1)$ consecutive "blocks" of time $O(\log N)$ each to get

$$\mathbb{P}\left[T > O\left(\log N\right)\right] \le \frac{1}{4},$$

which gives us the claimed mixing time.

5.4.2   Overview of Theorem 5.8

The main difficulty to prove this theorem is the existence of multiple unstable fixed points in the simplex from which the Markov chain should get away fast. As before, we study the time T required for two stochastic evolutions with arbitrary initial states $\mathbf{X}^{(0)}$ and $\mathbf{Y}^{(0)}$, guided by some function f, to collide. By the conditions

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of Theorem 5.8, function f has a unique stable fixed point $\mathbf{z}_0$ with

$$\mathrm{sp}\left(J(\mathbf{z}_0)\right) < \rho < 1.$$

Additionally, it has α-unstable fixed points. Moreover, for all starting points $\mathbf{x}_0 \in \Delta_m$, the sequence $(f^t(\mathbf{x}_0))_{t \in \mathbb{N}}$ has a limit. We can show that there exists constant c_0 such that $\mathbb{P}\left[T > c_0 \log N\right] \leq \frac{1}{4}$, from which it follows that $t_{\mathrm{mix}}(1/4) \leq c_0 \log N$. In order to show collision after $O(\log N)$ steps, it suffices first to run each chain *independently* for $O(\log N)$ steps. We first show that with probability $\Theta(1)$, each chain will reach $B(\mathbf{z}_0, \frac{1}{N^{1-\epsilon}})$ after at most $O(\log N)$ steps, for some $\epsilon > 0$.[5] As long as this is true, the coupling constructed for proving Theorem 5.7 can be used to show collision. To explain why our claim holds, we break the proof into three parts.

(a) First, it is shown that as long as the state of the Markov chain is within $o\left(\frac{\log^{2/3} N}{\sqrt{N}}\right)$ in ℓ_1 distance from some α-unstable fixed point $\mathbf{w}$, then, with probability $\Theta(1)$, it reaches distance $\Omega\left(\frac{\log^{2/3} N}{\sqrt{N}}\right)$ after $O(\log N)$ steps. Step (a) has the technical difficulty that as long as a chain starts from a $o(\frac{1}{\sqrt{N}})$ distance from an unstable fixed point, the variance of the process dominates the expansion due to the fact the fixed point is unstable.

(b) Assuming (a), we show that with probability $1 - \frac{1}{\mathrm{poly}(N)}$ the Markov chain reaches distance $\Theta(1)$ from any unstable fixed point after $O(\log N)$ steps.

(c) Finally, if the Markov chain has $\Theta(1)$ distance from any unstable fixed point (the fixed points have pairwise ℓ_1 distance independent of N, *i.e.*, they are "well separated"), it will reach some $\frac{1}{N^{1-\epsilon}}$-neighborhood of the stable fixed point $\mathbf{z}_0$ exponentially fast (*i.e.*, after $O(\log N)$ steps). For showing (a) and (b), we must prove an expansion argument for $\|f^t(\mathbf{x}) - \mathbf{w}\|_1$ as t increases, where $\mathbf{w}$ is an α-unstable fixed point and also taking care of the random perturbations due to the stochastic

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[5] $B(\mathbf{x}, r)$ denotes the open ball with center $\mathbf{x}$ and radius r in ℓ_1, which we call an *r-neighborhood* of $\mathbf{x}$.

evolution. Ideally what we want (but is not true) is the following to hold:

$$\left\|f^{t+1}(\mathbf{x}) - \mathbf{w}\right\|_1 \geq \alpha \left\|f^t(\mathbf{x}) - \mathbf{w}\right\|_1,$$

i.e., one step expansion. The first important fact is that f^{-1} is well-defined in a small neighborhood of $\mathbf{w}$ due to the Inverse Function Theorem, and it also holds that

$$\left\|f^t(\mathbf{x}) - \mathbf{w}\right\|_1 \approx \left\|J^{-1}(\mathbf{w})(f^{t+1}(\mathbf{x}) - \mathbf{w})\right\|_1 \leq \left\|J^{-1}(\mathbf{w})\right\|_1 \left\|f^{t+1}(\mathbf{x}) - \mathbf{w}\right\|_1,$$

where $\mathbf{x}$ is in some neighborhood of $\mathbf{w}$ and $J^{-1}(\mathbf{w})$ is the *pseudoinverse* of $J(\mathbf{w})$ (see the Remark 7 in Section 5.3). However even if $\mathbf{w}$ is α-unstable and $\operatorname{sp}(J^{-1}(\mathbf{w})) < \frac{1}{\alpha}$, it can hold that $\|J^{-1}(\mathbf{w})\|_1 > 1$. At this point, we use Gelfand's formula (Theorem 5.1). Since $\lim_{t \to \infty}(\|A^t\|_1)^{1/t} \to \operatorname{sp}(A)$, for all $\epsilon > 0$, there exists a k_0 such that for all $k \geq k_0$ we have

$$\left|\|A^k\|_1 - (\operatorname{sp}(A))^k\right| < \epsilon.$$

We use this important theorem to show for small $\epsilon > 0$, there exists a k such that

$$\left\|f^t(\mathbf{x}) - \mathbf{w}\right\|_1 \approx \left\|(J^{-1}(\mathbf{w}))^k(f^{t+k}(\mathbf{x}) - \mathbf{w})\right\|_1 \leq \frac{1}{\alpha^k} \left\|f^{t+k}(\mathbf{x}) - \mathbf{w}\right\|_1,$$

where we used the fact that

$$\left\|(J^{-1}(\mathbf{w}))^k\right\|_1 < (\operatorname{sp}(J^{-1}(\mathbf{w})))^k - \epsilon \leq \frac{1}{\alpha^k}.$$

By taking advantage of the continuity of the $J^{-1}(\mathbf{x})$ around the unstable fixed point $\mathbf{w}$, we can show expansion for every k steps of the dynamical system. It remains to show for (a) and (b) how one can handle the perturbations due to the randomness of the stochastic evolution. In particular, if $\left\|\mathbf{X}^{(0)} - \mathbf{w}\right\|_1$ is $o\left(\frac{1}{\sqrt{N}}\right)$, even with the expansion we have from the deterministic dynamics (as discussed above), variance dominates. We examine case (b) first, which is relatively easy (the *drift* dominates at this step). Due to Chernoff bounds, the difference $\left\|\mathbf{X}^{(t+k)} - \mathbf{w}\right\|_1 - \left\|f^k(\mathbf{X}^{(t)}) - \mathbf{w}\right\|_1$ is $O\left(\sqrt{\frac{\log N}{N}}\right)$ (this captures the deviation on running the stochastic evolution for

k steps vs running the deterministic dynamics for k steps, both starting from $\mathbf{X}^{(t)}$)
with probability $1 - \frac{1}{\text{poly}(N)}$. Since $\left\|\mathbf{X}^{(t)} - \mathbf{w}\right\|_1$ is $\Omega\left(\frac{\log^{2/3} N}{\sqrt{N}}\right)$, then

$$\left\|\mathbf{X}^{(t+k)} - \mathbf{w}\right\|_1 \geq (\alpha^k - o_N(1)) \left\|\mathbf{X}^{(t)} - \mathbf{w}\right\|_1.$$

For (a), first we show that with probability $\Theta(1)$, after one step the Markov chain has distance $\Omega(\frac{1}{\sqrt{N}})$ of $\mathbf{w}$. This claim just uses properties of the multinomial distribution. After reaching distance $\Omega\left(\frac{1}{\sqrt{N}}\right)$, we can use again the idea of expansion and being careful with the variance and we can show expansion with probability at least $\frac{1}{2}$, every k steps. Then we can show that with probability at least $\frac{1}{\log^{2/3} N}$, distance $\frac{\log^{2/3} N}{\sqrt{N}}$ is reached after $O(\log \log N)$ steps and basically we finish with (b). For (c), we use a couple of lemmas , *i.e.*, Lemma 5.18, Claim 58 and Lemma 5.25. Let Δ be some compact subset of Δ_m, where we have excluded all the α-unstable fixed points along with some open ball around each unstable fixed point of constant radius. We can show that given that the initial state of the Markov chain belongs to Δ, it reaches a $B(\mathbf{z}_0, \frac{1}{N^{1-\epsilon}})$ for some $\epsilon > 0$ as long as the dynamical system converges for all starting points in Δ (and it should converge to the stable fixed point $\mathbf{z}_0$). We have roughly that the dynamical system converges exponentially fast for every starting point in B to the stable fixed point $\mathbf{z}_0$ and that with probability $1 - \frac{1}{\text{poly}(n)}$ two arbitrary chains independently will reach a $\frac{1}{N^\epsilon}$ neighborhood of the stable fixed point $\mathbf{z}_0$. Therefore by $(a), (b), (c)$ and the coupling from the proof of Theorem 5.7, we conclude the proof of Theorem 5.8.

5.4.3 Overview of Theorems 5.9 and 5.10

To prove Theorem 5.10, we make use of Theorem 5.9, *i.e.*, we reduce the case of the stable limit cycle to the case of multiple stable fixed points. If s is the length of the limit cycle, roughly the bound $e^{\Omega(N)}$ on the mixing time loses a factor $\frac{1}{s}$ compared to the case of multiple stable fixed points. We now present the ideas behind the proof of Theorem 5.9. First as explained above, we can show contraction after k steps (for

some constant k) for the deterministic dynamics around a stable fixed point $\mathbf{z}$ with $\mathrm{sp}(J(\mathbf{z})) < \rho < 1$, *i.e.,*

$$\left\| f^{t+k}(\mathbf{x}) - \mathbf{z} \right\|_1 \approx \left\| J^k[\mathbf{z}] \right\|_1 \left\| f^t(\mathbf{x}) - \mathbf{z} \right\|_1 \leq \rho^k \left\| f^t(\mathbf{x}) - \mathbf{z} \right\|_1.$$

To do that, we use Gelfand's formula, Taylor's theorem and continuity of $J(\mathbf{x})$ where $\mathbf{x}$ lies in a neighborhood of the fixed point $\mathbf{z}$. Hence, due to the above contraction of the ℓ_1 norm and the concentration of Chernoff bounds, it takes a long time for the chain $\mathbf{X}^{(t)}$ to get out of the region of attraction of the fixed point $\mathbf{z}$. Technically, the error that aggregates due to the randomness of the stochastic evolution guided by f does not become large due to the convergence of the series $\sum_{i=0}^{\infty} \rho^i$. Hence, we focus on the error probability, namely the probability the stochastic evolution guided by f deviates a lot from the dynamical system with rule f if both have same starting point after one step. Since this probability is exponentially small, *i.e.,* it holds that

$$\left\| f(\mathbf{X}^{(0)}) - \mathbf{X}^{(1)} \right\|_1 > \epsilon m$$

with probability at most $2me^{-2\epsilon^2 N}$, an exponential number of steps is required for the above to be violated. Finally, as we have shown that it takes exponential time to get out of the region of attraction of a stable fixed point $\mathbf{z}$ we do the following easy (common) trick. Since the function has at least two fixed points, we start the Markov chain very close to the fixed point that its neighborhood has mass at most $1/2$ in the stationary distribution (this can happen since we have at least 2 fixed points that are well separated). Then, after exponential number of steps, it will follow that the total variation distance between the distribution of the chain and the stationary will be at least $1/4$.

5.4.4 Overview of Theorem 5.11

Our first step towards the proof of Theorem 5.11 is to show that the RSM model (see Section 5.7.1 for description of the model) can be seen as a stochastic evolution

guided by the function f defined by $f(\mathbf{p}) = \frac{(QA\mathbf{p})_t}{\|QA\mathbf{p}\|_1}$, where Q and A are matrices with positive entries. Then we show that the dynamical system with update rule f has a unique fixed point (due to Perron-Frobenius) and for all initial conditions in Δ_m, the dynamics converges to it (analogue to power method). Finally, we show that the spectral radius of the Jacobian of f at the unique fixed point is $\frac{\lambda_2}{\lambda_1}$ where λ_1, λ_2 are the largest and second largest eigenvalues in absolute value of QA, and hence < 1. Thus the conditions of Theorem 5.7 are satisfied and the result follows.

5.4.5 Overview of Theorem 5.12

Below we give the necessary ingredients of the proof of Theorem 5.12. Our previous results, along with some analysis on the fixed points of g (function of grammar acquisition dynamics) suffice to show the phase transition result. To prove Theorem 5.12, initially we show that the model (finite population) is essentially a stochastic evolution (see Definition 19) guided by g as defined in Section 5.7.3 and proceed as follows: We prove that in the interval $0 < \tau < \tau_c$, the function g has multiple fixed points whose Jacobian have spectral radius less than 1. Therefore due to Theorem 5.9 discussed above, the mixing time will be exponential in N. For $\tau = \tau_c$ a bifurcation takes place which results in function g of grammar acquisition dynamics having only one fixed point inside simplex (specifically, the uniform point $(1/m, \ldots, 1/m)$). In dynamical systems, a local bifurcation occurs when a parameter (in particular the mutation parameter τ) change causes two (or more) fixed points to collide or the stability of an equilibrium (or fixed point) to change. To prove fast mixing in the case $\tau_c < \tau \leq 1/m$, we make use of Theorem 5.7. One of the assumptions is that the dynamical system with g as update rule needs to converge to the unique fixed point for all initial points in simplex. To prove convergence to the unique fixed point, we define a Lyapunov function P such that

$$P(g(\mathbf{x})) > P(\mathbf{x}) \text{ unless } \mathbf{x} \text{ is a fixed point.} \tag{44}$$

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As a consequence, the (infinite population) grammar acquisition dynamics converge to the unique fixed point $(1/m, \ldots, 1/m)$. To show Equation (44), we use an inequality that dates back in 1967 (see Theorem 1.1), which intuitively states the discrete analogue of proving that for a gradient system $\frac{d\mathbf{x}}{dt} = \nabla V(\mathbf{x})$ it is true that $\frac{dV}{dt} \geq 0$.

5.5 Unique stable fixed point

5.5.1 Perturbed evolution near the fixed point

As discussed in 5.4, the crux of the proof of our main theorem is analyzing how the distance between two copies of a stochastic evolution guided by a smooth contractive evolution evolves in the presence of small perturbations at every step. In this section, we present our main tool, 5.13, to study this phenomenon. We then describe how the theorem, which itself is presented in a completely deterministic setting, applies to stochastic evolutions.

Fix any (L, B, ρ)-smooth contractive evolution f on Δ_m, with fixed point τ. As we noted in 5.4, since the Jacobian of f does not necessarily have operator (or $1 \to 1$) norm less than 1, we cannot argue that the effect of perturbations shrinks in every step. Instead, we need to argue that the condition on the spectral radius of the Jacobian of f at its fixed point implies that there is eventual contraction of distance between the two evolutions, even though this distance might increase in any given step. Indeed, the fact that the spectral radius $\mathrm{sp}\,(J)$ of the Jacobian at the fixed point τ of f is less than $\rho < 1$ implies that a suitable iterate of f has a Jacobian with operator (and $1 \to 1$) norm less than 1 at τ. This is because Gelfand's formula (5.1) implies that for all large enough positive integers k',

$$\left\| J^k(\tau) \right\|_1 < \rho^k.$$

We now use the above condition to argue that after k steps in the vicinity of the fixed point, there is indeed a contraction of the distance between two evolutions guided by f, even in the presence of adversarial perturbations, as long as those perturbations

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are small. The precise statement is given below; the vectors $\xi^{(i)}$ in the theorem model the small perturbations.

Theorem 5.13 (Perturbed evolution I). *Let f be a (L, B, ρ)-smooth contractive evolution, and let τ be its fixed point. For all positive integers $k > k_0$ (where k_0 is a constant that depends upon f) there exist $\epsilon, \delta \in (0, 1]$ depending upon f and k for which the following is true. Let $\left(\mathbf{x}^{(i)}\right)_{i=0}^k$, $\left(\mathbf{y}^{(i)}\right)_{i=0}^k$, and $\left(\xi^{(i)}\right)_{i=1}^k$ be sequences of vectors with $\mathbf{x}^{(i)}, \mathbf{y}^{(i)} \in \Delta_m$ and $\xi^{(i)}$ orthogonal to $\mathbf{1}$, which satisfy the following conditions:*

1. *(**Definition**). For $1 \leq i \leq k$, there exist vectors $\mathbf{u}^{(i)}$ and $\mathbf{v}^{(i)}$ such that*

$$\mathbf{x}^{(i)} = f(\mathbf{x}^{(i-1)}) + \mathbf{u}^{(i)}, \ \mathbf{y}^{(i)} = f(\mathbf{y}^{(i-1)}) + \mathbf{v}^{(i)}, \ and \ \xi^{(i)} = \mathbf{u}^{(i)} - \mathbf{v}^{(i)}.$$

2. *(**Closeness to fixed point**). For $0 \leq i \leq k$, $\left\|\mathbf{x}^{(i)} - \tau\right\|_1 \leq \epsilon$, $\left\|\mathbf{y}^{(i)} - \tau\right\|_1 \leq \epsilon$.*

3. *(**Small perturbations**). For $1 \leq i \leq k$, $\left\|\xi^{(i)}\right\|_1 \leq \delta \left\|\mathbf{x}^{(i-1)} - \mathbf{y}^{(i-1)}\right\|_1$.*

Then, we have

$$\left\|\mathbf{x}^{(k)} - \mathbf{y}^{(k)}\right\|_1 \leq \rho^k \left\|\mathbf{x}^{(0)} - \mathbf{y}^{(0)}\right\|_1.$$

In the theorem, the vectors $\mathbf{x}^{(i)}$ and $\mathbf{y}^{(i)}$ model the two chains, while the vectors $\mathbf{u}^{(i)}$ and $\mathbf{v}^{(i)}$ model the individual perturbations from the evolution dictated by f. The theorem says that if the perturbations $\xi^{(i)}$ to the *distance* are not too large, then the distance between the two chains indeed contracts after every k steps.

Proof. As observed above, we can use Gelfand's formula to conclude that there exists a positive integer k_0 (depending upon f) such that we have $\left\|J(\tau)^k\right\|_1 < \rho^k$ for all $k > k_0$. This k_0 will be the sought k_0 in the theorem, and we fix some appropriate $k > k_0$ for the rest of the section.

Since f is twice differentiable, J is continuous on Δ_m. This implies that the function on Δ_m^k defined by $\mathbf{z}_1, \mathbf{z}_2, \ldots, \mathbf{z}_k \mapsto \prod_{i=1}^k J(\mathbf{z}_i)$ is also continuous. Hence,

there exist $\epsilon_1, \epsilon_2 > 0$ smaller than 1 such that if $\|\mathbf{z}_i - \tau\| \le \epsilon_1$ for $1 \le i \le k$ then

$$\left\| \prod_{i=1}^{k} J(\mathbf{z}_i) \right\|_1 \le \rho^k - \epsilon_2. \tag{45}$$

Further, since Δ_m is compact and f is continuously differentiable, $\|J\|_1$ is bounded above on Δ_m by some positive constant L, which we assume without loss of generality to be greater than 1. Similarly, since f has bounded second derivatives, it follows from the multivariate Taylor's theorem that there exists a positive constant B (which we can again assume to be greater than 1) such that for any $\mathbf{x}, \mathbf{y} \in \Delta_m$, we can find a vector ν such that $\|\nu\|_1 \le Bm \|\mathbf{x} - \mathbf{y}\|_2^2 \le Bm \|\mathbf{x} - \mathbf{y}\|_1^2$ such that

$$f(\mathbf{x}) = f(\mathbf{y}) + J(\mathbf{y})(\mathbf{x} - \mathbf{y}) + \nu. \tag{46}$$

We can now choose

$$\epsilon = \min \left\{ \epsilon_1, \frac{\epsilon_2}{4Bmk(L+1)^{k-1}} \right\} \le 1, \text{ and } \delta = 2Bm\epsilon \le 1.$$

With this setup, we are now ready to proceed with the proof. Our starting point is the use of a first order Taylor expansion to control the error $\mathbf{x}^{(i)} - \mathbf{y}^{(i)}$ in terms of $\mathbf{x}^{(i-1)} - \mathbf{y}^{(i-1)}$. Indeed, Equation (46) when applied to this situation (along with the hypotheses of the theorem) yields for any $1 \le i \le k$ that

$$\mathbf{x}^{(i)} - \mathbf{y}^{(i)} = f(\mathbf{x}^{(i-1)}) - f(\mathbf{y}^{(i-1)}) + \xi^{(i)}$$
$$= J(\mathbf{y}^{(i-1)})(\mathbf{x}^{(i-1)} - \mathbf{y}^{(i-1)}) + (\nu^{(i)} + \xi^{(i)}), \tag{47}$$

where $\nu^{(i)}$ satisfies $\|\nu^{(i)}\|_1 \le Bm \|\mathbf{x}^{(i-1)} - \mathbf{y}^{(i-1)}\|_1^2$. Before proceeding, we first take note of a simple consequence of (47). Taking the ℓ_1 norm of both sides, and using the conditions on the norms of $\nu^{(i)}$ and $\xi^{(i)}$, we have

$$\left\| \mathbf{x}^{(i)} - \mathbf{y}^{(i)} \right\|_1 \le \left\| \mathbf{x}^{(i-1)} - \mathbf{y}^{(i-1)} \right\|_1 \left(L + \delta + Bm \left\| \mathbf{x}^{(i-1)} - \mathbf{y}^{(i-1)} \right\|_1 \right).$$

Since both $\mathbf{x}^{(i-1)}$ and $\mathbf{y}^{(i-1)}$ are within distance ϵ of τ by the hypothesis of the theorem, the above calculation and the definition of ϵ and δ imply that

$$\left\| \mathbf{x}^{(i)} - \mathbf{y}^{(i)} \right\|_1 \le (L + 4Bm\epsilon) \left\| \mathbf{x}^{(i-1)} - \mathbf{y}^{(i-1)} \right\|_1 \le (L + 1) \left\| \mathbf{x}^{(i-1)} - \mathbf{y}^{(i-1)} \right\|_1,$$

where in the last inequality we use $4Bm\epsilon \leq \epsilon_2 \leq 1$. This, in turn, implies via induction that for every $1 \leq i \leq k$,

$$\left\|\mathbf{x}^{(i)} - \mathbf{y}^{(i)}\right\|_1 \leq (L+1)^i \left\|\mathbf{x}^{(0)} - \mathbf{y}^{(0)}\right\|_1. \tag{48}$$

We now return to the proof. By iterating (47), we can control $\mathbf{x}^{(k)} - \mathbf{y}^{(k)}$ in terms of a product of k Jacobians, as follows:

$$\mathbf{x}^{(k)} - \mathbf{y}^{(k)} = \left(\prod_{i=1}^{i=k} J(\mathbf{y}^{(k-i)})\right)\left(\mathbf{x}^{(0)} - \mathbf{y}^{(0)}\right) + \sum_{i=1}^{k}\left(\prod_{j=0}^{j=k-i-1} J(\mathbf{y}^{(k-j)})\right)\left(\xi^{(i)} + \nu^{(i)}\right).$$

Since $\left\|\mathbf{y}^{(i)} - \tau\right\|_1 \leq \epsilon$ by the hypothesis of the theorem, we get from (66) that the leftmost term in the above sum has ℓ_1 norm less than $(\rho^k - \epsilon_2)\left\|\mathbf{x}^{(0)} - \mathbf{y}^{(0)}\right\|_1$.

We now proceed to estimate the terms in the summation. Our first step to use the conditions on the norms of $\nu^{(i)}$ and $\xi^{(i)}$ and the fact that $\|J\|_1 \leq L$ uniformly to obtain the upper bound

$$\sum_{i=1}^{k} L^{k-i} \left\|\mathbf{x}^{(i-1)} - \mathbf{y}^{(i-1)}\right\|_1 \left(Bm \left\|\mathbf{x}^{(i-1)} - \mathbf{y}^{(i-1)}\right\|_1 + \delta\right).$$

Now, recalling that $\mathbf{x}^{(i)}$ and $\mathbf{y}^{(i)}$ are both within an ϵ ℓ_1-neighborhood of τ so that $\left\|\mathbf{x}^{(i)} - \mathbf{y}^{(i)}\right\|_1 \leq 2\epsilon$, we can estimate the above upper bound as follows:

$$\sum_{i=1}^{k} L^{k-i} \left\|\mathbf{x}^{(i-1)} - \mathbf{y}^{(i-1)}\right\|_1 \left(Bm \left\|\mathbf{x}^{(i-1)} - \mathbf{y}^{(i-1)}\right\|_1 + \delta\right)$$

$$\leq (L+1)^{k-1} \left\|\mathbf{x}^{(0)} - \mathbf{y}^{(0)}\right\|_1 \sum_{i=1}^{k}\left(Bm \left\|\mathbf{x}^{(i-1)} - \mathbf{y}^{(i-1)}\right\|_1 + \delta\right)$$

$$\leq k(L+1)^{k-1}(2Bm\epsilon + \delta) \left\|\mathbf{x}^{(0)} - \mathbf{y}^{(0)}\right\|_1$$

$$\leq \epsilon_2 \left\|\mathbf{x}^{(0)} - \mathbf{y}^{(0)}\right\|_1,$$

where the first inequality is an application of (48), and the last uses the definitions of ϵ and δ. Combining with the upper bound of $(\rho^k - \epsilon_2)\left\|\mathbf{x}^{(0)} - \mathbf{y}^{(0)}\right\|_1$ obtained above for the first term, this yields the result. $\qquad\square$

Remark 9. *Note that k in the theorem can be chosen as large as we want. However, for simplicity, we fix some $k > k_0$ in the rest of the discussion, and revisit the freedom of choice of k only toward the end of the proof of the Theorem (5.7).*

5.5.2 Evolution under random perturbations.

We now explore some consequences of the above theorem for stochastic evolutions. Our main goal in this subsection is to highlight the subtleties that arise in ensuring that the third "small perturbations" condition during a random evolution, and strategies that can be used to avoid them. However, we first begin by showing the second condition, that of "closeness to the fixed point" is actually quite simple to maintain. It will be convenient to define for this purpose the notion of an *epoch*, which is simply the set of $(k + 1)$ initial and final states of k consecutive steps of a stochastic evolution.

Definition 23 (**Epoch**). *Let f be a smooth contractive evolution and let k be as in the statement of 5.13 when applied to f. An* epoch *is a set of $k+1$ consecutive states in a stochastic evolution guided by f. By a slight abuse of terminology we also use the same term to refer to a set of $k + 1$ consecutive states in a* pair *of stochastic evolutions guided by f that have been coupled using the optimal coupling.*

Suppose we want to apply 5.13 to a pair of stochastic evolutions guided by f. Recall the parameter ϵ in the statement of 5.13. Ideally, we would likely to show that if both the states in the pair at the beginning of an epoch are within some distance $\epsilon' < \epsilon$ of the fixed point τ, then (1) all the consequent steps in the epoch are within distance ϵ of the fixed point (so that the closeness condition in the theorem is satisfied), and more importantly (2) that the states at the last step of the epoch are *again* within the same distance ϵ' of the fixed point, so that we have the ability to apply the theorem to the *next* epoch. Of course, we also need to ensure that the condition on the perturbations being true also holds during the epoch, but as stated

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above, this is somewhat more tricky to maintain than the closeness condition, so we defer its discussion to later in the section. Here, we state the following lemma which shows that the closeness condition can indeed be maintained at the end of the epoch.

Lemma 5.14 (**Remaining close to the fixed point**). *Let $w < w' < 1/3$ be fixed constants. Consider a stochastic evolution $\mathbf{X}^{(0)}, \mathbf{X}^{(1)}, \ldots$ on a population of size N guided by a (L, B, ρ)-smooth contractive evolution $f : \Delta_m \to \Delta_m$ with fixed point τ. Suppose $\alpha > 1$ is such that $\left\| \mathbf{X}^{(0)} - \tau \right\|_1 \leq \frac{\alpha}{N^w}$. If N is chosen large enough (as a function of L, α, m, k, w, w' and ρ), then with probability at least $1 - 2mk \exp\left(-N^{w'}/2\right)$ we have*

- $\left\| \mathbf{X}^{(i)} - \tau \right\|_1 \leq \frac{(\alpha+m)(L+1)^i}{N^w}$, *for $1 \leq i \leq k - 1$.*

- $\left\| \mathbf{X}^{(k)} - \tau \right\|_1 \leq \frac{\alpha}{N^w}$.

To prove the lemma, we need the following simple concentration result.

Lemma 5.15. *Let $\mathbf{X}^{(0)}, \mathbf{X}^{(1)}, \ldots$ be a stochastic evolution on a population of size N which is guided by a (L, B, ρ)-smooth contractive evolution $f : \Delta_m \to \Delta_m$ with fixed point τ. For any $t > 0$ and $\gamma \leq 1/3$, it holds with probability at least $1 - 2mt \exp\left(-N^\gamma/2\right)$ that*

$$\left\| \mathbf{X}^{(i)} - f^i(\mathbf{X}^{(0)}) \right\|_1 \leq \frac{(L+1)^i m}{N^\gamma} \text{ for all } 1 \leq i \leq t.$$

Proof. Fix a coordinate $j \in [m]$. Since $\mathbf{X}^{(i)}$ is the normalized frequency vector obtained by taking N independent samples from the distribution $f(\mathbf{X}^{(i-1)})$, Hoeffding's inequality yields that

$$\mathbb{P}\left[\left| X_j^{(i)} - f(\mathbf{X}^{(i-1)})_j \right| > N^{-\gamma} \right] \leq 2 \exp\left(-N^{1-2\gamma}\right) \leq 2 \exp\left(-N^\gamma\right),$$

where the last inequality holds because $\gamma \leq 1/3$. Taking a union bound over all $j \in [m]$, we therefore have that for any fixed $i \leq t$,

$$\mathbb{P}\left[\left\| \mathbf{X}^{(i)} - f(\mathbf{X}^{(i-1)}) \right\|_1 > \frac{m}{N^\gamma} \right] \leq 2m \exp\left(-N^\gamma\right). \tag{49}$$

For ease of notation let us define the quantities $s^{(i)} := \left\| \mathbf{X}^{(i)} - f^i(\mathbf{X}^{(0)}) \right\|_1$ for $0 \le i \le t$. Our goal then is to show that it holds with high probability that $s^{(i)} \le \frac{(L+1)^i m}{N^\gamma}$ for all i such that $0 \le i \le t$.

Now, by taking an union bound over all values of i in (49), we see that the following holds for all i with probability at least $1 - 2mt \exp\left(-N^\gamma\right)$:

$$s^{(i)} = \left\| \mathbf{X}^{(i)} - f^i(\mathbf{X}^{(0)}) \right\|_1 \le \left\| \mathbf{X}^{(i)} - f(\mathbf{X}^{(i-1)}) \right\|_1 + \left\| f(\mathbf{X}^{(i-1)}) - f^i(\mathbf{X}^{(0)}) \right\|_1 \quad (50)$$

$$\le \frac{m}{N^\gamma} + Ls^{(i-1)}, \quad (51)$$

where the first term is estimated using the probabilistic guarantee from (49) and the second using the upper bound on the $1 \to 1$ norm of the Jacobian of f. However, (51) implies that $s^{(i)} \le \frac{m(L+1)^i}{N^\gamma}$ for all $0 \le i \le t$, which is what we wanted to prove. To see the former claim, we proceed by induction. Since $s_0 = 0$, the claim is trivially true in the base case. Assuming the claim is true for $s^{(i)}$, we then apply (51) to get

$$s^{(i+1)} \le \frac{m}{N^\gamma} + Ls^{(i)} \le \frac{m}{N^\gamma}\left(1 + L(L+1)^i\right) \le \frac{m}{N^\gamma} \cdot (L+1)^{i+1}. \qquad \square$$

Proof of 5.14. Lemma 5.15 implies that with probability at least $1 - 2mk \exp\left(-N^{w'}/2\right)$ we have

$$\left\| \mathbf{X}^{(i)} - f^i(\mathbf{X}^{(0)}) \right\|_1 \le \frac{(L+1)^i m}{N^{w'}}, \text{ for } 1 \le i \le k. \quad (52)$$

On the other hand, the fact that $\max \|J(\mathbf{x})\|_1 \le L$ implies that

$$\left\| f^{i+1}(\mathbf{X}^{(0)}) - \tau \right\|_1 = \left\| f^{i+1}(\mathbf{X}^{(0)}) - f(\tau) \right\|_1 \le L \left\| f^i(\mathbf{X}^{(0)}) - \tau \right\|_1,$$

so that

$$\left\| f^i(\mathbf{X}^{(0)}) - \tau \right\|_1 \le L^i \left\| \mathbf{X}^{(0)} - \tau \right\|_1 \le \frac{\alpha L^i}{N^w}, \text{ for } 1 \le i \le k. \quad (53)$$

Combining (52),(53), we already get the first item in the lemma. However, for $i = k$, we can do much better than the above estimate (and indeed, this is the most important part of the lemma). Recall the parameter ϵ in 5.13. If we choose N large enough so that

$$\frac{(\alpha + m)(L+1)^k}{N^w} \le \epsilon, \quad (54)$$

then the above argument shows that with probability at least $1 - 2mk \exp\left(-N^{w'}\right)$, the sequences $\mathbf{y}^{(i)} = f^i(\mathbf{X}^{(0)})$ and $\mathbf{z}^{(i)} = \tau$ (for $0 \leq i \leq k$) satisfy the hypotheses of 5.13: the perturbations in this case are simply 0. Hence, we get that

$$\left\| f^k(\mathbf{X}^{(0)}) - \tau \right\|_1 \leq \rho^k \left\| \mathbf{X}^{(0)} - \tau \right\|_1 \leq \frac{\alpha \rho^k}{N^w}. \tag{55}$$

Using (55) with the $i = k$ case of (52), we then have

$$\left\| \mathbf{X}^{(k)} - \tau \right\|_1 \leq \frac{(L+1)^k m}{N^{w'}} + \frac{\rho^k \alpha}{N^w}.$$

Thus, (since $\rho < 1$) we only need to choose N so that

$$N^{w'-w} \geq \frac{(L+1)^k m}{\alpha(1 - \rho^k)} \tag{56}$$

in order to get the second item in the lemma. Since $w > 0$ and $w' > w$, it follows that all large enough N will satisfy the conditions in both (54), (56), and this completes the proof. $\qquad \square$

5.5.3 Controlling the size of random perturbations.

We now address the "small perturbations" condition of 5.13. For a given smooth contractive evolution f, let α, w, w' be any constants satisfying the hypotheses of Lemma 5.14 (the precise values of these constants will specified in the next section). For some N as large as required by the lemma, consider a pair $\mathbf{X}^{(t)}, \mathbf{Y}^{(t)}$ of stochastic evolutions guided by f on a population of size N, which are coupled according to the optimal coupling. Now, let us call an epoch *decent* if the first states $\mathbf{X}^{(0)}$ and $\mathbf{Y}^{(0)}$ in the epoch satisfy $\left\| \mathbf{X}^{(0)} - \tau \right\|_1, \left\| \mathbf{Y}^{(0)} - \tau \right\|_1 \leq \alpha N^{-w}$. The lemma (because of the choice of N made in 54) shows that if an epoch is decent, then except with probability that is sub-exponentially small in N,

1. the current epoch satisfies the "closeness to fixed point" condition in 5.13, and

2. the *next* epoch is decent as well.

Thus, the lemma implies that if a certain epoch is decent, then with all but sub-exponential (in N) probability, a polynomial (in N) number of subsequent epochs are also decent, and hence satisfy the "closeness to fixed point" condition of Theorem 5.13. Hypothetically, if these epochs also satisfied the "small perturbation" condition, then we would be done, since in such a situation, the distance between the two chains will drop to less than $1/N$ within $O(\log N)$ time, implying that they would collide. This would in turn imply a $O(\log N)$ mixing time.

However, as alluded to above, ensuring the "small perturbations" condition turns out to be more subtle. In particular, the fact that the perturbations $\xi^{(i)}$ need to be *multiplicatively* smaller than the actual differences $\left\|\mathbf{x}^{(i)} - \mathbf{y}^{(i)}\right\|_1$ pose a problem in achieving adequate concentration, and we cannot hope to prove that the "small perturbations" condition holds with very high probability over an epoch when the staring difference $\left\|\mathbf{X}^{(0)} - \mathbf{Y}^{(0)}\right\|_1$ is very small. As such, we need to break the arguments into two stages based on the starting differences at the start of the epochs lying in the two stages.

To make this more precise (and to state a result which provides examples of the above phenomenon and will also be a building block in the coupling proof), we define the notion of an epoch being *good* with a *goal g*. As before let $\mathbf{X}^{(t)}$ and $\mathbf{Y}^{(t)}$ be two stochastic evolutions guided by f which are coupled according to the optimal coupling, and let $\xi^{(i)}$ be the perturbations as defined in 5.13. Then, we say that a decent epoch (which we can assume, without loss of generality, to start at $t = 0$) is *good* with goal g if one of following two conditions holds. Either (1) there is a j, $0 \leq j \leq k - 1$ such that $\left\|f(\mathbf{X}^{(j)}) - f(\mathbf{Y}^{(j)})\right\|_1 \leq g$, or otherwise, (2) it holds that the next epoch is also decent, and, further

$$\left\|\xi^{(i)}\right\|_1 \leq \delta \left\|\mathbf{X}^{(i)} - \mathbf{Y}^{(i)}\right\|_1 \text{ for } 0 \leq i \leq k,$$

where δ again is as defined in 5.13. Note that if an epoch is good with goal g, then either the expected difference between the two chains drops below g sometime

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during the epoch, or else, all conditions of 5.13 are satisfied during the epoch, and the distance between the chains drops by a factor of ρ^k. Further, in terms of this notion, the preceding discussion can be summarized as "the probability of an epoch being good depends upon the goal g, and can be small if g is too small". To make this concrete, we prove the following theorem which quantifies this trade-off between the size of the goal g and the probability with which an epoch is good with that goal.

Theorem 5.16 (**Goodness with a given goal**). *Let the chains* $\mathbf{X}^{(t)}$, $\mathbf{Y}^{(t)}$, *and the quantities* $N, m, w, w', k, L, \epsilon$ *and* δ *be as defined above, and let* $\beta < (\log N)^2$. *If* N *is large enough, then a decent epoch is good with goal* $g := \frac{4L^2 m \beta}{\delta^2 N}$ *with probability at least* $1 - 2mk \left(\exp(-\beta/3) + \exp(-N^{w'}/2) \right)$.

Proof. Let $\mathbf{X}^{(0)}$ and $\mathbf{Y}^{(0)}$ denote the first states in the epoch. Since the current epoch is assumed to be decent, 5.14 implies that with probability at least $1 - 2mk \exp(-N^{-w'}/2)$, the "closeness to fixed point" condition of 5.13 holds throughout the epoch, and the next epoch is also decent. If there is a $j \leq k - 1$ such that $\left\| f(\mathbf{X}^{(j)}) - f(\mathbf{Y}^{(j)}) \right\|_1 \leq g$, then the current epoch is already good with goal g. So let us assume that

$$\left\| f(\mathbf{X}^{(i-1)}) - f(\mathbf{Y}^{(i-1)}) \right\|_1 \geq g = \frac{4L}{\delta^2} \cdot \frac{\beta m}{N} \text{ for } 1 \leq i \leq k.$$

However, in this case, we can apply the concentration result in 5.6 with $c = 4L^2/\delta^2$ and $t = \beta$ to get that with probability at least $1 - 2mk \exp(-\beta/3)$,

$$\left\| \xi^{(i)} \right\|_1 \leq \frac{\delta}{L} \left\| f(\mathbf{X}^{(i-1)}) - f(\mathbf{Y}^{(i-1)}) \right\|_1 \leq \delta \left\| \mathbf{X}^{(i-1)} - \mathbf{Y}^{(i-1)} \right\|_1 \text{ for } 1 \leq i \leq k.$$

Hence, both conditions ("closeness to fixed point" and "small perturbations") for being good with goal g hold with the claimed probability. $\square$

Note that we need to take β to a large constant, at least $\Omega(\log(mk))$, even to make the result non-trivial. In particular, if we take $\beta = 3 \log(4mk)$, then if N is

large enough, the probability of success is at least $1/e$. However, with a slightly larger goal g, it is possible to reduce the probability of an epoch not being good to $o_N(1)$: if we choose $\beta = \log N$, then a decent epoch is good with the corresponding goal with probability at least $1 - N^{-1/4}$, for N large enough.

In the next section, we use both these settings of parameters in the above theorem to complete the proof of the mixing time result. As described in 5.4, the two settings above will be used in different stages of the evolution of two coupled chains in order to argue that the time to collision of the chains is indeed small.

Proof of the main theorem: Analyzing the coupling time.

Our goal is now to show that if we couple two stochastic evolutions guided by the same smooth contractive evolution f using the optimal coupling, then irrespective of their starting positions, they reach the same state in a small number of steps, with reasonably high probability. More precisely, our proof would be structured as follows. Fix any starting states $\mathbf{X}^{(0)}$ and $\mathbf{Y}^{(0)}$ of the two chains, and couple their evolutions according to the optimal coupling. Let T be the first time such that $\mathbf{X}^{(T)} = \mathbf{Y}^{(T)}$. Suppose that we establish that $\mathbb{P}\left[T < t\right] \geq q$, where t and p do not depend upon the starting states $(\mathbf{X}^{(0)}, \mathbf{Y}^{(0)})$. Then, we can dovetail this argument for ℓ "windows" of time t each to see that $\mathbb{P}\left[T > \ell \cdot t\right] \leq (1-q)^{\ell}$: this is possible because the probability bounds for T did not depend upon the starting positions $(\mathbf{X}^{(0)}, \mathbf{Y}^{(0)})$ and hence can be applied again to the starting positions $(\mathbf{X}^{(t)}, \mathbf{Y}^{(t)})$ if $\mathbf{X}^{(t)} \neq \mathbf{Y}^{(t)}$. By choosing ℓ large enough so that $(1-q)^{\ell}$ is at most $1/e$ (or any other constant less than $1/2$), we obtain a mixing time of ℓt. We therefore proceed to obtain an upper bound on $\mathbb{P}\left[T < t\right]$ for some $t = \Theta(\log N)$.

As discussed earlier, we need to split the evolution of the chains into several stages in order to complete the argument outlined above. We now describe these four different stages. Recall that f is assumed to be a (L, B, ρ)-smooth contractive evolution. Without loss of generality we assume that $L > 1$. The parameter r appearing below

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is a function of these parameters and k and is defined in 5.18. Further, as we noted after the proof of 5.13, k can be chosen to be as large as desired. We now exercise this choice by choosing k to be large enough so that

$$\rho^k \leq e^{-1}. \tag{57}$$

The other parameters below are chosen to ease the application of the framework developed in the previous section.

1. **Approaching the fixed point**. We define T_{start} to be the first time such that

$$\left\|\mathbf{X}^{(T_{\text{start}}+i)} - \tau\right\|_1, \left\|\mathbf{Y}^{(T_{\text{start}}+i)} - \tau\right\|_1 \leq \frac{\alpha}{N^w} \text{ for } 0 \leq i \leq k-1,$$

where $\alpha := m + r$ and $w = \min\left(\frac{1}{6}, \frac{\log(1/\rho)}{6\log(L+1)}\right)$. We show below that

$$\mathbb{P}\left[T_{\text{start}} > t_{\text{start}} \log N\right] \leq 4mkt_o \log N \exp\left(-N^{1/3}\right), \tag{58}$$

where $t_{\text{start}} := \frac{1}{6\log(L+1)}$. The probability itself is upper bounded by $\exp\left(-N^{1/4}\right)$ for N large enough.

2. **Coming within distance** $\Theta\left(\frac{\log N}{N}\right)$. Let $\beta_0 := (8/\rho^k)\log(17mk)$ and $h = \frac{4L^2 m}{\delta^2}$. Then, we define T_0 to be the smallest number of steps needed after T_{start} such that either

$$\left\|\mathbf{X}^{(T_{\text{start}}+T_0)} - \mathbf{Y}^{(T_{\text{start}}+T_0)}\right\|_1 \leq \frac{h\beta_0 \log N}{N} \text{ or}$$

$$\left\|f(\mathbf{X}^{(T_{\text{start}}+T_0)}) - f(\mathbf{Y}^{(T_{\text{start}}+T_0)})\right\|_1 \leq \frac{h\beta_0 \log N}{N(1+\delta)}.$$

We prove below that when N is large enough

$$\mathbb{P}\left[T_0 > kt_0 \log N\right] \leq \frac{1}{N^{\beta_0/7}}, \tag{59}$$

where $t_0 := \frac{1}{k\log(1/\rho)}$.

3. **Coming within distance** $\Theta(1/N)$. Let β_0 and h be as defined in the last item. We now define a sequence of $\ell_1 := \left\lceil \frac{\log\log N}{k\log(1/\rho)} \right\rceil$ random variables $T_1, T_2, \ldots T_\ell$. We

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begin by defining the stopping time $S_0 := T_{\text{start}} + T_0$. For $i \geq 1$, T_i is defined to be the smallest number of steps after S_{i-1} such that the corresponding stopping time $S_i := S_{i-1} + T_i$ satisfies

either $\left\| \mathbf{X}^{(S_i)} - \mathbf{Y}^{(S_i)} \right\|_1 \leq \dfrac{h\rho^{ik}\beta_0 \log N}{N}$ or $\left\| f(\mathbf{X}^{(S_i)}) - f(\mathbf{Y}^{(S_i)}) \right\|_1 \leq \dfrac{h\rho^{ik}\beta_0 \log N}{N(1+\delta)}$.

Note that T_i is defined to be 0 if setting $S_i = S_{i-1}$ already satisfies the above conditions. Define $\beta_i = \rho^{ik}\beta_0$. We prove below that when N is large enough

$$\mathbb{P}\left[T_i > k+1\right] \leq 4mk \exp\left(-(\beta_i \log N)/8\right), \text{ for } 1 \leq i \leq \ell_1. \tag{60}$$

4. **Collision**. Let β_0 and h be as defined in the last two items. Note that after time S_{ℓ_1}, we have

$$\left\| f(\mathbf{X}^{(S_{\ell_1})}) - f(\mathbf{Y}^{(S_{\ell_1})}) \right\|_1 \leq \frac{Lh\beta_{\ell_1} \log N}{N} = \frac{Lh\beta_0\rho^{k\ell_1} \log N}{N} \leq \frac{Lh\beta_0}{N}.$$

Then, from the properties of the optimal coupling we have that $\mathbf{X}^{(S_{\ell_1}+1)} = \mathbf{Y}^{(S_{\ell_1}+1)}$ with probability at least $\left(1 - \frac{Lh\beta_0}{2N}\right)^N$ which is at least $\exp\left(-L\beta_0 h\right)$ when N is so large that $N > hL\beta_0$.

Assuming (60), (59), (58), we can complete the proof of 5.7 as follows.

Proof of 5.7. Let $\mathbf{X}^{(0)}$, $\mathbf{Y}^{(0)}$ be the arbitrary starting states of two stochastic evolutions guided by f, whose evolution is coupled using the optimal coupling. Let T be the minimum time t satisfying $\mathbf{X}^{(t)} = \mathbf{Y}^{(t)}$. By the Markovian property and the probability bounds in items 1 to 4 above, we have (for large enough N)

$\mathbb{P}\left[T \leq t_{\text{start}} \log N + kt_0 \log N + (k+1)\ell_1\right]$

$\geq \mathbb{P}\left[T_{\text{start}} \leq t_{\text{start}} \log N\right] \cdot \mathbb{P}\left[T_0 \leq kt_0 \log N\right] \cdot \left(\prod_{i=1}^{\ell_1} \mathbb{P}\left[T_i \leq k+1\right]\right) \cdot e^{-L\beta_0 h}$

$\geq e^{-L\beta_0 h}\left(1 - \exp(-N^{1/4})\right)\left(1 - N^{-\beta/7}\right) \cdot \prod_{i=1}^{\ell_1}\left(1 - 4mk\exp(-(\rho^{ik}\beta_0 \log N)/8)\right)$

$\geq \exp\left(-L\beta_0 h - 1\right) \cdot \left(1 - 4mk\sum_{i=1}^{\ell_1} \exp(-(\rho^{ik}\beta_0 \log N)/8)\right)$

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where the last inequality is true for large enough N. Applying 5.19 to the above sum (with the parameters x and α in the lemma defined as $x = \exp(-(\beta_0 \log N)/8)$ and $\alpha = \rho^k \leq 1/e$ by the assumption in 57), we can put a upper bound on it as follows:

$$\sum_{i=1}^{\ell_1} \exp(-(\rho^{ik}\beta_0 \log N)/8) \leq \frac{1}{\exp(\rho^k \beta_0/8) - 1}$$

$$= \frac{1}{17mk - 1} \leq \frac{1}{16mk},$$

where the first inequality follows from the lemma and the fact that $\frac{\log \log N}{k \log(1/\rho)} \leq \ell_1 \leq 1 + \frac{\log \log N}{k \log(1/\rho)}$, and the last inequality uses the definition of β_0 and $m, k \geq 1$. Thus, for large enough N, we have

$$\mathbb{P}\left[T \leq c \log N\right] \geq q,$$

where $c := 2(t_{\text{start}} + kt_0)$ and $q := (3/4) \exp\left(-L\beta_0 h - 1\right)$. Since this estimate does not depend upon the starting states, we can bootstrap the estimate after every $c \log N$ steps to get

$$\mathbb{P}\left[T > c\ell \log N\right] < (1 - q)^\ell \leq e^{-q\ell},$$

which shows that

$$\frac{c}{q} \cdot \log N$$

is the mixing time of the chain for total variation distance $1/e$, when N is large enough. $\qquad\square$

We now proceed to prove the claimed equations, starting with (58). Let $t := t_{\text{start}} \log N$ for convenience of notation. From Lemma 5.18 we have

$$\left\|f^t(\mathbf{X}^{(0)}) - \tau\right\|_1 \leq r\rho^t.$$

On the other hand, applying 5.15 to the chain $\mathbf{X}^{(0)}, \mathbf{X}^{(1)}, \ldots$ with $\gamma = 1/3$, we have

$$\left\|f^t(\mathbf{X}^{(0)}) - \mathbf{X}^{(t)}\right\|_1 \leq \frac{(L+1)^t m}{N^{1/3}}$$

with probability at least $1 - 2mt \exp(-N^{1/3})$. From the triangle inequality and the definition of t, we then see that with probability at least $1 - 2mt \exp\left(-N^{1/3}\right)$, we have

$$\left\|\mathbf{X}^{(t)} - \tau\right\|_1 \leq \frac{m}{N^{1/6}} + \frac{r}{N^{t_{\text{start}} \log(1/\rho)}} \leq \frac{m + r}{N^w} = \frac{\alpha}{N^w},$$

where α, w are as defined in item 1 above. Now, if we instead looked at the chain starting at some $i < k$, the same result would hold for $\mathbf{X}^{(t+i)}$. Further, the same analysis applies also to $\mathbf{Y}^{(t+i)}$. Taking an union bound over these $2k$ events, we get the required result.

Before proceeding with the proof of the other two equations, we record an important consequences of 58. Let w, α be as defined above, and let $w' > w$ be such that $w' < 1/3$. Recall that an epoch starting at time 0 is decent if both $\mathbf{X}^{(t)}$ and $\mathbf{Y}^{(t)}$ are within distance α/N^w of τ.

Observation 5.17. *For large enough N, it holds with probability at least $1 - \exp(-N^{w'/4})$ that for $1 \leq i \leq kN$, $\mathbf{X}^{(T_{\text{start}}+i)}, \mathbf{Y}^{(T_{\text{start}}+i)}$ are within ℓ_1 distance α/N^w of τ.*

Proof. We know from item 1 that the epochs starting at times $T_{\text{start}} + i$ for $0 \leq i < k$ are all decent. For large enough N, 5.14 followed by a union bound implies that the N consecutive epochs starting at $T + j + k\ell$ where $\ell \leq N$ and $0 \leq j \leq N$ are also all decent with probability at least $1 - 2mk^2N \exp(-N^{w'/2})$, which upper bounds the claimed probability for large enough N. $\qquad\square$

We denote by E the event that the epochs starting at $T_{\text{start}} + i$ for $1 \leq i \leq kN$ are all decent. The above observation says that $P(E) \geq 1 - \exp(-N^{-w'/4})$ for N large enough.

We now consider T_0. Let $g_0 := \frac{h\beta_0 \log N}{N(1+\delta)}$, where h is as defined in items 2 and 3 above. From 5.16 followed by a union bound, we see that the first $t_1 \log N$ consecutive epochs starting at $T_{\text{start}}, T_{\text{start}} + k, T_{\text{start}} + 2k, \ldots$ are good with goal g_0 (they are already known to be decent with probability at least $P(E)$ from the above observation)

with probability at least

$$1 - 2mkt_1 \left(N^{-\beta_0/(3(1+\delta))} + \exp(-N^{w'}/4) \right) \log N - P(\neg E),$$

which is larger than $1 - N^{-\beta_0/7}$ for N large enough (since $\delta < 1$). Now, if we have $\left\| f(\mathbf{X}^{(i)}) - f(\mathbf{Y}^{(i)}) \right\|_1 \leq g$ for some time i during these $t_1 \log N$ good epochs then $T_0 \leq kt_1 \log N$ follows immediately. Otherwise, the goodness condition implies that the hypotheses of 5.13 are satisfied across all these epochs, and we get

$$\left\| \mathbf{X}^{(T_{\text{start}}+kt_1 \log N)} - \mathbf{Y}^{(T_{\text{start}}+kt_1 \log N)} \right\|_1 \leq \rho^{kt_1 \log N} \left\| \mathbf{X}^{(T_{\text{start}})} - \mathbf{Y}^{(T_{\text{start}})} \right\|_1$$
$$\leq \rho^{kt_1 \log N} \frac{\alpha}{N^w}$$
$$\leq g_0 \leq \frac{h\beta_0 \log N}{N},$$

where the second last inequality is true for large enough N.

Finally, we analyze T_i for $i \geq 1$. For this, we need to consider cases according to the state of the chain at time S_{i-1}. However, we first observe that plugging our choice of h into 5.16 shows that any decent epoch is good with goal $g_i := \frac{h\beta_i \log N}{N(1+\delta)}$ with probability at least

$$1 - 2mk \left(\exp(-(\beta_i \log N)/(3(1+\delta))) + \exp(-N^{w'}/4) \right),$$

which is at least $1 - 2mk \exp(-(\beta_i \log N)/7)$ for N large enough (since $\delta < 1$). Further, since we can assume via the above observation that all the epochs we consider are decent with probability at least $P(E)$, it follows that the epoch starting at S_{i-1} (and also the one starting at $S_{i-1} + 1$) is good with goal g_i with probability at least

$$p := 1 - 2mk \exp(-(\beta_i \log N)/7) - P(\neg E) \geq 1 - 2mk \exp(-(\beta_i \log N)/8),$$

where the last inequality holds whenever $\beta_i \leq \log N$ and N is large enough (we will use at most one of these two epochs in each of the exhaustive cases we consider below). Note that if at any time $S_{i-1} + j$ (where $j \leq k + 1$) during one of these two good

epochs it happens that $\left\| f(\mathbf{X}^{(S_{i-1}+j)}) - f(\mathbf{Y}^{(S_{i-1}+j)}) \right\|_1 \leq g_i$, then we immediately get $T_i \leq k+1$ as required. We can therefore assume that this does not happen, so that the hypotheses of 5.13 are satisfied across these epochs.

Now, the first case to consider is $\left\| \mathbf{X}^{(S_{i-1})} - \mathbf{Y}^{(S_{i-1})} \right\|_1 \leq \frac{h\beta_{i-1}\log N}{N}$. Since we are assuming that 5.13 is satisfied across the epoch starting at S_{i-1}, we get

$$\left\| \mathbf{X}^{(S+i-1+k)} - \mathbf{Y}^{(S_{i-1}+k)} \right\|_1 \leq \rho^k \left\| \mathbf{X}^{(S_{i-1})} - \mathbf{Y}^{(S_{i-1})} \right\|_1 \leq \rho^k \frac{h\beta_{i-1}\log N}{N} = \frac{h\beta_i \log N}{N}.$$

(61)

Thus, in this case, we have $T_i \leq k$ with probability at least p as defined in the last paragraph.

Even simpler is the case $\left\| f(\mathbf{X}^{(S_{i-1})}) - f(\mathbf{Y}^{(S_{i-1})}) \right\|_1 \leq \frac{h\beta_i \log N}{N}$ in which case T_i is zero by definition. Thus the only remaining case left to consider is

$$\frac{h\beta_i \log N}{N} < \left\| f(\mathbf{X}^{(S_{i-1})}) - f(\mathbf{Y}^{(S_{i-1})}) \right\|_1 \leq \frac{h\beta_{i-1}\log N}{N(1+\delta)}.$$

Since $h = \frac{4L^2 m}{\delta^2}$, the first inequality allows us to use 5.6 with the parameters c and t in that lemma set to $c = 4/\delta^2$ and $t = \beta_i L^2 \log N$, and we obtain

$$\left\| \mathbf{X}^{(S_{i-1}+1)} - \mathbf{Y}^{(S_{i-1}+1)} \right\|_1 \leq (1+\delta) \left\| f(\mathbf{X}^{(S_{i-1})}) - f(\mathbf{Y}^{(S_{i-1})}) \right\|_1 \leq \frac{h\beta_{i-1}\log N}{N},$$

with probability at least $1 - 2m \exp\left(-(\beta_i L^2 \log N)/3\right)$. Using the same analysis as the first case from this point onward (the only difference being that we need to use the epoch starting at $S_{i-1}+1$ instead of the epoch starting at S_{i-1} used in that case), we get that

$$\mathbb{P}\left[T_i \leq 1+k\right] \geq p - 2m \exp\left(-(\beta_i L^2 \log N)/3\right)$$

$$\geq 1 - 4mk \exp\left(-(\beta_i \log N)/8\right),$$

since $L, k > 1$. Together with (61), this completes the proof of (60).

5.5.4 Proofs omitted from Section 5.5

Lemma 5.18 (Exponential convergence I). *Let f be a smooth contractive evolution, and let τ and ρ be as in the conditions described in Section 5.3.2. Then, there*

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exist a positive r such that for every $\mathbf{z} \in \Delta_m$, and every positive integer t,

$$\left\| f^t(\mathbf{z}) - \tau \right\|_1 \leq r\rho^t.$$

Proof. Let ϵ and k be as defined in 5.13. From the "convergence to the fixed point" condition, we know that there exists an ℓ such that for all $\mathbf{z} \in \Delta_m$,

$$\left\| f^\ell(\mathbf{z}) - \tau \right\|_1 \leq \frac{\epsilon}{L^k}. \tag{62}$$

Note that this implies that $f^{\ell+i}(\mathbf{z})$ is within distance ϵ of τ for $i = 0, 1, \ldots, k$, so that 5.13 can be applied to the sequence of vectors $f^\ell(\mathbf{z}), f^{\ell+1}(\mathbf{z}), \ldots, f^{\ell+k}(\mathbf{z})$ and $\tau, f(\tau) = \tau, \ldots, f^k(\tau) = \tau$ (the perturbations are simply 0). Thus, we get

$$\left\| f^{\ell+k}(\mathbf{z}) - \tau \right\|_1 \leq \rho^k \left\| f^\ell(\mathbf{z}) - \tau \right\|_1 \leq \frac{\rho^k \epsilon}{L^k}.$$

Since $\rho < 1$, we see that the epoch starting at $\ell + k$ also satisfies (62) and hence we can iterate this process. Using also the fact that the $1 \rightarrow 1$ norm of the Jacobian of f is at most L (which we can assume without loss of generality to be at least 1), we therefore get for every $\mathbf{z} \in \Delta_m$, and every $i \geq 0$ and $0 \leq j < k$

$$\begin{aligned}
\left\| f^{\ell+ik+j}(\mathbf{z}) - \tau \right\|_1 &\leq \rho^{ki+j} \frac{L^j}{\rho^j} \left\| f^\ell(\mathbf{z}) - \tau \right\|_1 \\
&\leq \rho^{ki+j+\ell} \frac{L^{j+\ell}}{\rho^{j+\ell}} \left\| \mathbf{z} - \tau \right\|_1 \\
&\leq \rho^{ki+j+\ell} \frac{L^{k+\ell}}{\rho^{k+\ell}} \left\| \mathbf{z} - \tau \right\|_1
\end{aligned}$$

where in the last line we use the facts that $L > 1$, $\rho < 1$ and $j < k$. Noting that any $t \geq \ell$ is of the form $\ell + ki + j$ for some i and j as above, we have shown that for every $t \geq \ell$ and every $\mathbf{z} \in \Delta_m$

$$\left\| f^t(\mathbf{z}) - \tau \right\|_1 \leq \left(\frac{L}{\rho} \right)^{k+\ell} \rho^t \left\| \mathbf{z} - \tau \right\|_1. \tag{63}$$

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Similarly, for $t < \ell$, we have, for any $\mathbf{z} \in \Delta_m$

$$\left\| f^t(\mathbf{z}) - \tau \right\|_1 \leq L^t \left\| \mathbf{z} - \tau \right\|_1$$

$$\leq \left(\frac{L}{\rho} \right)^t \rho^t \left\| \mathbf{z} - \tau \right\|_1 \tag{64}$$

$$\leq \left(\frac{L}{\rho} \right)^\ell \rho^t \left\| \mathbf{z} - \tau \right\|_1, \tag{65}$$

where in the last line we have again used $L > 1, \rho < 1$ and $t < \ell$. From (65), (63), we get the claimed result with $r := \left(\frac{L}{\rho} \right)^{k+\ell}$. $\qquad \square$

5.5.5 Sums with exponentially decreasing exponents

The following technical lemma is used in the proof of 5.7.

Lemma 5.19. *Let x, α be positive real numbers less than 1 such that $\alpha < \frac{1}{e}$. Let ℓ be a positive integer, and define $y := x^{\alpha^\ell}$. Then*

$$\sum_{i=0}^{\ell} x^{\alpha^i} \leq \frac{y}{1-y}.$$

Proof. Note that since both x and α are positive and less than 1, so is y. We now have

$$\sum_{i=0}^{\ell} x^{\alpha^i} = \sum_{i=0}^{\ell} x^{\alpha^{\ell-i}} = y \sum_{i=0}^{\ell} y^{\alpha^{-i}-1}$$

$$\leq y \sum_{i=0}^{\ell} y^{i \log(1/\alpha)}, \text{ since } 0 < y \leq 1 \text{ and } \alpha^{-i} \geq 1 + i \log(1/\alpha),$$

$$\leq y \sum_{i=0}^{\ell} y^i, \text{ since } 0 < y \leq 1 \text{ and } \alpha < 1/e,$$

$$\leq \frac{y}{1-y}. \qquad \square$$

5.6 Multiple fixed points

5.6.1 One stable, many unstable fixed points

We start this section by proving some technical lemmas that will be very useful for the proofs. The following lemma roughly states that there exists a k (derived

from Theorem 5.1) such that after k steps in the vicinity a stable fixed point $\mathbf{z}$, there is as expected a contraction of the ℓ_1 distance between the frequency vector of the deterministic dynamics and the fixed point.

Lemma 5.20 (Perturbed evolution II). *Let $f : \Delta_m \to \Delta_m$ and $\mathbf{z}$ be a stable fixed point of f with $\mathrm{sp}\,(J(\mathbf{z})) < \rho$. Assume that f is continuously differentiable for all $\mathbf{x}$ with $\|\mathbf{x} - \mathbf{z}\|_1 < \delta$ for some positive δ. From Gelfand's formula (Theorem 5.1) consider a positive integer k such that $\left\|J^k[\mathbf{z}]\right\|_1 < \rho^k$. There exist $\epsilon \in (0,1], \epsilon$ depending upon f and k for which the following is true. Let $\left(\mathbf{x}^{(i)}\right)_{i=0}^{k}$ be sequences of vectors with $\mathbf{x}^{(i)} \in \Delta_m$ which satisfy the following conditions:*

1. For $1 \le i \le k$, it holds that

$$\mathbf{x}^{(i)} = f(\mathbf{x}^{(i-1)}).$$

2. For $0 \le i \le k$, $\left\|\mathbf{x}^{(i)} - \mathbf{z}\right\|_1 \le \epsilon$.

Then, we have

$$\left\|\mathbf{x}^{(k)} - \mathbf{z}\right\|_1 \le \rho^k \left\|\mathbf{x}^{(0)} - \mathbf{z}\right\|_1.$$

Proof. We denote the set $\{\mathbf{x} : \|\mathbf{x} - \mathbf{z}\|_1 < \delta\}$ by $B(\mathbf{z}, \delta)$. Since f is continuously differentiable on $B(\mathbf{z}, \delta)$, $\nabla f_i(\mathbf{x})$ is continuous on $B(\mathbf{z}, \delta)$ for $i = 1, ..., m$. Let $A(\mathbf{y}_1, \ldots, \mathbf{y}_m)$ be a matrix so that $A_{ij}(\mathbf{y}_1, ..., \mathbf{y}_m) = (\nabla f_i(\mathbf{y}_i))_j$.[6] This implies that the function on $\times_{i=1}^{mk} B(\mathbf{z}, \delta)$ defined by $\mathbf{w}_{11}, \mathbf{w}_{12}, \ldots, \mathbf{w}_{1m}, \mathbf{w}_{21}, \ldots \mathbf{w}_{mk} \mapsto \prod_{i=1}^{k} A(\mathbf{w}_{i1}, \ldots, \mathbf{w}_{im})$ is also continuous. Hence, there exist $\epsilon_1, \epsilon_2 > 0$ smaller than 1 such that if $\|\mathbf{w}_{ij} - \mathbf{z}\| \le \epsilon_1$ for $1 \le i \le k, 1 \le j \le m$ then

$$\left\|\prod_{i=1}^{k} A(\mathbf{w}_{i1}, \ldots, \mathbf{w}_{im})\right\|_1 \le \left\|J^k[\mathbf{z}]\right\|_1 - \epsilon_2 < \rho^k. \tag{66}$$

From Taylor's theorem (Theorem 5.3) we have that $\mathbf{x}^{(t+1)} = A(\xi_1^{(k-t)}, \ldots, \xi_m^{(k-t)})(\mathbf{x}^{(t)} - \mathbf{z})$ where $\xi_i^{(k-t)}$ lies in the line segment from $\mathbf{z}$ to $\mathbf{x}^{(t)}$ for $i = 1, \ldots, m$. By induction

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[6]Easy to see that $A(\mathbf{z}, \ldots, \mathbf{z}) = J(\mathbf{z})$.

we get that

$$\mathbf{x}^{(k)} - \mathbf{z} = \prod_{j=1}^{k} A(\xi_1^{(j)}, \ldots, \xi_m^{(j)})(\mathbf{x}^{(0)} - \mathbf{z}).$$

We choose $\epsilon = \min(\epsilon_1, \delta)$. Therefore since $\xi_i^{(j)} \in B(\mathbf{z}, \epsilon)$ for $i = 1, \ldots, m$ and $j = 1, \ldots, k$, from inequality 66 we get that $\left\| \mathbf{x}^{(k)} - \mathbf{z} \right\|_1 < \rho^k \left\| \mathbf{x}^{(0)} - \mathbf{z} \right\|_1$. $\qquad\square$

Lemma 5.21 below roughly says that the stochastic evolution guided by f does not deviate by much from the deterministic dynamics with update rule f after t steps, for t some small positive integer.

Lemma 5.21. *Let $f : \Delta_m \to \Delta_m$ be continuously differentiable in the interior of Δ_m. Let $\mathbf{X}^{(0)}$ be the state of a stochastic evolution guided by f at time 0. Then with probability $1 - 2t \cdot m \cdot e^{-2\epsilon^2 N}$ we have that $\left\| \mathbf{X}^{(t)} - f^t(\mathbf{X}^{(0)}) \right\|_1 \leq t\beta^t \epsilon m$, where $\beta := \sup_{\mathbf{x} \in \Delta_m} \| J(\mathbf{x}) \|_1$.*

Proof. We proceed by induction. For $t = 1$ the result follows from concentration (Chernoff bounds, Theorem 5.5). Using the triangle inequality we get that

$$\left\| \mathbf{X}^{(t+1)} - f^{t+1}(\mathbf{X}^{(0)}) \right\|_1 \leq \left\| \mathbf{X}^{(t+1)} - f(\mathbf{X}^{(t)}) \right\|_1 + \left\| f(\mathbf{X}^{(t)}) - f^{t+1}(\mathbf{X}^{(0)}) \right\|_1.$$

With probability at least $1 - 2m \cdot e^{-2\epsilon^2 N}$ (Chernoff bounds, Theorem 5.5) we have

$$\left\| \mathbf{X}^{(t+1)} - f(\mathbf{X}^{(t)}) \right\|_1 \leq \epsilon m, \tag{67}$$

and also by the fact that $\| f(\mathbf{x}) - f(\mathbf{x}') \|_1 \leq \beta \| \mathbf{x} - \mathbf{x}' \|_1$ and induction we get that with probability at least $1 - 2t \cdot m \cdot e^{-2\epsilon^2 N}$

$$\left\| f(\mathbf{X}^{(t)}) - f^{t+1}(\mathbf{X}^{(0)}) \right\|_1 \leq \beta \left\| \mathbf{X}^{(t)} - f^t(\mathbf{X}^{(0)}) \right\|_1 \leq \beta \cdot t\beta^t \epsilon m. \tag{68}$$

It is easy to see that $\epsilon m + t\beta^{t+1} \epsilon m \leq (t+1)\beta^{t+1} \epsilon m$, hence from inequalities 67 and 68 the result follows with probability at least $1 - 2(t+1) \cdot m \cdot e^{-2\epsilon^2 N}$. $\qquad\square$

Existence of Inverse function. For the rest of this section when we talk about the inverse of the Jacobian of a function f at an α-unstable fixed point, we mean the pseudoinverse which also has left eigenvector all ones $\mathbf{1}^\top$ with eigenvalue 0 (see also Remark 7). Since we use a lot the inverse of a function f around a neighborhood of α-unstable fixed points in our lemmas, we need to prove that the inverse is well defined.

Lemma 5.22. *Let $f : \Delta_m \to \Delta_m$ be continuously differentiable in the interior of Δ_m. Let $\mathbf{z}$ be an α-unstable fixed point ($\alpha > 1$). Then $f^{-1}(\mathbf{x})$ is well-defined in a neighborhood of $\mathbf{z}$ and is also continuously differentiable in that neighborhood. Also $J_{f^{-1}}(\mathbf{z}) = J^{-1}(\mathbf{z})$ where $J_{f^{-1}}(\mathbf{z})$ is the Jacobian of f^{-1} at $\mathbf{z}$.*

Proof. This comes from the Inverse function theorem. It suffices to show that $J(\mathbf{z})\mathbf{x} = 0$ iff $\sum_i x_i = 0$, namely the differential is invertible on the simplex Δ_m. This is true by assumption since the minimum eigenvalue $\lambda_{\min}$ of $(J(\mathbf{z}))$, excluding the one with left eigenvector $\mathbf{1}^\top$, will satisfy $\lambda_{\min} > \alpha > 1 > 0$. Finally the Jacobian of f^{-1} at $\mathbf{z}$ is just the pseudoinverse $J^{-1}(\mathbf{z})$ (which will have as well $\mathbf{1}^\top$ as a left eigenvector with eigenvalue 0). □

Distance $\Omega\left(\frac{\log^{2/3} N}{\sqrt{N}}\right)$.

Lemma 5.23. *Let $f : \Delta_m \to \Delta_m$ be continuously differentiable in the interior of Δ_m. Let $\mathbf{X}^{(0)}$ be the state of a stochastic evolution guided by f at time 0 and also $\mathbf{z}$ be an α-unstable fixed point of f such that $\left\|\mathbf{X}^{(0)} - \mathbf{z}\right\|_1$ is $O\left(\frac{\log^{2/3} N}{\sqrt{N}}\right)$. Then with probability at least $\Theta(1)$ we get that*

$$\left\|\mathbf{X}^{(t)} - \mathbf{z}\right\|_1 \geq \frac{\log^{2/3} N}{\sqrt{N}}$$

after at most $O(\log N)$ steps.

Proof. We assume that $\mathbf{X}^{(t)}$ is in a neighborhood of $\mathbf{z}$ which is $o_N(1)$ for the rest of the proof, otherwise the lemma holds trivially. Let q be a positive integer such that

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$\left\|(J^{-1}(\mathbf{z}))^q\right\|_1 < \frac{1}{\alpha^q} < \frac{2}{5}$ (using Gelfand's formula 5.1 and the fact that $\alpha > 1$). First of all, it is easy to see that if $\left\|X^{(0)} - \mathbf{z}\right\|_1$ is $o\left(\frac{1}{\sqrt{N}}\right)$ then with probability at least $\Theta(1) = c_1$ we have after one step that $\left\|X^{(1)} - \mathbf{z}\right\|_1 > \frac{c}{\sqrt{N}}$ (this is true because the variance of binomial is $\Theta(N)$ and by CLT). We choose $c = \sqrt{2}\log(4mq)q\beta^q m$ where $\beta := \sup_{\mathbf{x} \in \Delta_m} \|J(\mathbf{x})\|_1$. From Lemma 5.21 we get that with probability at least $\frac{1}{2}$ the deviation between the deterministic dynamics and the stochastic evolution after q steps is at most $\frac{\log(4mq)q\beta^q m}{\sqrt{2N}}$ (by substitute $\epsilon = \frac{\log(4mq)}{\sqrt{2N}}$ in Lemma 5.21). Hence, using Lemma 5.20 for the function $h = f^{-1}$ around $\mathbf{z}$ and $k = q$, $\mathrm{sp}\,(J-1[\mathbf{z}]) < \frac{1}{\alpha}$, after q steps we get that $\left\|f^q(\mathbf{X}^{(1)}) - \mathbf{z}\right\|_1 \geq \alpha^q \left\|\mathbf{X}^{(1)} - \mathbf{z}\right\|_1$ with probability at least $\frac{1}{2}c_1$. From Lemma 5.21 and using the facts that $\alpha^q > 5/2$ and $\left\|\mathbf{X}^{(1)} - \mathbf{z}\right\|_1 \geq 2\frac{\log(4mq)q\beta^q m}{\sqrt{2N}}$ we conclude that

$$\begin{aligned}
\left\|\mathbf{X}^{(q+1)} - \mathbf{z}\right\|_1 &\geq \left\|f^q(\mathbf{X}^{(1)}) - \mathbf{z}\right\|_1 - \frac{\log(4mq)q\beta^q m}{\sqrt{2N}} \\
&\geq \alpha^q \left\|\mathbf{X}^{(1)} - \mathbf{z}\right\|_1 - \frac{\log(4mq)q\beta^q m}{\sqrt{2N}} \geq 2\left\|\mathbf{X}^{(1)} - \mathbf{z}\right\|_1.
\end{aligned}$$

By induction, we conclude that $\left\|\mathbf{X}^{(qt+1)} - \mathbf{z}\right\|_1 \geq \frac{\log^{2/3} N}{\sqrt{N}}$ with t to be at most $2/3(\log\log N)$ with probability at least $\frac{c_1}{(\log N)^{2/3}}$. Since we have made no assumptions on the position of the chain (except the distance), it follows that after at most $c_2 (\log N)^{2/3} \cdot (\log\log N) = O(\log N)$ steps, the Markov chain has reached distance greater than $\frac{\log^{2/3} N}{\sqrt{N}}$ from the fixed point with probability $\Theta(1)$. $\qquad\square$

Distance $\Theta(1)$. Combining Lemma 5.23 with the lemma below we can show that after $O(\log N)$ number of steps, the Markov chain will have distance from an α-unstable fixed point lower bounded by a constant $\Theta(1)$ with sufficient probability.

Lemma 5.24. *Let $f : \Delta_m \to \Delta_m$ be continuously differentiable in the interior of Δ_m. Let $\mathbf{X}^{(0)}$ be the state of a stochastic evolution guided by f at time 0 and also $\mathbf{z}$ be an α-unstable fixed point of f such that $\left\|\mathbf{X}^{(0)} - \mathbf{z}\right\|_1 \geq \frac{\log^{2/3} N}{\sqrt{N}}$. Then with probability $1 - \frac{1}{poly(N)}$ we have that $\left\|\mathbf{X}^{(t)} - \mathbf{z}\right\|_1$ is $r := \Theta(1)$ after at most $O(\log N)$ steps.*

Proof. Let r be such that we can apply Lemma 5.20 for f^{-1} with fixed point $\mathbf{z}$ and parameters $\rho = \frac{1}{a}$ and q such that $a^q < \frac{1}{2}$ since $\text{sp}\left(J^{-1}(\mathbf{z})\right) < \frac{1}{a}$ and q is given from Gelfand's formula. Using Lemma 5.21 for $\epsilon = \sqrt{\frac{\gamma \log N}{N}}$ we get that $\mathbf{X}^{(1)}, \ldots, \mathbf{X}^{(q)}$ have ℓ_1 distance $\Omega\left(\frac{\log^{2/3} N}{\sqrt{N}}\right)$ from $\mathbf{z}$, with probability at least $1 - 2\frac{mq}{N^{2\gamma}}$. Then by induction for some t follows that

$$\left\|\mathbf{X}^{(t)} - \mathbf{z}\right\|_1 \geq \left\|f^q(\mathbf{X}^{(t-q)}) - \mathbf{z}\right\|_1 - q\beta^q m \sqrt{\frac{\gamma \log N}{N}}$$

$$= (1 - o_N(1)) \left\|f^q(\mathbf{X}^{(t-q)}) - \mathbf{z}\right\|_1$$

$$\geq (1 - o_N(1))\alpha^q \left\|\mathbf{X}^{(t-q)} - \mathbf{z}\right\|_1 > 2\left\|\mathbf{X}^{(t-q)}\right\|_1. \quad \text{(Lemma 5.21)}$$

Therefore, after at most $T = q \log N$ steps we get that $\left\|\mathbf{X}^{(T)} - \mathbf{z}\right\|_1 \geq r$ with probability at least $1 - \frac{2mq^2 \log N}{N^{2\gamma}}$ from union bound (and choose $\gamma = 2$). $\qquad \square$

Below we show the last technical lemma of the section. Intuitively says that given a dynamical system where the update rule is defined in the simplex, if for every initial condition, the dynamics converges to some fixed point $\mathbf{z}$, then $\mathbf{z}$ cannot be an α-unstable unless the initial condition is $\mathbf{z}$.

Lemma 5.25. *Let $f : \Delta_m \to \Delta_m$ be continuously differentiable and assume that f has $\mathbf{z}_0, \ldots, \mathbf{z}_{l+1}$ (l is finite) fixed points, where $\mathbf{z}_0$ is stable such that $\text{sp}\left(J(\mathbf{z}_0)\right) < \rho < 1$ and $\mathbf{z}_1, \ldots, \mathbf{z}_{l+1}$ are α-unstable with $\alpha > 1$. Assume also that $\lim_{q \to \infty} f^q(\mathbf{x})$ exists for all $\mathbf{x} \in \Delta_m$ (and it is some fixed point). Let $B = \cup_{i=1}^l B(\mathbf{z}_i, r_i)$, where $B(\mathbf{z}_i, r_i)$ denotes the open ball of radius r_i around $\mathbf{z}_i$ and set $\Delta = \Delta_m - B$. Then for every ϵ, there exists a t such that*

$$\left\|f^t(\mathbf{x}) - \mathbf{z}_0\right\|_1 < \epsilon$$

for all $\mathbf{x} \in \Delta$.

Proof. If Δ is empty, then it holds trivially. By assumption we have that for all $\mathbf{x} \in \Delta$, $\lim_{q \to \infty} f^q(\mathbf{x}) = \mathbf{z}_i$ for some $i = 0, \ldots, l+1$. Let $\mathbf{z}$ be an α-unstable fixed point. We claim that the if $\lim_{t \to \infty} f^t(\mathbf{x}) = \mathbf{z}$ then $\mathbf{x} = \mathbf{z}$. Let us prove this claim.

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Assume $\mathbf{x}_0 \in \Delta$ and that $\mathbf{x}_0$ is not a fixed point. By assumption $\lim_{q\to\infty} f^q(\mathbf{x}_0) = \mathbf{z}_i$ for some $i > 0$, hence for every $\delta > 0$, there exists a q_0 such that for $q \geq q_0$ we get that $\|f^q(\mathbf{x}_0) - \mathbf{z}_i\|_1 \leq \delta$. We choose some k such that $\mathrm{sp}\left((J^{-1}(\mathbf{z}_i))^k\right) < \frac{1}{\alpha^k}$ and we consider an ϵ such that Theorem 5.20 holds for function f^{-1} and k. We pick $\delta = \frac{\min(\epsilon, r_i)}{2}$ and assume a q_0 such that by convergence assumption $\|f^q(\mathbf{x}_0) - \mathbf{z}_i\|_1 \leq \delta$ for $q \geq q_0$. Hence Theorem 5.20 holds for the trajectory $(f^{t+q_0}(\mathbf{x}_0))_{t\in\mathbb{N}}$. Set $s = \|f^{q_0}(\mathbf{x}_0) - \mathbf{z}_i\|_1$ and observe that for $t = q_0 + k\left\lceil \frac{\log_\alpha \frac{2\delta}{s}}{k} \right\rceil$ it holds that $\|f^t(\mathbf{x}_0) - \mathbf{z}_i\|_1 \geq a^{t-q_0} \|f^{q_0}(\mathbf{x}_0) - \mathbf{z}\|_1 \geq 2\delta$ (due to Lemma 5.20), *i.e.,* we reached a contradiction. Hence $\lim_{t\to\infty} f^t(\mathbf{x}) = \mathbf{z}_0$ for all $\mathbf{x} \in \Delta$. The rest follows from Lemma 5.26 which is stated below. $\qquad\square$

Lemma 5.26. *Let $S \subset \Delta_m$ be compact and assume that $\lim_{t\to\infty} f^t(\mathbf{x}) = \mathbf{z}$ for all $\mathbf{x} \in S$. Then for every ϵ, there exists a q such that*

$$\|f^q(\mathbf{x}) - \mathbf{z}\|_1 < \epsilon$$

for all $\mathbf{x} \in S$.

Proof. Because of the convergence assumption, for every $\epsilon > 0$ and every $x \in S$, there exists an $d = d_x$ (depends on $\mathbf{x}$) such that

$$\left\|f^d(\mathbf{x}) - \mathbf{z}\right\|_1 < \epsilon.$$

Define the sets $A_i = \{\mathbf{y} \in S \mid \|f^i(\mathbf{y}) - \mathbf{z}\|_1 < \epsilon\}$ for each positive integer i. Then, since f^i is continuous, the sets A_i are open in S, and therefore, by the above condition, form an open cover of S (since every $\mathbf{y}$ must lie in some A_i). By compactness, some finite collection of them must therefore cover S, and hence by taking q to be the maximum of the indices of the sets in this finite collection the lemma follows. $\qquad\square$

We are now able to prove the main theorem of the section, *i.e.,* Theorem 5.8.

Proof of Theorem 5.8. Consider $r_1, \ldots, r_l$ as can occur from Lemma 5.23 and assume without loss of generality that the open balls $B(\mathbf{z}_i, r_i)$ for $i = 1, \ldots, l$, with center $\mathbf{z}_i$ and radius r_i (in ℓ_1 distance) are disjoint sets and that $\Delta := \Delta_m \setminus \cup_{i=1}^l B(\mathbf{z}_i, r_i)$ is not empty (otherwise we could decrease r_i's since they remain constants and Lemma 5.23 would still hold). We consider two chains $\mathbf{X}^{(0)}, \mathbf{Y}^{(0)}$. We claim that with probability $\Theta(1)$ (which can be boosted to any constant) each chain reaches within $\frac{1}{N^w}$ distance of the stable fixed point $\mathbf{z}_0$ for some $w > 0$, after at most $T = O(\log N)$ steps. Then the coupling constructed to prove 5.7 works because it uses the smoothness of f and the stability of the fixed point, as long as the two chains are within $\frac{1}{N^w}$ for some $w > 0$ distance of $\mathbf{z}_0$. Due to the coupling, as the two chains reach within $\frac{1}{N^w}$ distance of $\mathbf{z}_0$, they collide after $O(\log N)$ steps (with probability $\Theta(1)$ which also can be boosted to any constant) and hence the mixing time will be $O(\log N)$. To prove the claim, we first use Lemmas 5.24 and 5.23. It occurs that with probability say $\Theta(1)$ after at most $O(\log^{2/3} N \log \log N) + O(\log N)$ steps, each chain will have reached the compact set Δ. Moreover, from Lemma 5.28 we have that for all $\mathbf{x} \in \Delta$, $f^t(\mathbf{x})$ converges to fixed point $\mathbf{z}_0$ exponentially fast. Hence, using claim (58) (by choosing $\mathbf{z}_0, \rho, \Delta$ same as in the proof of Theorem 5.8 and r from Lemma 5.28) follows that after $O(\log N)$ steps, each chain that started in Δ comes within $\frac{1}{N^w}$ distance of $\mathbf{z}_0$ with sufficiently enough probability. $\square$

5.6.2 Multiple stable fixed points and limit cycles

Staying close to fixed point. We prove the main lemma of this section, then our second result will be a corollary. The main lemma states that as long as the Markov chain starts from a neighborhood of one stable fixed point, it takes at least exponential time to get away from that neighborhood with probability say $\frac{9}{10}$.

Lemma 5.27. *Let $f : \Delta_m \to \Delta_m$ be continuously differentiable in the interior of Δ_m with stable fixed points $\mathbf{z}_1, \ldots, \mathbf{z}_l$ and k (independent of N) be such that $\left\| J(\mathbf{z}_i)^k \right\|_1 <$*

$\rho_i^k < 1$ for all $i = 1, \ldots, l$. Let $\mathbf{X}^{(0)}$ be the state of a stochastic evolution guided by f at time 0. There exists a small constant ϵ_i (independent of N) such that given that $\mathbf{X}^{(0)}$ satisfies $\left\|\mathbf{X}^{(0)} - \mathbf{z}_i\right\|_1 \leq m\epsilon_i$ for some stable fixed point $\mathbf{z}_i$, after $t = \frac{e^{2\epsilon_i^2 N}}{20mk}$ steps it holds that $\left\|\mathbf{X}^{(t)} - \mathbf{z}_i\right\|_1 \leq \frac{(k+1)\beta^k \epsilon_i m}{1-\rho_i}$ with probability at least $\frac{9}{10}$.

Proof. ϵ_i will be chosen later. By Lemma 5.21 it follows that

$$\left\|\mathbf{X}^{(t)} - \mathbf{z}\right\|_1 \leq \left\|f^t(\mathbf{X}^{(0)}) - \mathbf{z}\right\|_1 + t\beta^t \epsilon_i m$$

with probability at least $1 - 2m \cdot ke^{-2\epsilon_i^2 N}$ for $t = 1, \ldots, k$. Since $\left\|f^t(\mathbf{X}^{(0)}) - \mathbf{z}\right\|_1 \leq \beta^t \left\|\mathbf{X}^{(0)} - \mathbf{z}\right\|_1$, it follows that $\left\|\mathbf{X}^{(t)} - \mathbf{z}\right\|_1 \leq (t+1)\beta^t \epsilon_i m$ with probability at least $1 - 2m \cdot ke^{-2\epsilon_i^2 N}$ for $t = 1, \ldots, k-1$. Assume that $\left\|\mathbf{X}^{(t)} - \mathbf{z}\right\|_1 \leq (t+1)\beta^t \epsilon_i m$ is true for $t = 1, \ldots, k-1$. We choose ϵ_i small enough constant such that Lemma 5.20 holds with $\epsilon = \frac{(k+1)\beta^k \epsilon_i m}{1-\rho_i}$. To prove the lemma, we use induction on t and show that $\left\|\mathbf{X}^{(t)} - \mathbf{z}_i\right\|_1 \leq \left((k+1)\beta^k \epsilon_i m\right) \cdot \left(\sum_{j=0}^t \rho_i^j\right) < \frac{\left((k+1)\beta^k \epsilon_i m\right)}{1-\rho_i} < \epsilon$ and hence Lemma 5.20 will hold. For $t = k$ we have that

$$\left\|\mathbf{X}^{(k)} - \mathbf{z}_i\right\|_1 \leq \left\|f^k(\mathbf{X}^{(0)}) - \mathbf{z}_i\right\|_1 + \left\|f^k(\mathbf{X}^{(0)}) - \mathbf{X}^{(k)}\right\|_1 \quad \text{(triangle inequality)}$$

$$\leq \rho_i^k \left\|\mathbf{X}^{(0)} - \mathbf{z}_i\right\|_1 + k\beta^k \epsilon_i m \quad \text{(Lemma 5.20 and Lemma 5.21)}$$

$$< (1 + \rho_i^k)(k+1)\beta^k \epsilon_i m < (\sum_{j=0}^k \rho_i^j)(k+1)\beta^k \epsilon_i m.$$

Let $t' = t - k$, be a time index. We do the same trick as for the base case and we get that

$$\left\|\mathbf{X}^{(t)} - \mathbf{z}_i\right\|_1 \leq \left\|f^k(\mathbf{X}^{(t')}) - \mathbf{z}_i\right\|_1 + \left\|f^k(\mathbf{X}^{(t')}) - \mathbf{X}^{(t)}\right\|_1$$

$$\leq \rho_i^k \left\|\mathbf{X}^{(t')} - \mathbf{z}\right\|_1 + k\beta^k \epsilon_i m$$

$$\leq \rho_i^k \left((k+1)\beta^k \epsilon_i m\right) \cdot \left(\sum_{j=0}^{t'} \rho_i^j\right) + (k+1)\beta^k \epsilon_i m \quad \text{(induction)}$$

$$= \left((k+1)\beta^k \epsilon_i m\right) \cdot \left(1 + \sum_{j=k}^t \rho_i^j\right) < \left((k+1)\beta^k \epsilon_i m\right) \cdot \left(\sum_{j=0}^t \rho_i^j\right).$$

The error probability, *i.e.*, at least one of the steps above fails and the chain gets larger noise than $k\beta^k\epsilon_1 m$, by union bound will be at most $\frac{e^{2\epsilon_i^2 N}}{20mk} \cdot 2mk \cdot e^{-2\epsilon_i^2 N} = \frac{1}{10}$ (by Lemma 5.21). $\qquad\square$

We can now prove Theorem 5.9 which follows as a corollary from Lemma 5.27.

Proof of Theorem 5.9. Two stable fixed points suffice; let $\mathbf{z}_1, \mathbf{z}_2$. Consider the ϵ_i's from the previous lemma (Lemma 5.27) and set $S_i = \{\mathbf{x} : \|\mathbf{x} - \mathbf{z}_i\|_1 \leq \frac{(k+1)\beta^k\epsilon_i m}{1-\rho_i}\}$ for $i = 1, 2$ where $\beta := \sup_{\mathbf{x}\in\Delta_m}\|J(\mathbf{x})\|_1$. We can choose ϵ_1, ϵ_2 so small such that $S_1 \cap S_2 = \varnothing$ (by continuity). Let μ be the stationary distribution. Set $S = S_1, T = \frac{e^{2\epsilon_1^2 N}}{20mk}$ and $\mathbf{y} = \mathbf{z}_1$ if $\mu(S_1) \leq \frac{1}{2}$, otherwise set $S = S_2, T = \frac{e^{2\epsilon_2^2 N}}{20mk}$ and $\mathbf{y} = \mathbf{z}_2$. Assume $\|X^{(0)} - \mathbf{y}\|_1 \leq \epsilon m$. Therefore from Lemma 5.27 we get that $\mathbb{P}\left[X^{(T)} \in \bar{S}\right] \leq \frac{1}{10}$. and also by assumption $\mu(\bar{S}) \geq \frac{1}{2}$. Let $\nu^{(T)}$ be the distribution of $X^{(T)}$. However

$$\left\|\mu, \nu^{(T)}\right\|_{\text{TV}} \geq \left|\mu(\bar{S}) - \mathbb{P}\left[X^{(T)} \in \bar{S}\right]\right| > \frac{1}{4}$$

and the result follows, *i.e.*, $t_{mix}(1/4)$ is $e^{\Omega(N)}$. $\qquad\square$

Stable limit cycle. This part technically is small, because it depends on the previous section. We denote by $\mathbf{w}_1, \ldots, \mathbf{w}_s$ $(s \geq 2)$ the points in the stable limit cycle. Again we assume that $\mathbf{w}_i$'s are *well separated*.

Proof of Theorem 5.10. Let $h(\mathbf{x}) = f^s(\mathbf{x})$. It is clear to see that the Markov chain guided by h satisfies the assumptions of 5.9. The fixed points of h are just the points in the limit cycle, *i.e.*, $\mathbf{w}_1, \ldots, \mathbf{w}_s$. Additionally, it easy to see (via chain rule) that $J_{f^s}(\mathbf{w}_i) = J_{f^{s-1}}(f(\mathbf{w}_i))J(\mathbf{w}_i) = J_{f^{s-1}}(\mathbf{w}_{i+1})J(\mathbf{w}_i)$, where we denote by J_{f^i} the Jacobian of function $f^i(\mathbf{x})$ and $\mathbf{w}_{l+1} = \mathbf{w}_1$. Therefore

$$J_h(\mathbf{w}_i) = \prod_{j=1}^{i-1} J(\mathbf{w}_{i-j}) \prod_{j=i}^{s} J(\mathbf{w}_{s+i-j}).$$

Matrices don't commute in general but it is true that AB, BA have the same eigenvalues hence $\text{sp}\,(J_h(\mathbf{w}_i)) < \rho$ is the same for all $i = 1, \ldots, s$. Finally, let k be such that

$\left\|J_{f^s}(\mathbf{w}_i)^k\right\|_1 < \rho^k$ (using Gelfand's formula 5.1). For each $\mathbf{w}_i$ consider ϵ_i as in the proof of 5.27, for function h and upper bound ρ on the spectral radius of $J_{f^s}(w_i)$. Then analogously for $t = \frac{e^{2\epsilon_i^2 N}}{20mk\cdot s}$ with probability at least $\frac{9}{10}$ we have $\left\|\mathbf{X}^{(t)} - \mathbf{w}_i\right\|_1 \leq \frac{(k+1)\beta^k \epsilon_i m}{1-\rho}$ and the proof for $e^{\Omega(N)}$ mixing comes from Theorem 5.9. $\qquad\square$

5.6.3 Proofs omitted from Section 5.6

Lemma 5.28 (**Exponential convergence II**). *Choose $\mathbf{z}_0, \rho, \Delta$ as in the proof of Theorem 5.8, and set $\beta := \sup_{\mathbf{x} \in \Delta_m} \|J[\mathbf{x}]\|_1$. Then there exist a positive r such that for every $\mathbf{x} \in \Delta$, and every positive integer t,*

$$\left\|f^t(\mathbf{x}) - \mathbf{z}_0\right\|_1 \leq r\rho^t.$$

Proof. This is almost identical to the proof of Lemma 5.18. Let ϵ and k be as defined in 5.20. From Lemma 5.25, we know that there exists an ℓ such that for all $\mathbf{x} \in \Delta$,

$$\left\|f^\ell(\mathbf{x}) - \mathbf{z}_0\right\|_1 \leq \frac{\epsilon}{\beta^k}. \tag{69}$$

Note that this implies that $f^{\ell+i}(\mathbf{x})$ is within distance ϵ of $\mathbf{z}_0$ for $i = 0, 1, \ldots, k$, so that 5.20 can be applied to the sequence of vectors $f^\ell(\mathbf{x}), f^{\ell+1}(\mathbf{x}), \ldots, f^{\ell+k}(\mathbf{x})$ and $\mathbf{z}_0$. Thus, we get

$$\left\|f^{\ell+k}(\mathbf{x}) - \mathbf{z}_0\right\|_1 \leq \rho^k \left\|f^\ell(\mathbf{x}) - \mathbf{z}_0\right\|_1 \leq \frac{\rho^k \epsilon}{\beta^k}.$$

Since $\rho < 1$, we can iterate this process. Using also the fact that the $1 \to 1$ norm of the Jacobian of f is at most β (which we can assume without loss of generality to be at least 1), we therefore get for every $\mathbf{x} \in \Delta$, and every $i \geq 0$ and $0 \leq j < k$

$$\left\|f^{\ell+ik+j}(\mathbf{x}) - \mathbf{z}_0\right\|_1 \leq \rho^{ki+j} \frac{\beta^j}{\rho^j} \left\|f^\ell(\mathbf{x}) - \mathbf{z}_0\right\|_1$$

$$\leq \rho^{ki+j+\ell} \frac{\beta^{j+\ell}}{\rho^{j+\ell}} \left\|\mathbf{x} - \mathbf{z}_0\right\|_1 \leq \rho^{ki+j+\ell} \frac{\beta^{k+\ell}}{\rho^{k+\ell}} \left\|\mathbf{x} - \mathbf{z}_0\right\|_1$$

where in the last line we use the facts that $\beta > 1$, $\rho < 1$ and $j < k$. Noting that any $t \geq \ell$ is of the form $\ell + ki + j$ for some i and j as above, we have shown that for every

$t \geq \ell$ and every $\mathbf{x} \in \Delta$

$$\left\| f^t(\mathbf{x}) - \mathbf{z}_0 \right\|_1 \leq \left(\frac{\beta}{\rho} \right)^{k+\ell} \rho^t \left\| \mathbf{x} - \mathbf{z}_0 \right\|_1 . \tag{70}$$

Similarly, for $t < \ell$, we have, for any $\mathbf{z} \in \Delta$

$$\left\| f^t(\mathbf{x}) - \mathbf{z}_0 \right\|_1 \leq \beta^t \left\| \mathbf{x} - \mathbf{z}_0 \right\|_1$$
$$\leq \left(\frac{\beta}{\rho} \right)^t \rho^t \left\| \mathbf{x} - \mathbf{z}_0 \right\|_1 \leq \left(\frac{\beta}{\rho} \right)^\ell \rho^t \left\| \mathbf{x} - \mathbf{z}_0 \right\|_1 , \tag{71}$$

where in the last line we have again used $\beta > 1, \rho < 1$ and $t < \ell$. From (71), (70), we get the claimed result with $r := \left(\frac{\beta}{\rho} \right)^{k+\ell}$. $\qquad \square$

5.7 Models of Evolution and Mixing times

5.7.1 Eigen's model (RSM)

An individual of type i has a *fitness* (that translates to the ability to reproduce) which is specified by a positive integer a_i, and captured as a whole by a diagonal $m \times m$ matrix A whose (i,i)th entry is a_i. The reproduction is error-prone and this is captured by an $m \times m$ stochastic matrix Q whose (i,j)th entry captures the probability that the jth type will mutate to the ith type during reproduction.[7] The population is assumed to be infinite and its evolution deterministic. The population is assumed to be *unstructured*, meaning that only the type of each member of the population matters and, thus, it is sufficient to track the fraction of each type. One can then track the fraction of each type at step t of the evolution by a vector $\mathbf{x}^{(t)} \in \Delta_m$ (the probability simplex of dimension m) whose evolution is then governed by the difference equation $\mathbf{x}^{(t+1)} = \frac{QA\mathbf{x}^{(t)}}{\|QA\mathbf{x}^{(t)}\|_1}$. Of interest is the steady state[8] or the limiting distribution of this process and how it changes as one changes the evolutionary parameters Q and A. This model was proposed in the pioneering work of Eigen and co-authors [43, 45]. One stochastic version of this dynamics, motivated by the Wright-Fisher model in

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[7]We follow the convention that a matrix if stochastic if its *columns* sum up to 1.
[8]Note that there is a unique steady state, called the *quasispecies*, when $QA > 0$.

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population genetics, was studied by Dixit *et al.* [39]. Here, the population is again assumed to be unstructured and fixed to a size N. Thus, after normalization, the composition of the population is captured by a random point in Δ_m; say $\mathbf{X}^{(t)}$ at time t. In the replication (R) stage, one first replaces an individual of type i in the current population by a_i individuals of type i: the total number of individuals of type i in the intermediate population is therefore $a_i N X_i^{(t)}$. In the selection (S) stage, the population is culled back to size N by sampling with replacement N individuals from this intermediate population. In analogy with the Wright-Fisher model, we assume that the N individuals are sampled with replacement.[9] Finally, since the evolution is error prone, in the mutation (M) stage, one then mutates each individual in this intermediate population independently and stochastically according to the matrix Q. The vector $\mathbf{X}^{(t+1)}$ then is the normalized frequency vector of the resulting population. In the next section we show a rapid mixing result for RSM (Theorem 5.11).

5.7.2 Mixing time for Eigen model

We first show that the Eigen or RSM model discussed in Section 5.7.2 is a special case of the abstract model defined in the last section, and hence satisfies the mixing time bound in Theorem 5.7. Our first step is to show that the RSM model can be seen as a stochastic evolution guided by the function f defined by $f(\mathbf{p}) = \frac{(QA\mathbf{p})_t}{\|QA\mathbf{p}\|_1}$, where Q and A are matrices with positive entries, with Q stochastic (*i.e.,* columns summing up to 1), as described in the introduction. We will then show that this f is a smooth contractive evolution, which implies that Theorem 5.7 applies to the RSM process.

We begin by recalling the definition of the RSM process. Given a starting population of size N on m types represented by a $1/N$-integral probability vector $\mathbf{p} =$

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[9]Culling via sampling without replacement was considered in [39], but the Wright-Fisher inspired sampling with replacement is the natural model for culling in the more general setting that we consider in this chapter.

$(p_1, p_2, \ldots, p_m)$, the RSM process produces the population at the next step by independently sampling N times from the following process:

1. Sample a type T from the probability distribution $\frac{A\mathbf{p}}{\|A\mathbf{p}\|_1}$.

2. Mutate T to the result type S with probability Q_{ST}.

We now show that sampling from this process is exactly the same as sampling from the multinomial distribution $f(\mathbf{p}) = \frac{QA\mathbf{p}}{\|QA\mathbf{p}\|_1}$. To do this, we only need to establish the following claim:

Claim 5.29. *For any type $t \in [m]$, $\mathbb{P}\left[S = t\right] = \frac{\sum_j Q_{tj} A_{jj} p_j}{\sum_j A_{jj} p_j} = \frac{(QA\mathbf{p})_t}{\|QA\mathbf{p}\|_1}$.*

Proof. We first note that $\|QA\mathbf{p}\|_1 = \sum_{ij} Q_{ij} A_{jj} p_j = (\sum_i Q_{ij}) \cdot (\sum_j A_{jj} p_j) = \sum_j A_{jj} p_j = \|A\mathbf{p}\|_1$, where in the last equality we used the fact that the columns of Q sum up to 1. Now, we have

$$\mathbb{P}\left[S = t\right] := \sum_i^m Q_{ti} \cdot \frac{(A\mathbf{p})_i}{\|A\mathbf{p}\|_1} = \frac{\sum_{i=1} Q_{ti} A_{ii} p_i}{\sum_j A_{jj} p_j} = \frac{(QA\mathbf{p})_t}{\|QA\mathbf{p}\|_1}. \qquad \square$$

From 5.29, we see that producing N independent samples from the process described above (which corresponds exactly to the RSM model) produces the same distribution as producing N independent samples from the distribution $\frac{(QA\mathbf{p})}{\|QA\mathbf{p}\|_1}$. Thus, the RSM process is a stochastic evolution guided by $f(\mathbf{x}) := \frac{QA\mathbf{x}}{\|QA\mathbf{x}\|_1}$. We now proceed to verify that this f is a smooth contractive evolution. We first note that the "smoothness" condition is directly implied by the definition of f. For the "uniqueness of fixed point" condition, we observe that every fixed point of $\frac{QA\mathbf{x}}{\|QA\mathbf{x}\|_1}$ in the simplex Δ_m must be an eigenvector of QA. Since QA is a matrix with positive entries, the Perron-Frobenius theorem implies that it has a unique positive eigenvector $\mathbf{v}$ (for which we can assume without loss of generality that $\|\mathbf{v}\|_1 = 1$) with a positive eigenvalue λ_1. Therefore $f(\mathbf{x})$ has a unique fixed point $\tau = \mathbf{v}$ in the simplex Δ_m which is in its interior. The Perron-Frobenius theorem also implies that for every $\mathbf{x} \in \Delta_m$, $\lim_{t \to \infty} (QA)^t \mathbf{x} / \lambda_1^t \to \mathbf{v}$. In fact, this convergence can be made uniform

over Δ_m (meaning that given an $\epsilon > 0$ we can choose t_0 such that for all $t > t_0$, $\|(QA)^t\mathbf{x}/\lambda_1^t - \mathbf{v}\|_1 < \epsilon$ for all $\mathbf{x} \in \Delta_m$) since each point $\mathbf{x} \in \Delta_m$ is a convex combination of the extreme points of Δ_m and the left hand side is a linear function of $\mathbf{x}$. From this uniform convergence, it then follows easily that $\lim_{t\to\infty} f^t(\mathbf{x}) = \mathbf{v}$, and that the convergence in this limit is also uniform. The "convergence to fixed point" condition follows directly from this observation.

Finally, we need to establish that the spectral radius of the Jacobian $J := J(\mathbf{v})$ of f at its fixed point is less than 1. A simple computation shows that the Jacobian at $\mathbf{v}$ is $J = \frac{1}{\lambda_1}(I - V)QA$ where V is the matrix each of whose columns is the vector $\mathbf{v}$. Since QA has positive entries, we know from the Perron-Frobenius theorem that λ_1 as defined above is real, positive, and strictly larger in magnitude than any other eigenvalue of QA. Let $\lambda_2, \lambda_3, \ldots, \lambda_m$ be the other, possibly complex, eigenvalues arranged in decreasing order of magnitude (so that $\lambda_1 > |\lambda_2|$). We now establish the following claim from which it immediately follows that $\mathrm{sp}\,(J) = \frac{|\lambda_2|}{\lambda_1} < 1$ as required.

Claim 5.30. *The eigenvalues of $M := (I - V)QA$ are $\lambda_2, \lambda_3, \ldots, \lambda_m, 0$.*

Proof. Let D be the Jordan canonical form of QA, so that $D = U^{-1}QAU$ for some invertible matrix U. Note that D is an upper triangular matrix with $\lambda_1, \lambda_2, \ldots, \lambda_m$ on the diagonal. Further, the Perron-Frobenius theorem applied to QA implies that λ_1 is an eigenvalue of both algebraic and geometric multiplicity 1, so that we can assume that the topmost Jordan block in D is of size 1 and is equal to λ_1. Further, we can assume the corresponding first column of U is equal to the corresponding positive eigenvector $\mathbf{v}$ satisfying $\|\mathbf{v}\|_1 = 1$. It therefore follows that $U^{-1}V = U^{-1}\mathbf{v}\mathbf{1}^T$ is the matrix $\mathbf{e}_1\mathbf{1}^T$, where $\mathbf{e}_1$ is the first standard basis vector.

Now, since U is invertible, M has the same eigenvalues as $U^{-1}MU = (U^{-1} - U^{-1}V)QAU = (I - \mathbf{e}_1\mathbf{1}^TU)D$, where in the last line we use $UD = QAU$. Now, note that all rows except the first of the matrix $\mathbf{e}_1\mathbf{1}^TU$ are zero, and its $(1,1)$ entry is 1 since the first column of U is $\mathbf{v}$, which in turn is chosen so that $\mathbf{1}^T\mathbf{v} = 1$. Thus, we

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get that $(I - \mathbf{e}_1 \mathbf{1}^T U)D$ is an upper triangular matrix with the same diagonal entries as D except that its $(1, 1)$ entry is 0. Since the $(1, 1)$ entry of D was λ_1 while its other diagonal entries were $\lambda_2, \lambda_3, \ldots, \lambda_m$, it follows that the eigenvalues of $(I - \mathbf{e}_1 \mathbf{1}^T U)D$ (and hence those of M) are $\lambda_2, \lambda_3, \ldots, \lambda_m, 0$, as claimed. $\qquad \square$

We thus see that the RSM process satisfies the condition of being guided by a smooth contractive evolution and hence has the mixing time implied by Theorem 5.7.

5.7.3 Dynamics of grammar acquisition and sexual evolution

We begin by describing the evolutionary processes for grammar acquisition and sexual evolution. As we will explain, the two turn out to be identical and hence we primarily focus on the model for grammar acquisition in the remainder of the section.

The starting point of the model is Chomsky's *Universal Grammar* theory [27].[10] In his theory, language learning *is facilitated by a predisposition that our brains have for certain structures of language.* This universal grammar (UG) is believed to be innate and embedded in the neuronal circuitry. Based on this theory, an influential model for how children acquire grammar was given by appealing to evolutionary dynamics for infinite and finite populations respectively in [101] and [71]. We first describe the infinite population model, which is a dynamical system that guides the stochastic, finite population model. Each individual speaks exactly one of the m grammars from the set of inherited UGs $\{G_1, \ldots, G_m\}$; denote by x_i the fraction of the population using G_i. The model associates a *fitness* to every individual on the basis of the grammar she *and others* use. Let A_{ij} be the probability that a person who speaks grammar j understands a randomly chosen sentence spoken by an individual using grammar i. This can be viewed as the fraction of sentences according to grammar i that are also valid according to grammar j. Clearly, $A_{ii} =$

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[10]Like any important problem in the sciences, Chomsky's theory is not uncontroversial; see [52] for an in-depth discussion.

1. The pairwise *compatibility* between two individuals speaking grammars i and j is $B_{ij} := \frac{A_{ij}+A_{ji}}{2}$, and the fitness of an individual using G_i is $f_i := \sum_{j=1}^{m} x_j B_{ij}$, *i.e.,* the probability that such an individual is able to meaningfully communicate with a randomly selected member of the population.

In the reproduction phase each individual produces a number of offsprings proportional to her fitness. Each child speaks one grammar, but the exact learning model can vary and allows for the child to incorrectly learn the grammar of her parent. We define the matrix Q where the entry Q_{ij} denotes the probability that the child of an individual using grammar i learns grammar j (*i.e., Q* is column stochastic matrix); once a child learns a grammar it is fixed and she does not later use a different grammar. Thus, the frequency x_i' of the individuals that use grammar G_i in the next generation will be

$$x_i' = g_i(\mathbf{x}) := \sum_{j=1}^{m} \frac{Q_{ji} x_j (B\mathbf{x})_j}{\mathbf{x}^\top B \mathbf{x}}$$

(with $g : \Delta_m \mapsto \Delta_m$ encoding the update rule). Nowak *et al.* [101] study the symmetric case, *i.e.,* $B_{ij} = b$ and $Q_{ij} = \tau \in (0, 1/m]$ for all $i \neq j$ and observe a threshold: When τ, which can be thought of as quantifying the *error of learning or mutation,* is above a critical value, the only stable fixed point is the uniform distribution (all $1/m$) and below it, there are multiple stable fixed points.

Finite population models can be derived from the grammar acquisition dynamics in a standard way. We describe the Wright-Fisher finite population model for the grammar acquisition dynamics. The population size remains N at all times and the generations are non-overlapping. The current state of the population is described by the frequency vector $\mathbf{X}^{(t)}$ at time t which is a random vector in Δ_m and notice also that the population that uses G_i is $N X_i^{(t)}$. In the replication (R) stage, one first replaces the individuals that speak grammar G_i in the current population by

$NX_i^{(t)}(B(N\mathbf{X}^{(t)}))_i$ and the total population has size $N^2\mathbf{X}^{(t)\top}B\mathbf{X}^{(t)}$.[11] In the selection (S) stage, one selects N individuals from this population by sampling independently with replacement. Since the evolution is error prone, in the mutation (M) stage, the grammar of each individual in this intermediate population is mutated independently at random according to the matrix Q to obtain frequency vector $\mathbf{X}^{(t+1)}$. Given these rules, note that

$$\mathbb{E}[\mathbf{X}^{(t+1)}|\mathbf{X}^{(t)}] = g(\mathbf{X}^{(t)}).$$

In other words, in expectation, fixing $\mathbf{X}^{(t)}$, the next generation's frequency vector $\mathbf{X}^{(t+1)}$ is exactly $g(\mathbf{X}^{(t)})$, where g is the grammar acquisition dynamics. Of course, this holds only for one step of the process. This process is a Markov chain with state space $\{(y_1, \ldots, y_m) : y_i \in \mathbb{N}, \sum_i y_i = N\}$ of size $\binom{N+m-1}{m-1}$. If $Q > 0$ then it is ergodic (*i.e.,* it is irreducible and aperiodic) and thus has a unique stationary distribution. In our analysis, we consider the symmetric case as in Nowak *et al.* [101], *i.e.,* $B_{ij} = b$ and $Q_{ij} = \tau \in (0, 1/m]$ for all $i \neq j$.

Note that the grammar acquisition model described above can also be seen as a (finite population) sexual evolution model: Assume there are N individuals and m types. Let $\mathbf{Y}^{(t)}$ be a vector of frequencies at time t, where $\mathbf{Y}_i^{(t)}$ denotes the fraction of individuals of type i. Let F be a fitness matrix where F_{ij} corresponds to the number of offspring of type i, if an individual of type i chooses to mate with an individual of type j (assume $F_{ij} \in \mathbb{N}$). At every generation, each individual mates with every other individual. It is not hard to show that the number of offspring after the matings will be $N^2(\mathbf{Y}^{(t)\top}F\mathbf{Y}^{(t)})$ and there will be $N^2\mathbf{Y}_i^{(t)}(F\mathbf{Y}^{(t)})_i$ individuals of type i. After the reproduction step, we select N individuals at random with replacement, *i.e.,* we sample an individual of type i with probability $\frac{\mathbf{Y}_i^{(t)}(F\mathbf{Y}^{(t)})_i}{\mathbf{Y}^{(t)\top}F\mathbf{Y}^{(t)}}$. Finally in the mutation step, every individual of type i mutates with probability τ (*mutation parameter*) to

---

[11]Here we assume that B_{ij} is an positive integer and thus $N^2X_i^{(t)}(B\mathbf{X}^{(t)})_i$ is an integer since the individuals are whole entities; this can be achieved by scaling and is without loss of generality.

some type j. Let $F_{ii} = A$, $F_{ij} = B$ for all $i \neq j$ with $A > B$ (this is called homozygote advantage) and set $b = \frac{B}{A} < 1$. It is self-evident that this sexual evolution model is identical with the (finite population) grammar acquisition model described above since both end up having the same reproduction, selection and mutation rule. It holds that $E[\mathbf{X}^{(t+1)}|\mathbf{X}^{(t)}] = g(\mathbf{X}^t)^{12}$ with

$$g_i(\mathbf{x}) = (1 - (m-1)\tau)\frac{N^2 x_i(B\mathbf{x})_i}{N^2(\mathbf{x}^\top B\mathbf{x})} + \sum_{j \neq i} \tau \frac{N^2 x_j(B\mathbf{x})_j}{N^2(\mathbf{x}^T B\mathbf{x})} = (1 - m\tau)\frac{x_i(B\mathbf{x})_i}{(\mathbf{x}^\top B\mathbf{x})} + \tau$$

where $B_{ii} = 1, B_{ij} = b$ with $i \neq j$.[13] For the aforementioned Markov chains (symmetric case), we prove Theorem 5.12 in the next section.

5.7.4 Mixing time for grammar acquisition and sexual evolution

Sampling from distribution $g(\mathbf{x})$. In this section, we prove that the finite population grammar acquisition model discussed in preliminaries can be seen as a stochastic evolution guided by the function g defined by $g(\mathbf{x}) = (1 - m\tau)\frac{x_i(B\mathbf{x})_i}{\mathbf{x}^\top B\mathbf{x}} + \tau$ (we assume that we have m grammars and $g : \Delta_m \to \Delta_m$, see Definition 19 to check what a stochastic evolution guided by a function is). Given a starting population of size N on m types represented by a $1/N$-integral probability vector $\mathbf{x} = (x_1, x_2, \ldots, x_m)$ we consider the following process P1:

1. Reproduction, *i.e.*, the number of individuals that use grammar G_i becomes $N^2 x_i(B\mathbf{x})_i$ and the total number is $N^2 \mathbf{x}^\top B\mathbf{x}$.

2. Each individual that uses grammar S can end up using grammar T with probability Q_{ST}.

We now show that sampling from P1 is exactly the same as sampling from the multinomial distribution $g(\mathbf{x})$. Taking one sample (individual) we compute the probability to use grammar t.

---

[12]We use same notation for the update rule as before, *i.e.*, g because it turns out to be the same function.

[13]Observe that this rule is invariant under scaling of fitness matrix B.

Claim 5.31. $\mathbb{P}\left[type\ t\right] = \frac{N^2 \sum_j Q_{jt} x_j (B\mathbf{x})_j}{N^2 \mathbf{x}^\top B\mathbf{x}} = (1 - m\tau) \frac{x_t (B\mathbf{x})_t}{\mathbf{x}^\top B\mathbf{x}} + \tau.$

Proof. We have

$$
\begin{aligned}
\mathbb{P}\left[type\ t\right] &:= \sum_{i=1}^{m} Q_{it} \cdot \frac{x_i (B\mathbf{x})_i}{\mathbf{x}^\top B\mathbf{x}} \\
&= (1 - m\tau) \frac{x_t (B\mathbf{x})_t}{\mathbf{x}^\top B\mathbf{x}} + \tau \frac{x_t (B\mathbf{x})_t}{\mathbf{x}^\top B\mathbf{x}} + \tau \sum_{i \neq t} \frac{x_i (B\mathbf{x})_i}{\mathbf{x}^\top B\mathbf{x}} \\
&= (1 - m\tau) \frac{x_t (B\mathbf{x})_t}{\mathbf{x}^\top B\mathbf{x}} + \tau \frac{\mathbf{x}^\top B\mathbf{x}}{\mathbf{x}^\top B\mathbf{x}}. \qquad \square
\end{aligned}
$$

From 5.31, we see that producing N independent samples from the process P1 described above (which is the finite grammar acquisition model discussed in the introduction) produces the same distribution as producing N independent samples from the distribution $g(\mathbf{x})$. So, we assume that the finite grammar acquisition model is a stochastic evolution guided by g (see Definition 19).

Analyzing the Infinite Population Dynamics. In this section we prove several structural properties of the grammar acquisition dynamics. We start this section by proving that the grammar acquisition dynamics converges to fixed points. [14]

Theorem 5.32 (Convergence of grammar acquisition dynamics). *The grammar acquisition dynamics converges to fixed points. In particular, the Lyapunov function $P(\mathbf{x}) = (x^\top Bx)^{\frac{1}{\tau} - m} \prod_i x_i^2$ is strictly increasing along the trajectories for $0 \leq \tau \leq 1/m$.*

Proof. We first prove the results for rational τ; let $\tau = \kappa/\lambda$. We use the theorem of Baum and Eagon [14]. Let

$$
L(\mathbf{x}) = (x^\top Bx)^{\lambda - m\kappa} \prod_i x_i^{2\kappa}.
$$

---

[14] This requires proof since convergence to limit cycles or the existence of strange attractors are a priori not ruled out.

Then

$$x_i \frac{\partial L}{\partial x_i} = 2\kappa L + \frac{2x_i(B\mathbf{x})_i(\lambda - m\kappa)L}{\mathbf{x}^\top B\mathbf{x}}.$$

It follows that

$$
\begin{aligned}
\frac{x_i \frac{\partial L}{\partial x_i}}{\sum_i x_i \frac{\partial L}{\partial x_i}} &= \frac{2\kappa L + \frac{2x_i(B\mathbf{x})_i(\lambda - m\kappa)L}{\mathbf{x}^\top B\mathbf{x}}}{2m\kappa L + 2(\lambda - m\kappa)L} \\
&= \frac{2\kappa L}{2\lambda L} + \frac{2L(\lambda - m\kappa)x_i(B\mathbf{x})_i}{2\lambda L\mathbf{x}^\top B\mathbf{x}} \\
&= (1 - m\tau)x_i\frac{(B\mathbf{x})_i}{\mathbf{x}^\top B\mathbf{x}} + \tau
\end{aligned}
$$

where the first equality comes from the fact that $\sum_{i=1}^m x_i(B\mathbf{x})_i = \mathbf{x}^\top B\mathbf{x}$. Since L is a homogeneous polynomial of degree 2λ, from Theorem 1.1 we get that L is strictly increasing along the trajectories, namely

$$L(g(\mathbf{x})) > L(\mathbf{x})$$

unless $\mathbf{x}$ is a fixed point. So $P(\mathbf{x}) = L^{1/\kappa}(\mathbf{x})$ is a potential function for the dynamics. To prove the result for irrational τ, we just have to see that the proof of [14] holds for all homogeneous polynomials with degree d, even irrational.

To finish the proof let $\Omega \subset \Delta_m$ be the set of limit points of an orbit $\mathbf{x}(t)$ (frequencies at time t for $t \in \mathbb{N}$). $P(\mathbf{x}(t))$ is increasing with respect to time t by above and so, because P is bounded on Δ_m, $P(\mathbf{x}(t))$ converges as $t \to \infty$ to $P^* = \sup_t\{P(\mathbf{x}(t))\}$. By continuity of P we get that $P(\mathbf{y}) = \lim_{t\to\infty} P(\mathbf{x}(t)) = P^*$ for all $\mathbf{y} \in \Omega$. So P is constant on Ω. Also $\mathbf{y}(t) = \lim_{n\to\infty} \mathbf{x}(t_n + t)$ as $n \to \infty$ for some sequence of times $\{t_i\}$ and so $\mathbf{y}(t)$ lies in Ω, *i.e.*, Ω is invariant. Thus, if $\mathbf{y} \equiv \mathbf{y}(0) \in \Omega$ the orbit $\mathbf{y}(t)$ lies in Ω and so $P(\mathbf{y}(t)) = P^*$ on the orbit. But P is strictly increasing except on equilibrium orbits and so Ω consists entirely of fixed points. $\qquad\square$

Fixed points and bifurcation. Let $\mathbf{z}$ be a fixed point. $\mathbf{z}$ satisfies the following equations:

$$\frac{z_i - \tau}{z_i(B\mathbf{z})_i} = \frac{z_j - \tau}{z_j(B\mathbf{z})_j} = \frac{1 - m\tau}{\mathbf{z}^T B\mathbf{z}} \text{ for all } i, j. \tag{72}$$

The previous equations can be derived by solving $z_i = (1 - m\tau)z_i \frac{z_i(B\mathbf{z})_i}{\mathbf{z}^\top B\mathbf{z}} + \tau$. By solving with respect to τ we get that

$$\tau = \frac{z_i z_j((B\mathbf{z})_i - (B\mathbf{z})_j)}{z_i(B\mathbf{z})_i - z_j(B\mathbf{z})_j} \text{ for } z_i(B\mathbf{z})_i \neq z_j(B\mathbf{z})_j.$$

Fact 5.33. *The uniform point $(^1/m, \ldots, ^1/m)$ is a fixed point of the dynamics for all values of τ.*

To see why 5.33 is true, observe that $g_i(1/m, \ldots, 1/m) = (1 - m\tau)\frac{1}{m} + \tau = \frac{1}{m}$ for all i and hence $g(1/m, \ldots, 1/m) = (1/m, \ldots, 1/m)$. The fixed points satisfy the following property:

Lemma 5.34 (Two Distinct Values). *Let $(x_1, \ldots, x_m)$ be a fixed point. Then $x_1, \ldots, x_m$ take at most two distinct values.*

Proof. Let $x_i \neq x_j$ for some i, j. Then it follows that

$$\tau = \frac{x_i x_j((B\mathbf{x})_i - (B\mathbf{x})_j)}{x_i(B\mathbf{x})_i - x_j(B\mathbf{x})_j} = \frac{x_i x_j(1 - b)}{(1 - b)(x_i + x_j) + b}.$$

Hence if $x_{j'} \neq x_i$ then

$$\frac{x_{j'}}{(1 - b)(x_i + x_{j'}) + b} = \frac{x_j}{(1 - b)(x_i + x_j) + b}$$

from which follows that $x_j = x_{j'}$. Finally, the uniform fixed point satisfies trivially the property. $\square$

We shall compute the threshold τ_c such that for $0 < \tau < \tau_c$ the dynamics has multiple fixed points and for $^1/m \geq \tau > \tau_c$ we have only one fixed point (which by Fact 5.33 must be the uniform one). Let

$$h(x) = -x^2(m - 2)(1 - b) - 2x(1 + b(m - 2)) + 1 + b(m - 2).$$

By Bolzano's theorem and the fact that $h(0) = 1 + b(m - 2) > 0$ and $h(-1) < 0$, $h(1) = 1 - m < 0$, it follows that there exists one positive solution for $h(x) = 0$ which is between 0 and 1; we denote it by s_1.

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We can now define

$$\tau_c := \frac{(1-b)s_1(1-s_1)}{(m-1)b+(1-b)(1+(m-2)s_1)}.$$

Lemma 5.35 (Bifurcation). *If $\tau_c < \tau \le {}^1/m$ then the only fixed point is the uniform one. If $0 \le \tau < \tau_c$ then there exist multiple fixed points.*

Proof. Assume that there are multiple fixed points (apart from the uniform, see 5.33) and let $(x_1, \ldots, x_m)$ be a fixed point, where x and y being the two values that the coordinates x_i take (by Lemma 5.34). Let $k \ge 1$ be the number of coordinates with value x and $m - k$ the coordinates with values y where $m > k$ and $kx + (m-k)y = 1$ (in case $k = 0$ or $m = k$ we get the uniform fixed point). Solving by τ we get that $\tau = \frac{xy(1-b)}{b+(1-b)(x+y)}$. We set $y = \frac{1-kx}{m-k}$ and we analyze the function

$$f(x,k) = \frac{(1-b)x(1-kx)}{(m-k)b+(1-b)(1+(m-2k)x)}$$

It follows that f is decreasing with respect to k (assuming $x < {}^1/{k+1}$ such that $y > 0$, see Appendix A.3 for Mathematica code for proving $f(x,k)$ is decreasing with respect to k). Hence the maximum is attained for $k = 1$. Hence, we can consider

$$f(x) := f(x,1) = \frac{(1-b)x(1-x)}{(m-1)b+(1-b)(1+(m-2)x)}.$$

By solving $\frac{df}{dx} = 0$ it follows that $h(x) = 0$ (where $h(x)$ is the numerator of the derivative of f). This occurs at s_1. For $\tau > \tau_c$ there exist no fixed points whose coordinates can take on more than one value by construction of f, namely the only fixed point is the uniform one. □

Stability analysis. The equations of the Jacobian are given below:

$$\frac{\partial g_i}{\partial x_i} = (1 - m\tau)\left(\frac{(B\mathbf{x})_i + x_i B_{ii}}{\mathbf{x}^\top B\mathbf{x}} - \frac{x_i(B\mathbf{x})_i \cdot 2(B\mathbf{x})_i}{(\mathbf{x}^\top B\mathbf{x})^2}\right), \tag{73}$$

$$\frac{\partial g_j}{\partial x_i} = (1 - m\tau)\left(\frac{x_j B_{ji}}{\mathbf{x}^\top B\mathbf{x}} - \frac{x_j(B\mathbf{x})_j \cdot 2(B\mathbf{x})_i}{(\mathbf{x}^\top B\mathbf{x})^2}\right) \text{ for } j \ne i. \tag{74}$$

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Fact 5.36. *The all ones vector $(1, \ldots, 1)$ is a left eigenvector of the Jacobian with corresponding eigenvalue 0.*

Proof. This can be derived by computing

$$\sum_{j=1}^{m} \frac{\partial g_j}{\partial x_i} = (1 - m\tau)\left(\frac{2(B\mathbf{x})_i}{\mathbf{x}^\top B\mathbf{x}} - \frac{2\mathbf{x}^\top B\mathbf{x}(B\mathbf{x})_i}{(\mathbf{x}^\top B\mathbf{x})^2}\right) = 0.$$

$\square$

We will focus on two specific classes of fixed points. The first one is the uniform, i.e., $(1/m, \ldots, 1/m)$ which we denote by $\mathbf{z}_u$ and the other one is $(y, \ldots, y, \underbrace{x}_{i^{th}}, y, \ldots, y)$ with $x + (m-1)y = 1$ and $x > s_1$, which we denote by $\mathbf{z}_i$ (for $1 \leq i \leq m$).

Stability of $\mathbf{z}_u$. Let

$$\tau_u := \frac{1-b}{m(2 - 2b + mb)}.$$

Lemma 5.37. *If $\tau_u < \tau \leq 1/m$, then $\mathrm{sp}\,(J(z_u)) < 1$ and if $0 \leq \tau < \tau_u$, then $\mathrm{sp}\,(J(z_u)) > 1$.*

Proof. The Jacobian of the uniform fixed point has diagonal entries equal to $(1 - m\tau)\left(1 - \frac{2}{m} + \frac{1}{1+(m-1)b}\right)$ and non-diagonal entries $(1 - m\tau)\left(\frac{b}{1+(m-1)b} - \frac{2}{m}\right)$. Consider the matrix

$$W_u := J(\mathbf{z}_u) - (1 - m\tau)\left(1 + \frac{1-b}{1+(m-1)b}\right)I_m$$

where I_m is the identity matrix of size $m \times m$. The matrix W_u has eigenvalue 0 with multiplicity $m - 1$ and eigenvalue $m(1 - m\tau)\left(\frac{b}{1+(m-1)b} - \frac{2}{m}\right)$ with multiplicity 1. Hence the eigenvalues of $J(\mathbf{z}_u)$ are 0 with multiplicity 1 and $(1 - m\tau)(1 + \frac{1-b}{1+(m-1)b})$ with multiplicity $m - 1$. Thus, the Jacobian of $\mathbf{z}_u$ has spectral radius less than one if and only if $-1 < (1 - m\tau)(1 + \frac{1-b}{1+(m-1)b}) < 1$. By solving with respect to τ it follows that

$$\frac{1-b}{m(2-2b+mb)} < \tau < \frac{3 - 3b + 2bm}{m(2 - 2b + mb)}.$$

Because $1/m < \frac{3-3b+2bm}{m(2-2b+mb)}$ (as $b \leq 1$), the first part of the lemma follows. In case $0 \leq \tau < \frac{1-b}{m(2-2b+mb)}$ then $(1 - m\tau)(1 + \frac{1-b}{1+(m-1)b})$ and the second part follows. $\square$

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Hence, we conclude that τ_u is the threshold below which the uniform fixed point satisfies $\mathrm{sp}\left(J(\mathbf{z}_u)\right) > 1$ and above which $\mathrm{sp}\left(J(\mathbf{z}_u)\right) < 1$.

Stability of $\mathbf{z}_i$.

Lemma 5.38. *If $0 \leq \tau < \tau_c$ then $\mathrm{sp}\left(J(z_i)\right) < 1$.*

Proof. Consider the matrix

$$W_i := J(\mathbf{z}_i) - (1 - m\tau)\frac{y + b + (1 - 2b)y}{\mathbf{z}_i^\top B\mathbf{z}_i}I_m$$

where I_m is the identity matrix of size $m \times m$. The matrix W_i has eigenvectors of the form

$$(w_1, \ldots, w_{i-1}, 0, w_{i+1}, \ldots, w_m)$$

with $\sum_{j=1,j\neq i}^{m} w_j = 0$ (the dimension of the subspace is $m - 2$) and corresponding eigenvalues 0. Hence the Jacobian has $m - 2$ eigenvalues of value $(1 - m\tau)\frac{y+b+(1-2b)y}{\mathbf{z}_i^\top B\mathbf{z}_i}$.

It is true that $0 < (1 - m\tau)\frac{y+b+(1-2b)y}{\mathbf{z}_i^\top B\mathbf{z}_i} < 1$ (see Appendix A.3 for Mathematica code). Finally, since $J(z_i)$ has an eigenvalue zero (see Fact 5.36), the last eigenvalue is

$$\mathrm{Tr}(J(z_i)) - (1 - m\tau)(m - 2)\frac{y + b + (1 - 2b)y}{\mathbf{z}_i^\top B\mathbf{z}_i} = (1 - m\tau)\cdot$$
$$\left(\frac{2b + (2 - b)x + ((m - 3)b + 2)y}{\mathbf{z}_i^\top B\mathbf{z}_i} - \frac{2x(b + (1 - b)x)^2 + 2(m - 1)y(b + (1 - b)y)^2}{(\mathbf{z}_i^\top B\mathbf{z}_i)^2}\right)$$

which is also less than 1 and greater than 0 (see Appendix A.3 for Mathematica code). $\square$

Remark 10. *In the case where $m = 2$ it follows that $\tau_u = \tau_c = \frac{1-b}{4}$. For $m > 2$ we have $\tau_u < \tau_c$ (see Mathematica code in Lemma A.3.3).*

Analyzing the Mixing Time. We prove our result concerning the grammar acquisition model (finite population). The structural lemmas proved in the previous section are used here. Now, we proceed by analysing the mixing time of the Markov chain for the two intervals $(0, \tau_c)$ and $(\tau_c, 1/m]$.

Regime $0 < \tau < \tau_c$.

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Lemma 5.39. *For the interval $0 < \tau < \tau_c$. the mixing time of the Markov chain is* $\exp(\Omega(N))$.

Proof. By Lemma 5.38 it is true that there exist m fixed points $\mathbf{z}_i$ with $\mathrm{sp}\left(J(\mathbf{z}_i)\right) < 1$ and their pairwise distance is some positive constant independent of N (well-separated). Hence using Theorem 5.9 and because the Markov chain is a stochastic evolution guided by g (see 5.31), we conclude that the mixing time is $e^{\Omega(N)}$. $\qquad\square$

Regime $\tau_c < \tau \le 1/m$. We prove the second part of Theorem 5.12.

Lemma 5.40. *For the interval $\tau_c < \tau \le 1/m$, the assumptions of Theorem 5.7 are satisfied, namely the mixing time of the Markov chain is $O(\log N)$.*

Proof. By Lemma 5.35, we know that in the interval $\tau_c < \tau \le 1/m$ there is a unique fixed point (the uniform $\mathbf{z}_u$) and also by Lemma 5.37 that $\mathrm{sp}\left(J(\mathbf{z}_u)\right) < 1$. It is trivial to check that g is twice differentiable with bounded second derivative. It suffices to show the 4th condition in the Definition 22. Due to Theorem 5.32 we have $\lim_{k\to\infty} g^k(\mathbf{x}) \to \mathbf{z}_u$ for all $\mathbf{x} \in \Delta_m$. The rest follows from Lemma 5.26 (by setting $S = \Delta_m$). $\qquad\square$

Our result on grammar acquisition model is a consequence of 5.39, 5.40.

Remark 11. *For $\tau = {}^1\!/m$ the Markov chain mixes in one step. This is trivial since g maps every point to the uniform fixed point $\mathbf{z}_u$.*

5.8   Conclusion and Remarks

The results of this chapter appear in [104, 105] and it is joint work with Piyush Srivastava and Nisheeth Vishnoi. We examine the mixing time of a class of Markov chains that are guided by dynamical systems on the simplex. We make an interesting connection between the mixing time of the Markov chains and the geometry of the underlying dynamical systems (structure of limit points, convergence, stability). We

prove that when the dynamical system has one stable fixed point then the mixing time of the corresponding Markov chain is rapidly mixing, something that is not true when there are multiple fixed points. We also provide two applications, *i.e.,* RSM and grammar acquisition models. We prove that the RSM model has mixing time $O(\log N)$ whereas in the grammar acquisition model we show a phase transition result. Questions that arise:

- Study the mixing at the threshold for the grammar acquisition model. More generally, how can we handle the case where the spectral radius of the Jacobian of the update rule of the dynamics is one?

- A natural next step is to study the evolution of *structured* populations. Roughly, this setting extends the evolutionary Markov chains by introducing an additional input parameter, a graph on N vertices. The graph provides structure to the population by locating each individual at a vertex, and the main difference from the is that at time $t + 1$, an individual determines its new vertex by sampling with replacement from among its neighbors in the graph at time t; see [76] for more details. Here, it is no longer sufficient to just keep track of the fraction of each type. The stochastic evolution model can be seen as a special case when the underlying graph is the complete graph on N vertices, so that the locations of the individuals in the population are of no consequence. Our results do not seem to apply directly to this setting and it is a challenging open problem to prove bounds in the general graph setting.

CHAPTER VI

AVERAGE CASE ANALYSIS IN POTENTIAL GAMES

6.1 Introduction

The study of game dynamics is a basic staple of game theory with several books
dedicated exclusively to it [61, 54, 142, 22, 121]. Historically, the golden standard for
classifying the behavior of learning dynamics in games has been to establish conver-
gence to equilibria. Thus, it is hardly surprising that a significant part of the work
on learning in games focuses on potential games (and slight generalizations thereof)
where many dynamics (*e.g.,* replicator, smooth fictitious play) are known to converge
to equilibrium sets. The structure of the convergence proofs is essentially universal
across different learning dynamics and boils down to identifying a Lyapunov/potential
function that strictly decreases along any nontrivial trajectory. In potential games,
as their name suggests, this function is part of the description of the game and pre-
cisely guides self-interested dynamics towards critical points of these functions that
correspond to equilibria of the learning process.

Potential games are also isomorphic to congestion games [89]. Congestion games
have been instrumental in the study of efficiency issues in games. They are amongst
the most extensively studied class of games from the perspective of price of anarchy
and price of stability with many tight characterization results for different subclasses
of games (*e.g.,* linear congestion games [120], symmetric load balancing [98] and
references therein).

Our contribution. We show that this is far from the case. We focus on simple
systems where replicator dynamic, arguably one of the most well studied game dy-
namics, is applied to linear congestion games and (network) coordination games. We

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resolve a number of basic open questions in the following results:

(A) Point-wise convergence to equilibrium. In the case of linear congestion games and (network) coordination games we prove convergence to equilibrium instead of equilibrium sets. Convergence to equilibrium sets implies that the distance of system trajectories from the sets of equilibria converges to zero (see Theorems 6.2, A.3). On the other hand, convergence to equilibrium, also referred to as point-wise convergence, implies that every system trajectory has a unique limit point, which is an equilibrium. In games with continuums of equilibria, (*e.g.,* N balls N bins games[1] with $N \geq 4$), the first statement is more inclusive that the second. In fact, system equilibration is not implied by set-wise convergence, and the limit set of a trajectory may have complex topology (*e.g.,* the limit of social welfare may not be well defined). Despite numerous positive convergence results in classes of congestion games [53, 17, 48, 16, 2], this is the first to our knowledge result about deterministic point-wise convergence for any concurrent dynamic. The proof is based on combining global Lyapunov functions arguments with local information theoretic Lyapunov functions around each equilibrium.

(B) Global stability analysis. Although the point-wise convergence result is interesting in itself, it critically enables all other results in the paper. Specifically, we establish that modulo point-wise convergence, all but a zero measure set of initial conditions converge to equilibrium points which are weakly stable Nash equilibria (see Definition 10, Theorem 6.4, Corollary 6.5). This is a technical result that combines game theoretic arguments with tools from dynamical systems (Center-Stable Manifold Theorem 1.3) and analysis (Lindelöf's lemma A.1).

(C) Invariant functions. Sometimes a game may have multiple (weakly) stable equilibria. In this case we would like to be able to predict which one will arise given

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[1]These are symmetric load balancing games with N agents and N machines where the cost function of each machine is the identity function.

a specific (or maybe a randomly chosen) initial condition. Systems invariants allows us to do exactly that. A system invariant is a function defined over the system state space such that it remains constant along every system trajectory. Establishing invariant properties of replicator dynamics in generalized zero-sum games has helped prove interesting topological properties of the system trajectories such as (near) cycles [112, 111, 106]. In the case of bipartite coordination games with fully mixed Nash equilibria, we can establish similar invariant functions. Specifically, the difference between the sum of the Kullback-Leibler (KL) divergences of the evolving mixed strategies of the agents on the left partition from their fully mixed Nash equilibrium strategy and the respective term for the agents in the right partition remains constant along any trajectory. In the special case of star graphs, we show how to produce n such invariants where n is the degree of the star. This allows for creating efficient oracles for predicting to which Nash equilibrium the system converges provably for any initial condition without simulating explicitly the system trajectory.

Applications. The tools that we have developed allow for novel insights in classic and well studied class of games. We group our results into two clusters, average case performance analysis and estimating risk dominance/regions of attraction:

Average Case Performance. We propose a novel quantitative framework for analyzing the efficiency of potential games with many equilibria. Informally, we define the expected system performance as the weighted average of the social costs of all equilibria where the weight of each equilibrium is proportional to the volume (or more generally measure) of its region of attraction. The main idea is as follows: The agents start participating in the game having some prior beliefs about which are the best actions for them. We will typically assume that the initial beliefs are chosen according to a uniform prior given that we want to assume no knowledge about the agents' internal beliefs[2]. Given this initial condition the agents start interacting through the

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[2]Our techniques extend to arbitrarily correlated beliefs, any prior over initial mixed strategies.

game and update their beliefs (*i.e.,* their randomized strategies) up until they reach equilibrium. At this point the measure of the region of attraction of an equilibrium captures exactly the likelihood that we will converge to that state. So the average case performance computes, as its names suggests, what will be the resulting system performance on average. As is typical in algorithmic game theory, we can normalize this quantity by dividing with the performance of the optimal state. We define this ratio as the *average price of anarchy*. In our convergent systems it always lies between the price of stability and the price of anarchy. We analyze the average price of anarchy in a number of settings which include, N balls N bins games, symmetric linear load balancing games (with agents of equal weights),[3] parametric versions of coordination games as well as star network extensions of them. These are games with large gaps between the price of stability and price of anarchy and replicator is shown to be able to zero in on the good equilibria with high enough probability so that the average price of anarchy is always a small constant. This measure of performance could help explain why some games are easy in practice, despite having large price of anarchy. We aggregate these results below:

	Average PoA	Techniques	PoS	Pure PoA	PoA
n balls n bins game	**1**	**A & B**	1	1	$\Theta(\log n/\log\log n)$
Symmetric Load Balancing	**[1, 1.5]**	**A & B**	1	1	$\Omega(\log n/\log\log n)$
w-Coordination Game	**[1.15, 1.21]**	**A & B & C**	1	$\Theta(w)$	$\Theta(w)$
N-Star w-Coordination Game[4]	**[1.15, 1.21]**	**A & B & C**	1	$\Theta(w)$	$\Theta(w)$

Table 2: Our APoA results

Risk dominance/Regions of attraction. Risk dominance is an equilibrium refinement process that centers around uncertainty about opponent behavior. A Nash equilibrium is considered risk dominant if it has the largest basin of attraction[5]. The benchmark example is the Stag Hunt game, shown in figure 10(a). In such symmetric

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[3]We focus mostly on the makespan as a measure of social cost.

[5]Although risk dominance [60] was originally introduced as a hypothetical model of the method by which perfectly rational players select their actions, it may also be interpreted [91] as the result of evolutionary processes.

2x2 coordination games a strategy is risk dominant if it is a best response to the uniformly random strategy of the opponent. We show that the likelihood of the risk dominant equilibrium of the Stag Hunt game is $\frac{1}{27}(9 + 2\sqrt{3}\pi) \approx 0.7364$ (instead of merely knowing that it is at least $^1/_2$, see Figure 11). The size of the region of attraction of the risk dominated equilibrium is 0.2636, whereas the mixed equilibrium has region of attraction of zero measure. Moving to networks of coordination games, we show how to construct an oracle that predicts the limit behavior of an arbitrary initial condition, in the case of coordination games played over a star network with N agents. This is the most economic class of games that exhibits two characteristics that intuitively seem to pose intractable obstacles to the quantitative analysis of nonlinear systems: i) they have (arbitrarily many) free variables, ii) they exhibit a continuum of equilibria.

6.2 Related work

A number of positive convergence results have been established for concurrent dynamics [53, 17, 48, 16, 2, 70], however, they usually depend on strong assumptions about network structure (*e.g.,* load balancing games) and/or symmetry of available strategies and/or are probabilistic in nature and/or establish convergence to approximate equilibria. On the contrary our convergence results are deterministic, hold for any network structure and in the case of the replicator dynamics are point-wise.

Apart from replicator dynamics, nonlinear dynamical systems have been studied quite extensively in a number of different fields including computer science. Specifically, quadratic dynamical systems [114] are known to arise in the study genetic algorithms [62]. These are a class of heuristics for combinatorial optimization based loosely on the mechanisms of natural selection [115, 13]. Both positive and negative computational complexity and convergence results are known for them, including convergence to a stationary distribution (analogous of classic theorems for Markov

chains) [113, 115, 9] depending on the specifics of the model. In contrast, replicator dynamic in linear congestion games defines a cubic dynamical system.

Price of anarchy-like bounds in potential games using equilibrium stability refinements (*e.g.,* stochastically stable states) have been explored before [30, 10, 2]. Our approach and techniques are more expansive in scope, since they also allow for computing the actual likelihoods of each equilibrium as well as the topology of the regions of attractions of different equilibria. Finally, in independent parallel work Zhang and Hofbauer have examined equilibrium selection issues in $2x2$ coordination games for replicator dynamics [143], however, their techniques do not scale to larger games and they do not analyze the average case performance of these games but mostly focus on which equilibrium is more likely to arise.

6.3 Definitions and basic tools

6.3.1 Average performance of a system

Let μ be the Lebesgue measure in $\mathbb{R}^n$ and assume that $\mu(\mathcal{S}) > 0$. Given a dynamical system (continuous time) we assume that $\lim_{t\to\infty} \phi_t(\mathbf{x})$ exists for all $\mathbf{x} \in \mathcal{S}$ (the limit is called a *limit point*); the system converges point-wise for all initial conditions. If that is true, by continuity occurs that every trajectory converges to some equilibrium of the dynamics[6].

We would like to understand the *average (long-term) behavior* of the convergent system, for example if the initial condition is chosen uniformly at random from $\mathcal{S}$. Intuitively, since the system converges to fixed points, we would like each fixed point $\mathbf{x}_0$ to be assigned weight proportional to its *region of attraction* denoted by $R_{\mathbf{x}_0}$. Let $\psi(\mathbf{x}) = \lim_{t\to\infty} \phi_t(\mathbf{x})$, *i.e.,* ψ maps each starting point $\mathbf{x}$ to the limit of the $\phi_t(\mathbf{x})$. It turns out that ψ is a measurable function.

Lemma 6.1. $\psi(\mathbf{x})$ *is a measurable function.*

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[6]If $\lim_{t\to\infty} h^t(\mathbf{x}) = \mathbf{y}$ and h continuous then $h(\mathbf{y}) = \mathbf{y}$. Set $h := \phi_1$.

Proof. For an arbitrary $c \in \mathbb{R}$ we have that

$$\{\mathbf{x} : \psi(\mathbf{x})_i < c\} = \cup_{k=1}^{\infty} \cup_{m=1}^{\infty} \cap_{n>m}^{\infty} \{\mathbf{x} : \phi_n(\mathbf{x})_i < c - \frac{1}{k}\}\}.$$

The set $\{\mathbf{x} : \phi_n(\mathbf{x})_i < c - \frac{1}{k}\}$ is measurable since $\phi_n(\mathbf{x})_i$ is a (Lebesgue) measurable function (by continuity). Therefore $\psi(\mathbf{x})_i$ is a measurable function. $\square$

Therefore, we can define the average (long-term) performance of the system under some function u. Let $u : \mathcal{S} \to \mathbb{R}$ be continuous, then the *average performance* of a system is defined as

$$\mathrm{ap}_u := \frac{\int_{\mathcal{S}} u \circ \psi d\mu}{\mu(\mathcal{S})} = \mathbb{E}_{x \sim U(\mathcal{S})}[u(\psi(\mathbf{x}))], \tag{75}$$

with $U(\mathcal{S})$ to be the uniform distribution on $\mathcal{S}$. u quantifies the quality of the points $\mathbf{x} \in \mathcal{S}$ (*e.g.,* social welfare in games). Observe that if $m := \min_{\mathbf{x} \in \mathrm{FP}} u(\mathbf{x}), M := \max_{\mathbf{x} \in \mathrm{FP}} u(\mathbf{x})$ where FP denotes the set of fixed points[7], then $m \le \mathrm{ap}_u \le M$ (a). We believe that computing/approximating average performance is a very important problem in order to understand the average behavior of a system.

To see the connection with game theory, think of $\mathcal{S}$ as the set of mixed (randomized) strategies, a fixed point with region of attraction of positive measure as a Nash equilibrium, u as the social cost/welfare. Then the integral (75) becomes a weighted average among the social cost/welfare of the Nash equilibria. Therefore, by observation (a) the average performance is sandwiched between the values (of social cost/welfare) of best and worst Nash. We use (continuous time) replicator dynamics on congestion and network coordination games as our benchmark. In that case, the set of Nash equilibria is a subset of the set of fixed points, we can show the dynamics converge point-wise and finally Nash equilibria are the only fixed points that get region of attraction of positive Lebesgue measure (they are linearly stable fixed points

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[7]The set of fixed points in $\mathcal{S}$ is closed.

of the dynamics). Later in this section we define the notion of *average price of anar-chy* which is essentially a scaled version of average performance, defined particularly for games.

Remark 12 (**Generalizations of average performance**). *It is remarkable that the definition of average performance can be used for point-wise convergent discrete time dynamical systems (function $\psi(\mathbf{x})$ will be equal to $\lim_{k\to\infty} g^k(\mathbf{x})$ where g is the rule of the discrete dynamics). Also, different measurement can be defined where the initial condition follows other distribution than the uniform (it should be called something different from average performance!).*

6.3.2 Definition of average price of anarchy (APoA)

In this section we define the notion of average price of anarchy, following the machinery from Section 6.3.1. It is natural to set $\mathcal{S}$ to be the product of simplexes Δ, but this is not the case since Δ has measure zero in $\mathbb{R}^M$, where $M := \sum_i |S_i|$. The reason is that the probabilities sum up to one for each player. To circumvent this issue (since from Section 6.3.1 we need $\mu(\mathcal{S}) > 0$), we consider a natural projection g of the points $\mathbf{p} \in \Delta$ to $\mathbb{R}^{M-N}$ by excluding a specific but arbitrarily chosen [8] variable for each player. We denote $g(\Delta)$ the "projected" product of simplexes and the projection of any point $\mathbf{p} \in \Delta$ by $g(\mathbf{p})$ (for example $(p_{1,a}, p_{1,b}, p_{1,c}, p_{2,a'}, p_{2,b'}) \to_g (p_{1,a}, p_{1,b}, p_{2,a'})$ where $p_{1,a} + p_{1,b} + p_{1,c} = 1$ and $p_{2,a'} + p_{2,b'} = 1$)). Given a dynamical system which describes the actions of rational agents for some particular game, is defined in $g(\Delta)$ (projected set of mixed strategies) and which converges point-wise to fixed points, we can define $\mathrm{ap}_{\mathrm{sc}}, \mathrm{ap}_{\mathrm{sw}}$ to be the average performance as in Section 6.3.1. For cost/utility functions the average price of anarchy is defined as follows:

$$\mathrm{APoA} = \frac{\mathrm{ap}_{\mathrm{sc}}}{\min_{\mathbf{s}^* \in \times_i S_i} \mathrm{sc}(\mathbf{s}^*)}, \quad \mathrm{APoA} = \frac{\max_{\mathbf{s}^* \in \times_i S_i} \mathrm{sw}(\mathbf{s}^*)}{\mathrm{ap}_{\mathrm{sw}}}.$$

---

[8]Choose an arbitrary ordering of the strategies of each agent and then exclude the last strategy.

Remark 13. *The definition of APoA does not rely on the fact that the games are congestion or network coordination and it does not rely on replicator dynamics. All it needs is that given a game, we have a dynamic that converges point-wise for all initial mixed strategies. Essentially APoA is a scaled version of the average performance. In the next section we show that replicator dynamics converges point-wise for congestion and network coordination games and also that the fixed points (of replicator on these 2 classes of games) with region of attraction of positive measure are Nash equilibria. In particular APoA is well-defined.*

6.4 Analysis of replicator dynamics in potential games

In this section we develop the mathematical machinery necessary for computing the average case performance of replicator dynamics in different classes of potential games. Specifically, we establish point-wise convergence of replicator dynamics for linear congestion games and arbitrary networks of coordination games (Theorem 6.2). This allows us to define properly the average case performance which is essentially equal to the weighted sum of the social cost/welfare of all equilibria weighted by the cumulative measure/volume of all initial conditions that converge to each (point-wise). Next, we show that the union of regions of attraction of (locally) unstable equilibria is of measure zero (Theorem 6.4). Combining this result with a game theoretic characterization of (un)stable equilibria in [70], known as weakly stable equilibria, establishes that only weakly stable equilibria affect the average case system performance. The analysis here is a strengthening of the techniques of [70] to carefully account for the possibility of continuums of unstable equilibria. Finally, we still need to compute for each weakly stable equilibrium the size of its region of attraction. The tool that is necessary for this is to establish invariants for replicator dynamics in different classes of games. We present an information theoretic invariant function (Theorem 6.7) for replicator dynamics for bipartite network coordination games.

6.4.1 Point-wise convergence

We show that replicator dynamics converges point-wise for the class of linear congestion and network coordination games. The proof of the theorem has two steps. The first step is standard, utilizes the potential function of the game and establishes convergence to equilibria sets. The critical, second step is to construct a *local* Lyapunov function in some small neighborhood of a limit point.

Theorem 6.2 (Point-wise convergence). *Given any initial condition replicator dynamics converges to a fixed point (point-wise convergence) in all linear congestion and network coordination games.*

Proof. We prove here the result in the case of linear congestion games. The argument for network coordination games follows similar lines and is in Appendix A.3.

We denote by $\hat{c}_i$ the expected cost of agent i under mixed strategy profile $\mathbf{p}$. Moreover, $c_{i\gamma}$ is his expected cost when he deviates to strategy γ and all other agents still play according to $\mathbf{p}$. We observe that $\Psi(\mathbf{p}) = \sum_i \hat{c}_i + \sum_{i,\gamma} \sum_{e \in \gamma} (b_e + a_e) p_{i\gamma}$ is a Lyapunov function since

$$
\frac{\partial \Psi}{\partial p_{i\gamma}} = c_{i\gamma} + \sum_{j \neq i} p_{j\gamma'} \frac{\partial c_{j\gamma'}}{\partial p_{i\gamma}} + \sum_{e \in \gamma} (b_e + a_e)
$$

$$
= c_{i\gamma} + \underbrace{\sum_{j \neq i} \sum_{\gamma'} \sum_{e \in \gamma \cap \gamma'} a_e p_{j\gamma'} + \sum_{e \in \gamma} (b_e + a_e)}_{c_{i\gamma}} = 2c_{i\gamma}
$$

and hence $\frac{d\Psi}{dt} = \sum_{i,\gamma} \frac{\partial \Psi}{\partial p_{i\gamma}} \frac{dp_{i\gamma}}{dt} = -\sum_{i,\gamma,\gamma'} p_{i\gamma} p_{i\gamma'} (c_{i\gamma} - c_{i\gamma'})^2 \leq 0$, with equality at fixed points. Hence (as in [70]) we have convergence to equilibria sets (compact connected sets consisting of fixed points). We will furthermore argue that each trajectory has a unique (equilibrium) limit point.

Let $\mathbf{q}$ be a limit point of the trajectory $\mathbf{p}(t)$ where $\mathbf{p}(t)$ is in the interior of Δ for all $t \in \mathbb{R}$ (since we started in the interior of Δ) then we have that $\Psi(\mathbf{q}) < \Psi(\mathbf{p}(t))$. We define the relative entropy $I(\mathbf{p}) = -\sum_i \sum_{\gamma : q_{i\gamma} > 0} q_{i\gamma} \ln(p_{i\gamma}/q_{i\gamma}) \geq 0$ (Jensen's ineq.)

and $I(\mathbf{p}) = 0$ iff $\mathbf{p} = \mathbf{q}$. We denote by $\hat{d}_i, d_{i\gamma}$ the expected costs of agent i under the mixed strategies $\mathbf{q}$.

$$
\begin{aligned}
\frac{dI}{dt} &= -\sum_i \sum_{\gamma:q_{i\gamma}>0} q_{i\gamma}(\hat{c}_i - c_{i\gamma}) = -\sum_i \hat{c}_i + \sum_{i,\gamma} q_{i\gamma} c_{i\gamma} \\
&= -\sum_i \hat{c}_i + \sum_{i,\gamma} \sum_{e \in \gamma} (b_e + a_e) q_{i\gamma} + \sum_{i,\gamma} \sum_{j \neq i} \sum_{\gamma'} \sum_{e \in \gamma \cap \gamma'} a_e q_{i\gamma} p_{j\gamma'} \\
&= -\sum_i \hat{c}_i + \sum_{i,\gamma} \sum_{e \in \gamma} (b_e + a_e) q_{i\gamma} + \sum_{i,\gamma} \sum_{j \neq i} \sum_{\gamma'} \sum_{e \in \gamma \cap \gamma'} a_e q_{j\gamma'} p_{i\gamma} \\
&= \sum_i \hat{d}_i - \sum_i \hat{c}_i + \sum_{i,\gamma} \sum_{e \in \gamma} (b_e + a_e) q_{i\gamma} - \sum_{i,\gamma} \sum_{e \in \gamma} (b_e + a_e) p_{i\gamma} - \sum_{i,\gamma} p_{i\gamma}(\hat{d}_i - d_{i\gamma}) \\
&= \Psi(\mathbf{q}) - \Psi(\mathbf{p}) - \sum_{i,\gamma} p_{i\gamma}(\hat{d}_i - d_{i\gamma}).
\end{aligned}
$$

We break the term $\sum_{i,\gamma} p_{i\gamma}(\hat{d}_i - d_{i\gamma})$ to positive and negative terms (zero terms are ignored), i.e., $\sum_{i,\gamma} p_{i\gamma}(\hat{d}_i - d_{i\gamma}) = \sum_{i,\gamma:\hat{d}_i>d_{i\gamma}} p_{i\gamma}(\hat{d}_i - d_{i\gamma}) + \sum_{i,\gamma:\hat{d}_i<d_{i\gamma}} p_{i\gamma}(\hat{d}_i - d_{i\gamma})$.

Claim 6.3. *There exists an $\epsilon > 0$ so that the function $Z(\mathbf{p}) = I(\mathbf{p}) + 2 \sum_{i,\gamma:\hat{d}_i<d_{i\gamma}} p_{i,\gamma}$ has $\frac{dZ}{dt} < 0$ for $\|\mathbf{p} - \mathbf{q}\|_1 < \epsilon$ and $\Psi(\mathbf{q}) < \Psi(\mathbf{p})$.*

Proof of Claim. To prove this claim, first assume that $\mathbf{p} \to \mathbf{q}$. We get $\hat{c}_i - c_{i\gamma} \to \hat{d}_i - d_{i\gamma}$ for all i, γ. Hence for small enough $\epsilon > 0$ with $\|\mathbf{p} - \mathbf{q}\|_1 < \epsilon$, we have that $\hat{c}_i - c_{i\gamma} \leq \frac{3}{4}(\hat{d}_i - d_{i\gamma})$ for the terms which $\hat{d}_i - d_{i\gamma} < 0$. Therefore

$$
\begin{aligned}
\frac{dZ}{dt} &= \Psi(\mathbf{q}) - \Psi(\mathbf{p}) - \sum_{i,\gamma:\hat{d}_i>d_{i\gamma}} p_{i\gamma}(\hat{d}_i - d_{i\gamma}) - \sum_{i,\gamma:\hat{d}_i<d_{i\gamma}} p_{i\gamma}(\hat{d}_i - d_{i\gamma}) + 2 \sum_{i,\gamma:\hat{d}_i<d_{i\gamma}} p_{i\gamma}(\hat{c}_i - c_{i\gamma}) \\
&\leq \Psi(\mathbf{q}) - \Psi(\mathbf{p}) - \sum_{i,\gamma:\hat{d}_i>d_{i\gamma}} p_{i\gamma}(\hat{d}_i - d_{i\gamma}) - \sum_{i,\gamma:\hat{d}_i<d_{i\gamma}} p_{i\gamma}(\hat{d}_i - d_{i\gamma}) + \frac{3}{2} \sum_{i,\gamma:\hat{d}_i<d_{i\gamma}} p_{i\gamma}(\hat{d}_i - d_{i\gamma}) \\
&= \underbrace{\Psi(\mathbf{q}) - \Psi(\mathbf{p})}_{<0} + \underbrace{\sum_{i,\gamma:\hat{d}_i>d_{i\gamma}} -p_{i\gamma}(\hat{d}_i - d_{i\gamma})}_{\leq 0} + \underbrace{\frac{1}{2} \sum_{i,\gamma:\hat{d}_i<d_{i\gamma}} p_{i\gamma}(\hat{d}_i - d_{i\gamma})}_{\leq 0} < 0,
\end{aligned}
$$

where we substitute $\frac{p_{i\gamma}}{dt} = p_{i\gamma}(\hat{c}_i - c_{i\gamma})$ (replicator equations), and the claim is proved. Notice that $Z(\mathbf{p}) \geq 0$ (sum of positive terms, $I(\mathbf{p}) \geq 0$) and is zero iff $\mathbf{p} = \mathbf{q}$. (i) $\square$

To finish the proof of the theorem, if $\mathbf{q}$ is a limit point of $\mathbf{p}(t)$, there exists an increasing sequence of times t_i, with $t_n \to \infty$ and $\mathbf{p}(t_n) \to \mathbf{q}$. We consider ϵ' such that the set $C = \{\mathbf{p} : Z(\mathbf{p}) < \epsilon'\}$ is inside $B = \|\mathbf{p} - \mathbf{q}\|_1 < \epsilon$ where ϵ is from claim above. Since $\mathbf{p}(t_n) \to \mathbf{q}$, consider a time t_N where $\mathbf{p}(t_N)$ is inside C. From the claim above we get that $Z(\mathbf{p})$ is decreasing inside B (and hence inside C), thus $Z(\mathbf{p}(t)) \leq Z(\mathbf{p}(t_N)) < \epsilon'$ for all $t \geq t_N$, hence the orbit will remain in C. By the fact that $Z(\mathbf{p}(t))$ is decreasing in C (claim above) and also $Z(\mathbf{p}(t_n)) \to Z(\mathbf{q}) = 0$ it follows that $Z(\mathbf{p}(t)) \to 0$ as $t \to \infty$. Hence $\mathbf{p}(t) \to \mathbf{q}$ as $t \to \infty$ using (i). $\square$

Remark 14. *If the fixed points of the dynamics are* isolated *then a (global) Lyapunov function suffices to show that the system converges point-wise (first step of the proof above). However, this is not the case even in linear congestion games (see Lemma 6.27, where there are uncountable many fixed points which are Nash equilibria).*

6.4.2   Global stability analysis

Replicator dynamics - in linear congestion games and network coordination games and essentially any dynamics that converges point-wise - induces a probability distribution over the fixed points. The probability for each fixed point is proportional to the volume of its region of attraction. The fixed points can be exponentially many or even accountable many, but as it is stated below (Corollary 6.5), only the weakly stable Nash equilibria (see Definition 10) have non-zero volumes of attraction.

In [70] Kleinberg *et al.* showed that in congestion games, every stable fixed point is a weakly stable Nash equilibrium. The following theorem (that assumes point-wise convergence) has a corollary that for all but measure zero initial conditions replicator dynamics converges to a weakly stable Nash equilibrium.

Theorem 6.4 (Replicator converges to stable fixed points). *The set of initial conditions for which the replicator converges to unstable fixed points has measure zero in Δ for linear congestion games and network coordination games.*

Proof. To prove the theorem we will use Center Stable Manifold Theorem (see Theorem 1.3). In order to do that we need a map whose domain is full-dimensional. However, a simplex in $\mathbb{R}^n$ has dimension $n-1$. Therefore, we need to take a projection of the domain space and accordingly redefine the map of the dynamical system. We note that the projection we take will be fixed-point dependent; this is to keep of the proof that every stable fixed point is a weakly stable Nash proved in [70] relatively less involved later. Let $\mathbf{q}$ be a point of our state space Δ and $\Sigma = |\cup_i S_i|$. Let $h_{\mathbf{q}} : [N] \to [\Sigma]$ be a function such that $h_{\mathbf{q}}(i) = \gamma$ if $q_{i\gamma} > 0$ for some $\gamma \in S_i$ (same definition with discrete case). Let $M = \sum |S_i|$ and g a fixed projection where you exclude the first coordinate of every player's distribution vector. We consider the mapping $z_{\mathbf{q}} : R^M \to R^{M-N}$ so that we exclude from each player i the variable $p_{i,h_{\mathbf{q}}(i)}$ ($z_{\mathbf{q}}$ plays the same role as g but we drop variables with specific property this time). We substitute the variables $p_{i,h_{\mathbf{q}}(i)}$ with $1 - \sum_{\substack{\gamma \neq h_{\mathbf{q}}(i) \\ \gamma \in S_i}} p_{i\gamma}$.

For $t = 1$ and an unstable fixed point $\mathbf{p}$ we consider the function $\psi_{1,\mathbf{p}}(\mathbf{x}) = z_{\mathbf{p}} \circ \phi_1 \circ z_{\mathbf{p}}^{-1}(\mathbf{x})$ which is C^1 diffeomorphism, where ϕ_1 is the time one map of the flow of the dynamical system in Δ (we assume we do the renormalization trick described in Section 1.1.1). Let $B_{z_{\mathbf{p}}(\mathbf{p})}$ be the ball that is derived from 1.3 and we consider the union of these balls (transformed in $\mathbb{R}^M$)

$$A = \cup_{\mathbf{p}} A_{z_{\mathbf{p}}(\mathbf{p})},$$

where $A_{z_{\mathbf{p}}(\mathbf{p})} = g \circ z_{\mathbf{p}}^{-1}(B_{z_{\mathbf{p}}(\mathbf{p})})$ ($z_{\mathbf{p}}^{-1}$ "returns" the set $B_{z_{\mathbf{p}}(\mathbf{p})}$ back to $\mathbb{R}^M$). Due to the Lindelöf's Lemma A.1, we can find a countable subcover for $A = \cup_{\mathbf{p}} A_{z_{\mathbf{p}}(\mathbf{p})}$, i.e., $A = \cup_{m=1}^\infty A_{z_{\mathbf{p}_m}(\mathbf{p}_m)}$.

Let $\psi_{n,\mathbf{p}}(\mathbf{x}) = z_{\mathbf{p}} \circ \phi_n \circ z_{\mathbf{p}}^{-1}(\mathbf{x})$. If a point $\mathbf{x} \in g(\Delta)$ (which corresponds to $g^{-1}(\mathbf{x})$ in our original Δ) has as unstable fixed point as a limit, there must exist a n_0 and m so that $\psi_{n,\mathbf{p}_m} \circ z_{\mathbf{p}_m} \circ g^{-1}(\mathbf{x}) \in B_{z_{\mathbf{p}_m}(\mathbf{p}_m)}$ for all $n \geq n_0$ and therefore again from 1.3 and the fact that Δ is invariant we get that we get that $\psi_{n_0,\mathbf{p}_m} \circ z_{\mathbf{p}_m} \circ g^{-1}(\mathbf{x}) \in (W_{loc\ z_{\mathbf{p}_m}(\mathbf{p}_m)}^{sc} \cap z_{\mathbf{p}_m}(\Delta))$, hence $\mathbf{x} \in g \circ z_{\mathbf{p}_m}^{-1} \circ \psi_{n_0,\mathbf{p}_m}^{-1}(W_{loc\ z_{\mathbf{p}_m}(\mathbf{p}_m)}^{sc} \cap z_{\mathbf{p}_m}(\Delta))$.

Hence, the set of points in $g(\Delta)$ whose ω-limit has an unstable equilibrium, is a subset of

$$C = \cup_{m=1}^{\infty} \cup_{n=1}^{\infty} g \circ z_{\mathbf{p}_m}^{-1} \circ \psi_{n,\mathbf{p}_m}^{-1} (W^{sc}_{loc\, z_{\mathbf{p}_m}(\mathbf{p}_m)} \cap z_{\mathbf{p}_m}(\Delta)) \tag{76}$$

Observe that the dimension of $W^{sc}_{loc\, z_{\mathbf{p}_m}(\mathbf{p}_m)}$ is at most $M - N - 1$ since we assume that $\mathbf{p}_m$ is unstable ($\mathcal{J}_{\mathbf{p}_m}$ has an eigenvalue with positive real part) [9] and thus $dimE^u \geq 1$, hence the set $(W^{sc}_{loc\, z_{\mathbf{p}_m}(\mathbf{p}_m)} \cap z_{\mathbf{p}_m}(\Delta))$ has Lebesgue measure zero in $\mathbb{R}^{M-N}$. Finally since $g \circ z_{\mathbf{p}_m}^{-1} \circ \psi_{n,\mathbf{p}_m}^{-1} : \mathbb{R}^{M-N} \to \mathbb{R}^{M-N})$ is continuously differentiable in an open neighborhood of $g(\Delta)$, $\psi_{n,\mathbf{p}_m}$ is C^1 and hence locally Lipschitz in that neighborhood (see [110] p.71) and it preserves the null-sets (see Lemma A.2). Namely, C is a countable union of measure zero sets, *i.e.,* is measure zero as well. Since the dynamical system after renormalization is topologically equivalent with the system before renormalization, Theorem 6.4 follows. $\qquad\square$

This theorem extends to all congestion games for which the replicator dynamics converges point-wise (*e.g.,* systems with finite equilibria). Combining theorem 6.4 with the weakly stable characterization of [70] which holds for all congestion/potential games, we get the following:

Corollary 6.5 (Replicator converges to pure NE). *For all but measure zero initial conditions, replicator dynamics converges to weakly stable Nash equilibria for linear congestion games and network coordination games.*

6.4.3 Invariant functions from information theory

We have established that all attracting ($\subseteq$ linearly stable) fixed points are weakly stable Nash equilibria. We still need to characterize and compute the regions of attraction of these equilibria. The key idea here is to characterize the boundaries of the regions of attraction. This is due to the following theorem.

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[9]Here we used the fact that the eigenvalues with absolute value less than one, one and greater than one of e^A correspond to eigenvalues with negative real part, zero real part and positive real part respectively of A

Theorem 6.6 ([69]). *If* **q** *is an asymptotically stable equilibrium point for a system* $\dot{x} = f(x)$ *where* $f \in C^1$, *then its region of attraction* $R_\mathbf{q}$ *is an invariant set whose boundaries are formed by trajectories.*

If we identify a (continuous) invariant function f, *i.e.,* a function that remains constant on any trajectory, and **q** is a (limit) point of the trajectory then the whole trajectory lies on the set $\{\mathbf{x} : f(\mathbf{x}) = f(\mathbf{q})\}$. If we identify more invariant functions $f_1, f_2, \ldots, f_k$ then the whole trajectory lies on the set $\{\mathbf{x} : f_1(\mathbf{x}) = f_1(\mathbf{q}) \wedge f_2(\mathbf{x}) = f_2(\mathbf{q}) \wedge \cdots \wedge f_k(\mathbf{x}) = f_k(\mathbf{q})\}$. By identifying enough invariant functions, we can derive an exact algebraic description of the trajectory.

By our point-wise convergence result (Theorems 6.2, A.3) each trajectory converges to an equilibrium. So each point of the state space that does not belong in the region of attraction of a weakly stable equilibrium, must converge to an unstable equilibrium. By computing the (union of) regions of attraction of all unstable equilibria we can understand how they partition the state space into regions of attractions for the asymptotically stable equilibria[10]. All points on this stable manifold of unstable fixed point **q** lie on the set $\{\mathbf{x} : f_1(\mathbf{x}) = f_1(\mathbf{q}) \wedge f_2(\mathbf{x}) = f_2(\mathbf{q}) \wedge \cdots \wedge f_k(\mathbf{x}) = f_k(\mathbf{q})\}$ where $f_1, \ldots, f_k$ the invariant functions of the dynamic. Such descriptions can allow for exact computation of volumes of regions of attraction (Section 6.5.1), approximate volume computation (Section 6.5.2), designing efficient oracles for testing if an initial condition belong in the region of attraction of an equilibrium (Section 6.6), and computing average system performance, amongst other applications.

The following lemma that identifies invariants functions in bipartite coordination games follows straightforwardly from prior work on identifying invariant functions for network generalizations of (linear transformations of) zero-sum games [112, 111]). To prove any such statement it suffices to compute the time derivatives of these functions

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[10]The region of attraction of an unstable equilibrium is referred to as the stable manifold of the (unstable) fixed point.

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along any trajectory and show them to be equal to zero. For completeness, we provide the proof below.

Lemma 6.7 (**Invariance of KL** [112, 111]). *Let* $\mathbf{p}(t) = (\mathbf{p}_1(t), ..., \mathbf{p}_N(t))$ *(with* $\mathbf{p}(0) \in \Delta$*) be a trajectory of replicator dynamics when applied to a bipartite network of coordination games that has a fully mixed Nash equilibrium* $\mathbf{q} = (\mathbf{q}_1, ..., \mathbf{q}_N)$ *then* $\sum_{i \in V_{left}} H(\mathbf{q}_i, \mathbf{p}_i(t)) - \sum_{i \in V_{right}} H(\mathbf{q}_i, \mathbf{p}_i(t))$ *is invariant, with* $H(\mathbf{x}, \mathbf{y}) = -\sum_i x_i \ln y_i$.

Proof. The derivative of $\sum_{i \in V_{left}} \sum_{\gamma \in S_i} q_{i\gamma} \cdot \ln(p_{i\gamma}) - \sum_{i \in V_{right}} \sum_{\gamma \in S_i} q_{i\gamma} \cdot \ln(p_{i\gamma})$ has as follows:

$$
\begin{aligned}
\sum_{i \in V_{left}} \sum_{\gamma \in S} q_{i\gamma} \frac{d \ln(p_{i\gamma})}{dt} - \sum_{i \in V_{right}} \sum_{\gamma \in S} q_{i\gamma} \frac{d \ln(p_{i\gamma})}{dt} &= \sum_{i \in V_{left}} \sum_{\gamma \in S} q_{i\gamma} \frac{\dot{p}_{i\gamma}}{p_{i\gamma}} - \sum_{i \in V_{right}} \sum_{\gamma \in S} q_{i\gamma} \frac{\dot{p}_{i\gamma}}{p_{i\gamma}} \\
&= \sum_{i \in V_{left}} \sum_{(i,j) \in E} \left(\mathbf{q_i}^T A_{ij} \mathbf{p_j} - \mathbf{p_i}^T A_{ij} \mathbf{p_j} \right) - \sum_{i \in V_{right}} \sum_{(i,j) \in E} \left(\mathbf{q_i}^T A_{ij} \mathbf{p_j} - \mathbf{p_i}^T A_{ij} \mathbf{p_j} \right) \\
&= \sum_{i \in V_{left}} \sum_{(i,j) \in E} \left(\mathbf{q_i}^T - \mathbf{p_i}^T \right) A_{ij} \mathbf{p_j} - \sum_{i \in V_{right}} \sum_{(i,j) \in E} \left(\mathbf{q_i}^T - \mathbf{p_i}^T \right) A_{ij} \mathbf{p_j} \\
&= \sum_{i \in V_{left}} \sum_{(i,j) \in E} \left(\mathbf{q_i}^T - \mathbf{p_i}^T \right) A_{ij} (\mathbf{p_j} - \mathbf{q_j}) - \sum_{i \in V_{right}} \sum_{(i,j) \in E} \left(\mathbf{q_i}^T - \mathbf{p_i}^T \right) A_{ij} (\mathbf{p_j} - \mathbf{q_j}) \\
&= - \sum_{(i,j) \in E, i \in V_{left}, j \in V_{right}} \left[\left(\mathbf{q_i}^T - \mathbf{p_i}^T \right) A_{ij} (\mathbf{q_j} - \mathbf{p_j}) - \left(\mathbf{q_j}^T - \mathbf{p_j}^T \right) A_{ji} (\mathbf{q_i} - \mathbf{p_i}) \right] = 0.
\end{aligned}
$$

$\square$

The cross entropy between the Nash $\mathbf{q}$ and the state of the system, however is equal to the summation of the K-L divergence between these two distributions and the entropy of $\mathbf{q}$. Since the entropy of $\mathbf{q}$ is constant, we derive the following corollary (rephrasing the previous lemma):

Corollary 6.8. *Let* $\mathbf{p}(t)$ *with* $\mathbf{p}(0) \in \Delta$ *be a trajectory of the replicator dynamic when applied to a bipartite network of coordination games that has a fully mixed Nash equilibrium* $\mathbf{q}$ *then the K-L divergence between* $\mathbf{q}$ *and the* $\mathbf{p}(t)$ *is constant, i.e., does not depend on* t.

	Stag	Hare
Stag	5, 5	0, 4
Hare	4, 0	2, 2

(a) Stag hunt game.

	Stag	Hare
Stag	1, 1	0, 0
Hare	0, 0	w, w

(b) w-coordination game

Figure 10: Stag hunt game

6.5   *Applications of average case analysis*

We use the tools we have developed in the previous section to compute the regions of attractions and find the average case performance of replicator dynamics for classic game theoretic settings. The game we examine are: the Stag Hunt game, (parametric) coordination games, polymatrix coordination games played over a star as well as symmetric linear load balancing games.

6.5.1   Exact quantitative analysis of risk dominance in stag hunt

The Stag Hunt game (Figure 10(a)) has two pure Nash equilibria, $(Stag, Stag)$ and $(Hare, Hare)$ and a symmetric mixed Nash equilibrium with each agent choosing strategy $Hare$ with probability ⅔. Stag Hunt replicator trajectories are equivalent those of a coordination game[11]. Coordination games are potential games where the potential function in each state is equal to the utility of each agent. Since the mixed Nash is not weakly stable replicator dynamics converges to pure Nash equilibria for all but a zero measure of initial conditions (Theorem 6.4). When we study the replicator dynamic here, it suffices to examine its projection in the subspace $p_{1s} \times p_{2s} \subset (0, 1)^2$ which captures the evolution of the probability that each agent assigns to strategy $Stag$ (see Figure 11). Using the invariant property of Lemma 6.7, we compute the size of each region of attraction in this space and thus provide a quantitative analysis of risk dominance in the classic Stag Hunt game.

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[11]If each agent reduces their payoff in their first column by 4, the replicator trajectories remain invariant. This results to a w-coordination game with $w = 2$.
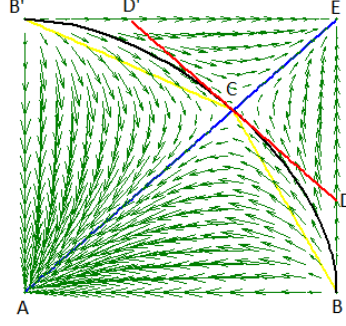
Figure 11: Vector field of replicator dynamics in Stag Hunt

Theorem 6.9. *The region of attraction of $(Hare, Hare)$ is the subset of $(0,1)^2$ that satisfies $p_{2s} < \frac{1}{2}(1 - p_{1s} + \sqrt{1 + 2p_{1s} - 3p_{1s}^2})$ and has Lebesgue measure $\frac{1}{27}(9 + 2\sqrt{3}\pi) \approx 0.7364$. The region of attraction of $(Stag, Stag)$ is the subset of $(0,1)^2$ that satisfies $p_{2s} > \frac{1}{2}(1 - p_{1s} + \sqrt{1 + 2p_{1s} - 3p_{1s}^2})$ and has Lebesgue measure $\frac{1}{27}(18 - 2\sqrt{3}\pi) \approx 0.2636$. The stable manifold of the mixed Nash equilibrium satisfies the equation $p_{2s} = \frac{1}{2}(1 - p_{1s} + \sqrt{1 + 2p_{1s} - 3p_{1s}^2})$ and has zero Lebesgue measure.*

Proof. In the case of stag hunt games, one can verify in a straightforward manner (via substitution) that $\frac{d\left(\frac{2}{3}\ln(\phi_{1s}(t,\mathbf{p})) + \frac{1}{3}\ln(\phi_{1h}(t,\mathbf{p})) - \frac{2}{3}\ln(\phi_{2s}(t,\mathbf{p})) - \frac{1}{3}\ln(\phi_{2h}(t,\mathbf{p}))\right)}{dt} = 0$, where $\phi_{i\gamma}(t,\mathbf{p})$, corresponds to the probability that each agent i assigns to strategy γ at time t given initial condition $\mathbf{p}$. This is a special case of Corollary 6.8. We use this invariant function to identify the stable and unstable manifold of the interior Nash $\mathbf{q}$.

Given any point $\mathbf{p}$ of the stable manifold of $\mathbf{q}$, we have that by definition

$$\lim_{t \to \infty} \phi(t, \mathbf{p}) = \mathbf{q}.$$

Similarly for the unstable manifold, we have that $\lim_{t \to -\infty} \phi(t, \mathbf{p}) = \mathbf{q}$. The time-invariant property implies that for all such points (belonging to the stable or unstable manifold), $\frac{2}{3}\ln(p_{1s}) + \frac{1}{3}\ln(1 - p_{1s}) - \frac{2}{3}\ln(p_{2s}) - \frac{1}{3}\ln(1 - p_{2s}) = \frac{2}{3}\ln(q_{1h}) + \frac{1}{3}\ln(1 - q_{1h}) - \frac{2}{3}\ln(q_{2h}) - \frac{1}{3}\ln(1 - q_{2h}) = 0$, since the fully mixed Nash equilibrium is symmetric. This condition is equivalent to $p_{1s}^2(1 - p_{1s}) = p_{2s}^2(1 - p_{2s})$, where $0 < p_{1s}, p_{2s} < 1$. It is

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straightforward to verify that this algebraic equation is satisfied by the following two distinct solutions, the diagonal line $(p_{2s} = p_{1s})$ and $p_{2s} = \frac{1}{2}(1-p_{1s}+\sqrt{1+2p_{1s}-3p_{1s}^2})$. Below, we show that these manifolds correspond indeed to the state and unstable manifold of the mixed Nash, by showing that this Nash equilibrium satisfies these equations and by establishing that the vector field is tangent everywhere along them.

The case of the diagonal is trivial and follows from the symmetric nature of the game. We verify the claims about $p_{2s} = \frac{1}{2}(1 - p_{1s} + \sqrt{1 + 2p_{1s} - 3p_{1s}^2})$. Indeed, the mixed equilibrium point in which $p_{1s} = p_{2s} = \frac{2}{3}$ satisfies the above equation. We establish that the vector filed is tangent to this manifold by showing in Lemma 6.10 that $\frac{\partial p_{2s}}{\partial p_{1s}} = \frac{\frac{dp_{2s}}{dt}}{\frac{dp_{1s}}{dt}} := \frac{p_{2s}\left(u_2(s)-(p_{2s}u_2(s)+(1-p_{2s})u_2(h))\right)}{p_{1s}\left(u_1(s)-(p_{1s}u_1(s)+(1-p_{1s})u_1(h))\right)}$, where the last equality is derived by the definition of replicator dynamics.

Lemma 6.10. *For any $0 < p_{1s}, p_{2s} < 1$, with $p_{2s} = \frac{1}{2}(1 - p_{1s} + \sqrt{1 + 2p_{1s} - 3p_{1s}^2})$ we have that:*

$$\frac{\partial p_{2s}}{\partial p_{1s}} = \frac{\frac{dp_{2s}}{dt}}{\frac{dp_{1s}}{dt}} = \frac{p_{2s}\left(u_2(s) - (p_{2s}u_2(s) + (1 - p_{2s})u_2(h))\right)}{p_{1s}\left(u_1(s) - (p_{1s}u_1(s) + (1 - p_{1s})u_1(h))\right)}.$$

Proof. By substitution of the stag hunt game utilities, we have that:

$$\frac{\zeta_{2s}}{\zeta_{1s}} = \frac{p_{2s}\left(u_2(s) - (p_{2s}u_2(s) + (1 - p_{2s})u_2(h))\right)}{p_{1s}\left(u_1(s) - (p_{1s}u_1(s) + (1 - p_{1s})u_1(h))\right)} = \frac{p_{2s}(1 - p_{2s})(3p_{1s} - 2)}{p_{1s}(1 - p_{1s})(3p_{2s} - 2)}. \quad (77)$$

However, $p_{2s}(1 - p_{2s}) = \frac{1}{2}p_{1s}(p_{1s} - 1 + \sqrt{1 + 2p_{1s} - 3p_{1s}^2})$. Combining this with (77),

$$\frac{\zeta_{2s}}{\zeta_{1s}} = \frac{(p_{1s} - 1 + \sqrt{1 + 2p_{1s} - 3p_{1s}^2})(3p_{1s} - 2)}{2(1 - p_{1s})(3p_{2s} - 2)} = \frac{1}{2}\frac{(\sqrt{1 + 3p_{1s}} - \sqrt{1 - p_{1s}})(3p_{1s} - 2)}{\sqrt{1 - p_{1s}} \cdot (3p_{2s} - 2)}. \quad (78)$$

Similarly, we have that $3p_{2s} - 2 = \frac{1}{2}\sqrt{1 + 3p_{1s}} \cdot (3\sqrt{1 - p_{1s}} - \sqrt{1 + 3p_{1s}})$. By multiplying and dividing equation (78) with $(\sqrt{1 + 3p_{1s}} + 3\sqrt{1 - p_{1s}})$ we get:

$$
\begin{aligned}
\frac{\zeta_{2s}}{\zeta_{1s}} &= \frac{1}{2}\frac{(\sqrt{1 + 3p_{1s}} + 3\sqrt{1 - p_{1s}})(\sqrt{1 + 3p_{1s}} - \sqrt{1 - p_{1s}})(3p_{1s} - 2)}{2\sqrt{1 - p_{1s}} \cdot \sqrt{1 + 3p_{1s}} \cdot (2 - 3p_{1s})} \\
&= -\frac{1}{4}\frac{(\sqrt{1 + 3p_{1s}} + 3\sqrt{1 - p_{1s}})(\sqrt{1 + 3p_{1s}} - \sqrt{1 - p_{1s}})}{\sqrt{1 + 2p_{1s} - 3p_{1s}^2})} \\
&= \frac{1}{2}\left(-1 + \frac{1 - 3p_{1s}}{\sqrt{1 + 2p_{1s} - 3p_{1s}^2}}\right) = \frac{\partial\left(\frac{1}{2}(1 - p_{1s} + \sqrt{1 + 2p_{1s} - 3p_{1s}^2})\right)}{\partial p_{1s}} = \frac{\partial p_{2s}}{\partial p_{1s}}.
\end{aligned}
$$

Finally, this manifold is indeed attracting to the equilibrium. Since the function $p_{2s} = y(p_{1s}) = \frac{1}{2}(1 - p_{1s} + \sqrt{1 + 2p_{1s} - 3p_{1s}^2})$ is a strictly decreasing function of p_{1s} in [0,1] and satisfies $y(2/3) = 2/3$, this implies that its graph is contained in the subspace $\left(0 < p_{1s} < 2/3 \cap 2/3 < p_{2s} < 1\right) \cup \left(2/3 < p_{1s} < 1 \cap 0 < p_{2s} < 2/3\right)$. In each of these subsets $\left(0 < p_{1s} < 2/3 \cap 2/3 < p_{2s} < 1\right), \left(2/3 < p_{1s} < 1 \cap 0 < p_{2s} < 2/3\right)$ the replicator vector field coordinates have fixed signs that "push" p_{1s}, p_{2s} towards their respective equilibrium values.

The stable manifold partitions the set $0 < p_{1s}, p_{2s} < 1$ into two subsets, each of which is flow invariant since the unstable manifold itself is flow invariant. Our convergence analysis for the generalized replicator flow implies that in each subset all but a measure zero of initial conditions must converge to its respective pure equilibrium. The size of the lower region of attraction[12] is equal to the following definite integral

$\int_0^1 \frac{1}{2}(1 - p_{1s} + \sqrt{1 + 2p_{1s} - 3p_{1s}^2})dx = \left[1/2\left(p_{1s} - \frac{p_{1s}^2}{2} + (-\frac{1}{6} + \frac{p_{1s}}{2})\sqrt{1 + 2p_{1s} - 3p_{1s}^2} - \frac{2arcsin[\frac{1}{2}(1-3p_{1s})]}{3\sqrt{3}} \right) \right]_0^1 = \frac{1}{27}(9 + 2\sqrt{3}\pi) = 0.7364$ and the theorem follows. □

6.5.2 Average price of anarchy analysis in coordination/consensus games via polytope approximations of regions of attraction

We focus on a parametric family of coordination games, as described in figure 10(b). We denote an instance of such a game a w-coordination/consensus game. We take the w parameter to be greater or equal to 1[13]. This game captures strategic situations where agents must learn to coordinate on a single action and where one pure equilibrium (consensus outcome) is preferable for both agents. The initial condition of the replicator dynamics captures each agent's initial bias. Both agents

---

[12]This corresponds to the risk dominant equilibrium $(Hare, Hare)$.

[13]It is easy to see that for any $0 < w < 1$, w-coordination game is isomorphic to $1/w$-coordination game after relabeling of strategies. Also, the replicator trajectories in the 2-coordination game are equivalent to the standard stag hunt game.

update their beliefs/distributions by applying the replicator and eventually the system converges to an equilibrium. Interestingly, since the mixed Nash is not weakly stable, Theorem 6.4 implies that the agents will reach a consensus with probability 1 as long as the initial conditions are chosen according to an arbitrary distribution F admitting a density with respect to the Lebesgue measure. A natural such prior (distribution) is the uniform one, since it encodes a total ignorance of the agents' initial biases. We wish to understand what is the expected system performance given a uniformly random initial condition. Although the inefficient equilibrium will arise with positive probability hopefully its probability is small enough that no matter the w efficiency gap between the two pure equilibria the average system performance is always within an absolute constant of the optimal, independent of w. We will show that this is indeed the case.

Theorem 6.11. *The average price of anarchy of the w-coordination game with $w \geq 1$ is at most $\frac{w^2+w}{w^2+1}$ and at least $\frac{w(w+1)^2}{w(w+1)^2-2w+2}$.*

For any w, a w-coordination game is a potential game and therefore it is payoff equivalent to a congestion game. The only two weakly stable equilibria are the pure ones, hence in order to understand the average case system performance it suffices to understand the size of regions of attraction for each of them. We focus on the projection of the system to the subspace $(p_{1s}, p_{2s}) \subset [0,1]^2$. We denote by ζ, ψ, the projected flow and vector field respectively.

Lemma 6.12. *All but a zero measure of initial conditions in the polytope (P_{Hare}):*

$$p_{2s} \leq -wp_{1s} + w$$
$$p_{2s} \leq -\frac{1}{w}p_{1s} + 1$$
$$0 \leq p_{1s}, p_{2s} \leq 1$$

converges to the $(Hare, Hare)$ equilibrium. All but a zero measure of initial conditions

in the polytope (P_{Stag}):

$$p_{2s} \geq -p_{1s} + \frac{2w}{w+1}$$

$$0 \leq p_{1s}, p_{2s} \leq 1$$

converges to the $(Stag, Stag)$ equilibrium.

Proof. First, we will prove the claimed property for polytope (P_{Stag}). Since the game is symmetric, the replicator dynamics are similarly symmetric with $p_{2s} = p_{1s}$ axis of symmetry. Therefore it suffices to prove the property for the polytope $P'_{Hare} = P_{Hare} \cap \{p_{2s} \leq p_{1s}\} = \{p_{2s} \leq p_{1s}\} \cap \{p_{2s} \leq -wp_{1s}+w\} \cap \{0 \leq p_{1s} \leq 1\} \cap \{0 \leq p_{2s} \leq 1\}$ We will argue that this polytope is forward flow invariant, *i.e.*, if we start from an initial condition $\mathbf{x} \in P'_{Hare}$ $\psi(t, \mathbf{x}) \in P'_{Hare}$ for all $t > 0$. On the p_{1s}, p_{2s} subspace P'_{Hare} defines a triangle with vertices $A = (0,0)$, $B = (1,0)$ and $C = (\frac{w}{w+1}, \frac{w}{w+1})$ (see Figure 11). The line segments AB, AC are trivially flow invariant. Hence, in order to argue that the ABC triangle is forward flow invariant, it suffices to show that everywhere along the line segment BC the vector field does not point "outwards" of the ABC triangle. Specifically, we need to show that for every point p on the line segment BC (except the Nash equilibrium C), $\frac{|\zeta_{1s}(\mathbf{p})|}{|\zeta_{2s}(\mathbf{p})|} \geq \frac{1}{w}$.

$$\frac{|\zeta_{1s}(\mathbf{p})|}{|\zeta_{2s}(\mathbf{p})|} = \frac{p_{1s}|p_{2s} - (p_{1s}p_{2s} + w(1-p_{1s})(1-p_{2s}))|}{p_{2s}|p_{1s} - (p_{1s}p_{2s} + w(1-p_{1s})(1-p_{2s}))|} = \frac{p_{1s}(1-p_{1s})(w - (w+1)p_{2s})}{p_{2s}(1-p_{2s})(-w + (w+1)p_{1s})}.$$

However, the points of the line passing through B, C satisfy $p_{2s} = w(1 - p_{1s})$.

$$
\begin{aligned}
\frac{|\zeta_{1s}(\mathbf{p})|}{|\zeta_{2s}(\mathbf{p})|} &= \frac{wp_{1s}(1-p_{1s})(1-(w+1)(1-p_{1s}))}{w(1-p_{1s})(1-w(1-p_{1s}))(-w+(w+1)p_{1s})} \\
&= \frac{p_{1s}(-w+(w+1)p_{1s})}{(1-w+wp_{1s})(-w+(w+1)p_{1s})} \\
&= \frac{p_{1s}}{1-w+wp_{1s}} \geq \frac{p_{1s}}{wp_{1s}} = \frac{1}{w}.
\end{aligned}
$$

We have established that the ABC triangle is forward flow invariant. Since the w-coordination game is a potential game, all but a zero measurable set of initial conditions converge to one of the two pure equilibria. Since ABC is forward invariant,

all but a zero measure of initial conditions converge to $(Hare, Hare)$. A symmetric argument holds for the triangle $AB'C$ with $B' = (0, 1)$. The union of ABC and $AB'C$ is equal to the polygon P_{Hare}, which implies the first part of the lemma.

Next, we will prove the claimed property for polytope (P_{Stag}). Again, due to symmetry, it suffices to prove the property for the polytope $P'_{Stag} = P_{Stag} \cap \{p_{2s} \leq p_{1s}\} = \{p_{2s} \leq p_{1s}\} \cap \{p_{2s} \geq -p_{1s} + \frac{2w}{w+1}\} \cap \{0 \leq p_{1s} \leq 1\} \cap \{0 \leq p_{2s} \leq 1\}$ We will argue that this polytope is forward flow invariant. On the p_{1s}, p_{2s} subspace P'_{Stag} defines a triangle with vertices $D = (1, \frac{w-1}{w+1})$, $E = (1, 1)$ and $C = (\frac{w}{w+1}, \frac{w}{w+1})$. The line segments CD, DE are trivially forward flow invariant. Hence, in order to argue that the CDE triangle is forward flow invariant, it suffices to show that everywhere along the line segment CD the vector field does not point "outwards" of the CDE triangle (see Figure 11) . Specifically, we need to show that for every point p on the line segment CD (except the Nash equilibrium C), $\frac{|\zeta_{1s}(\mathbf{p})|}{|\zeta_{2s}(\mathbf{p})|} \leq 1$.

$$\frac{|\zeta_{1s}(\mathbf{p})|}{|\zeta_{2s}(\mathbf{p})|} = \frac{p_{1s}|p_{2s} - (p_{1s}p_{2s} + w(1 - p_{1s})(1 - p_{2s}))|}{p_{2s}|p_{1s} - (p_{1s}p_{2s} + w(1 - p_{1s})(1 - p_{2s}))|} = \frac{p_{1s}(1 - p_{1s})(w - (w + 1)p_{2s})}{p_{2s}(1 - p_{2s})(-w + (w + 1)p_{1s})}.$$

However, the points of the line passing through C, D satisfy $p_{2s} = -p_{1s} + \frac{2w}{w+1}$.

$$\begin{aligned}
\frac{|\zeta_{1s}(\mathbf{p})|}{|\zeta_{2s}(\mathbf{p})|} &= \frac{p_{1s}(1 - p_{1s})(-w + (w + 1)p_{1s})}{(-p_{1s} + \frac{2w}{w+1})(-\frac{w-1}{w+1} + p_{1s})(-w + (w + 1)p_{1s})} \\
&= \frac{p_{1s}(1 - p_{1s})}{(-p_{1s} + \frac{2w}{w+1})(-\frac{w-1}{w+1} + p_{1s})} = \frac{p_{1s}(1 - p_{1s})}{\frac{2(w-1)}{w+1}(-\frac{w}{w+1} + p_{1s}) + p_{1s}(1 - p_{1s})} \leq 1.
\end{aligned}$$

We have established that the CDE triangle is forward flow invariant. Since the w-coordination is a potential game, all but a zero measurable set of initial conditions converge to one of the two pure equilibria. Since CDE is forward invariant, all but a zero measure of initial conditions converge to $(Stag, Stag)$. A symmetric argument holds for the triangle $CD'E$ with $D' = (\frac{w-1}{w+1}, 1)$. The union of CDE and $CD'E$ is equal to the polygon P_{Stag}, which implies the second part of the lemma. $\qquad\square$

Proof. The measure/size of $\mu(P_{Hare}) = 2|ABC| = \frac{w}{w+1}$, and similarly the measure of $\mu(P_{Stag}) = 2|CDE| = \frac{2}{(w+1)^2}$. The average limit performance of the replicator satisfies $\int_{g(\Delta)} sw(\psi(x))d\mu \geq 2w \cdot \mu(P_{Hare}) + 2\big(1 - \mu(P_{Hare})\big) = 2\frac{w^2+1}{w+1}$. Furthermore, $\int_{g(\Delta)} sw(\psi(x))d\mu \leq 2w\big(1 - \mu(P_{Stag})\big) + 2 \cdot \mu(P_{Stag}) = 2w(1 - \frac{2}{(w+1)^2}) + 2 \cdot \frac{2}{(w+1)^2} = 2w - 4\frac{w-1}{(w+1)^2}$. This implies that $\frac{w(w+1)^2}{w(w+1)^2-2w+2} \leq APoA \leq \frac{w^2+w}{w^2+1}$. $\qquad\square$

By combining the exact analysis of the standard Stag Hunt game (Theorem 6.9), Theorem 6.11 and optimizing over w we derive that:

Corollary 6.13. *The average price of anarchy of the class of w-coordination games with $w > 0$ is at least $\frac{2}{1+\frac{9+2\sqrt{3}\pi}{27}} \approx 1.15$ and at most $\frac{4+3\sqrt{2}}{4+2\sqrt{2}} \approx 1.21$. In comparison, the price of anarchy for this class of games is unbounded.*

6.6 Coordination/consensus games on a N-star graph

In this section we show how to estimate the topology of regions of attraction for star networks of w-coordination games. This corresponds to strategic settings where some agents again need to reach consensus but where there is an agent who works as a center communicating with all agents at once. The price of anarchy and stability of these games remain unchanged as we increase the size of the star. Specifically the price of stability is equal to 1 whereas the price of anarchy can become unbounded large for large w. We will argue that the average performance is approximately optimal.

This game has two pure Nash equilibria where all agents either play the first strategy *i.e., Stag*, or the second *i.e., Hare*. For simplicity in notation sometimes we denote the first strategy, *i.e., Stag*, as strategy A and the other strategy, *i.e., Hare*, as strategy B. This game has a continuum of mixed Nash equilibria. Our goal is to produce an oracle which given as input an initial condition outputs the resulting equilibrium that system converges to.

Example. In order to gain some intuition on the construction of these oracles let's focus on the minimal case with a continuum of equilibria ($N = 3$, center with two
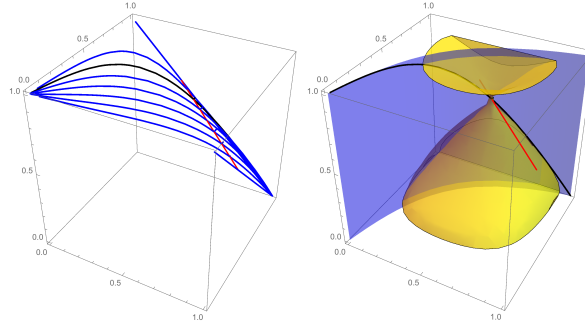
(a) Examples of stable manifolds for different mixed Nash.

(b) Stable manifolds lie on the intersection of level sets of invariant functions.

Figure 12: Star network coordination game with 3 agents

neighbors). Since each agent has two strategies it suffices to depict for each one the probability with which they choose strategy A (the "bad" *Stag* strategy). Hence, the phase space can be depicted in 3 dimensions. Figure 12 depicts this phase space. The point $(0, 0, 0)$ captures the good pure Nash (all B), whereas the point $(1, 1, 1)$ the bad pure Nash (all A). There is also a continuum of unstable mixed Nash equilibria. Specifically, as long as the center player chooses A with probability $w/(w + 1)$ and the summation of the probabilities that the two other agents assign to A is exactly $2w/(w + 1)$. In figure 12, we have chosen $w = 2$ this continuum of equilibria corresponds to the red straight line. These are unstable equilibria and by Theorem 6.4 almost all initial conditions are attracted to the two attracting pure Nash. For any mixed Nash equilibrium there exists a curve (co-dimension 2) of points that converge to it. Figure 12(a) depicts several such stable manifolds for sample mixed equilibria along the equilibrium line. The union of these stable manifolds partitions the state space into two regions, one attracting to equilibrium (A, A, A) and the other attracting to the equilibrium (B, B, B)). Hence, in order to construct our oracle its suffices to have a description of these attracting curves for the mixed equilibria. However, as shown in figure 12(b), we have identified two distinct invariant functions for the replicator dynamic in this system. Given any mixed Nash equilibrium, the set of

points of the state space which agree with the value of each of these invariant functions define a set of co-dimension one (the double hollow cone and the curved plane). Any points that converge to this equilibrium must lie on the intersection of these sets (black curve). In fact, due to our point-wise convergence theorem, it immediately follows that this intersection is exactly the stable manifold of the unstable equilibrium. The case for general N works analogously, but now we need to identify $N - 1 \, (= n)$ invariant functions in an algorithmic, efficient manner.

Here is the high level idea of the analysis: We start the analysis by showing that the only fixed points with region of attraction with positive measure are when all players choose strategy $Stag$ or all players choose strategy $Hare$. After that we show that the limit point will be either one of the two mentioned, or a fully mixed. Therefore we need to compute the regions of attraction of the 2 fixed points where all choose $Stag$ or all choose $Hare$. To do that, we need to compute the boundary of these two regions (namely the center/stable manifold of the fully mixed ones). This happens as follows: Given an initial point $(x_1, ..., x_n, y)$, we compute the possible fully mixed limit point $(x'_1, ..., x'_n, \frac{w}{w+1})$ (will be one possible because we have one variable of freedom due to Lemma 6.14 below) that is on the boundary of the two regions. If the initial condition is on the upper half space w.r.t to the possible fully mixed limit point $(x'_1, ..., x'_n, \frac{w}{w+1})$ the dynamics converge to the everyone playing $Stag$, otherwise to everyone playing $Hare$. To simplify notation in the remainder of this section, we rename strategy $Stag$ as strategy A and strategy $Hare$ as strategy B.

6.6.1   Structure of fixed points

If a "leaf" agent i applies a randomized/mixed strategy at a fixed point, it must be the case that the strategy of the center agent $y = \frac{w}{w+1}$. Otherwise, the "leaf" agent would strictly prefer either strategy A or strategy B. Hence the fixed points of the star graph game have the following structure: If the center agent has a pure

strategy, then all agents must be pure. If the center agent has a mixed strategy, then $\sum_i x_i = \frac{w}{w+1}n$. In that case, if all the "leaf" agents have pure strategies then y can have any value in $[0, 1]$, otherwise $y = \frac{w}{w+1}$.

6.6.2 Invariants and oracle

Lemma 6.14. $[\ln(x_i(t)) - \ln(1 - x_i(t))] - [\ln(x_j(t)) - \ln(1 - x_j(t))]$ *is invariant for all* i, j *(independent of t).*

Proof. By taking the derivative, we get $\frac{d}{dt}[\ln(x_i(t)) - \ln(1 - x_i(t))] = [y - w \cdot (1 - y)]$ and $\frac{d}{dt}[\ln(x_j(t)) - \ln(1 - x_j(t))] = [y - w \cdot (1 - y)]$ and claim follows. $\square$

Next, we will argue that if we start in the interior of Δ, the system can converge to fixed points, where either all agent play A or B, or to a fully mixed Nash where $y = \frac{w}{w+1}$ and $\sum x_i = \frac{w}{w+1}n$.

Lemma 6.15. *For all initial conditions in the interior of Δ, either the dynamic converges to all A's, i.e, $(1, \ldots, 1)$, or to all B's, i.e., $(0, \ldots, 0)$, or to some fully mixed fixed point, i.e, $(x_1, \ldots, x_n, \frac{w}{w+1})$ with $0 < x_i < 1$ for all i, and $\sum_i x_i = \frac{w}{w+1}n$.*

Proof. We consider the following two cases:

- If $x_i(t) \to 1$ for some i, then $\ln(x_i(t)) - \ln(1 - x_i(t)) \to +\infty$. So from Lemma 6.14 for every j we get that $\ln(x_j(t)) - \ln(1 - x_j(t)) \to +\infty$, hence $x_j(t) \to 1$. Due the structure of the equilibrium set and point-wise convergence, $y(t)$ must converge to 0 or 1. Due the fact that the fixed point $(1, \ldots, 1, 0)$ is repelling we get that the system converges to all A's. The same argument is used if $x_i(t) \to 0$ for some i.

- If the dynamic converges to an equilibrium were all "leaf" agents are mixed, then $y = \frac{w}{w+1}$ and $\sum_i x_i = \frac{w}{w+1}n$ because by the analysis of the structure of the fixed points that is the only possibility.

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□

Let $(x_1(0), \ldots, x_n(0), y(0))$ be the initial condition, where $x_i(0), y(0)$ are the probabilities agent i, center agent chooses A $(1 - x_i(0), 1 - y(0)$ will be the probability to choose $B)$ respectively. By Lemma 6.15, we know that the corresponding trajectory will converge either to the all A's equilibrium or the all B's equilibrium or a fully mixed one. Next, by using Lemma 6.14 we will narrow down the possibilities for this fully mixed equilibrium to a single one, which we denote by $(x_1, \ldots, x_n, \frac{w}{w+1})$.

For each leaf agent $i > 1$, we define a positive constant c_i such that

$$c_i = \frac{x_i(0)/(1 - x_i(0))}{x_1(0)/(1 - x_1(0))}.$$

Due to Lemma 6.14 the quantity $\frac{x_i(t)/(1 - x_i(t))}{x_1(t)/(1 - x_1(t))}$ is time invariant. Hence, the limit point $(x_1, \ldots, x_n, \frac{w}{w+1})$ must satisfy this condition, $i.e.,$

$$x_i = \frac{c_i x_1}{1 + (c_i - 1)x_1} \tag{79}$$

Moreover, by Lemma 6.15 it must satisfy $\sum x_i = \frac{w}{w+1}n$, which combined with (79) implies that:

$$\sum_i \frac{c_i x_1}{1 + (c_i - 1)x_1} = \frac{w}{w+1}n \tag{80}$$

where we have defined $c_1 = 1$.

Observe that the function $f(x) = \frac{cx}{1+(c-1)x}$ is strictly increasing in $[0, 1]$ (given any fixed positive c) and $f(0) = 0, f(1) = 1$. Therefore $g(x) = \sum_i \frac{c_i x}{1+(c_i-1)x} - \frac{w}{w+1}n$ is strictly increasing in $[0, 1]$ (as sum of strictly increasing functions in $[0, 1]$) and $g(0) = -\frac{w}{w+1}n < 0$ and $g(1) = n - \frac{w}{w+1}n > 0$. Thus, it has always a unique solution in $[0, 1]$ and equivalently the system of equations (79,80) has a unique solution. Together with $y = \frac{w}{w+1}$, the equilibrium limit point lies in the interior of Δ. Given $x_1(0), \ldots, x_n(0)$ we can compute (approximate with arbitrary small error ϵ) $x_1, \ldots, x_n$ via binary search (using Bolzano's theorem).

Lemma 6.16. *Since star graph is a bipartite graph from Lemma 6.7 we have that since* $(x_1, \ldots, x_n, y)$ *is a fully mixed Nash then along any system trajectory* $((x_1(t), \ldots, x_n(t), y(t)))$ *the function*

$$\frac{w}{w+1} \ln(y(t)) + \frac{1}{w+1} \ln(1-y(t)) - \sum_i [x_i \ln(x_i(t)) + (1-x_i) \ln(1-x_i(t))]$$

is (time) invariant, i.e. independent of t.

Lemma 6.17. *If* $y(t) \geq \frac{w}{w+1}$ *and* $\sum x_i(t) > \frac{w}{w+1}n$ *for some t, the trajectory converges to all A's and if* $y(t) \leq \frac{w}{w+1}$ *and* $\sum x_i(t) < \frac{w}{w+1}n$ *for some t, the trajectory converges to all B's.*

Proof. In the first case, $y(t)$ is increasing and $x_i(t)$ (for all i) are non-decreasing and thus $y(t') > \frac{w}{w+1}$ and $\sum x_i(t') > \frac{w}{w+1}n$ holds for all $t' > t$. In the second case $y(t)$ is decreasing and $x_i(t)$ (for all i) are non-increasing and thus $y(t') < \frac{w}{w+1}$ and $\sum x_i(t') < \frac{w}{w+1}n$ holds for all for $t' > t$. Combining this with Lemma 6.15, concludes the proof. $\qquad\square$

Therefore if a trajectory converges to the fully mixed equilibrium $(x_1, \ldots, x_n, \frac{w}{w+1})$ then at any time t we must have $\sum x_i(t) > \frac{w}{w+1}n$ and $y(t) < \frac{w}{w+1}$ ($x_1(t), \ldots, x_n(t)$ are decreasing and $y(t)$ increasing) or $\sum x_i(t) < \frac{w}{w+1}n$ and $y(t) > \frac{w}{w+1}$ ($x_1(t), \ldots, x_n(t)$ are increasing and $y(t)$ decreasing). Combining all the facts together, we get that the stable manifold of the fixed point $(x_1, \ldots, x_n, \frac{w}{w+1})$ can be described as follows: $(x_1(0), \ldots, x_n(0), y(0))$ lies on the stable manifold if $\sum_i x_i(0) > n\frac{w}{w+1}$ and $y(0) < \frac{w}{w+1}$ or $\sum_i x_i(0) < n\frac{w}{w+1}$ and $y(0) > \frac{w}{w+1}$ and by Lemma 6.16 we get that

$$y(0)^{\frac{w}{w+1}}(1-y(0))^{\frac{1}{w+1}} = c\prod_i x_i(0)^{x_i}(1-x_i(0))^{1-x_i}, \tag{81}$$

where $c = \frac{\left(\frac{w}{w+1}\right)^{\frac{w}{w+1}}\left(\frac{1}{w+1}\right)^{\frac{1}{w+1}}}{\prod_i (x_i)^{x_i}(1-x_i)^{1-x_i}}$.

Lemma 6.18. *The function* $x^w(1-x)$ *is strictly increasing in* $[0, \frac{w}{w+1}]$ *and decreasing in* $[\frac{w}{w+1}, 1]$.

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By Lemma 6.18 we have that there exist at most two $y(0)$ that satisfy (81), one which is $\geq \frac{w}{w+1}$ and one that $\leq \frac{w}{w+1}$. If $\sum x_i(0) < n\frac{w}{w+1}$, $y(0)$ should be the largest root of the two so that dynamics converges to the fully mixed, otherwise the smallest root. If now the initial condition $y(0)$ does not satisfy (81), then the dynamics converges to all A's if $y(0)$ is greater that it is supposed (so that dynamics converges to the fully mixed) and to all B's otherwise. Therefore we have the oracle below:

Oracle

1. Input: $(x_1, ..., x_n, y)$

2. Output: A or B or mixed

3. If $\sum x_i > (\geq)\frac{w}{w+1}n$ and $y \geq (>)\frac{w}{w+1}$ return A.

4. If $\sum x_i < (\leq)\frac{w}{w+1}n$ and $y \leq (<)\frac{w}{w+1}$ return B.

5. Set $c_i = \frac{x_i(1-x_1)}{x_1(1-x_i)}$ for $i \geq 2$ and $c_1 = 1$.

6. Solve equation $\sum_{i=1}^{n} \frac{x_1'c_i}{1+(c_i-1)x_1'} = \frac{w}{w+1}n$ (binary search) to compute x_1' and set $x_i' = \frac{c_i x_1'}{1+(c_i-1)x_1'}$ for $i \geq 2$.

7. Let $f(t) = \left(\frac{t(w+1)}{w}\right)^{\frac{w}{w+1}} [(1-t)(w+1)]^{\frac{1}{w+1}} - \prod_i \left(\frac{x_i}{x_i'}\right)^{x_i'} \left(\frac{1-x_i}{1-x_i'}\right)^{1-x_i'}$.

8. If $(\sum_i x_i > \frac{w}{w+1}n$ and $f(y) < 0)$ or $(\sum_i x_i < \frac{w}{w+1}n$ and $f(y) > 0)$ return B.

9. If $(\sum_i x_i > \frac{w}{w+1}n$ and $f(y) > 0)$ or $(\sum_i x_i < \frac{w}{w+1}n$ and $f(y) < 0)$ return A.

10. return mixed.

Table 3: Oracle algorithm

Remark 15. *Given any point from Δ uniformly at random, under the assumption of solving exactly the equations to compute $x_1', ..., x_n'$ and infinite precision the probability that the oracle above returns mixed is zero.*

Given this oracle it is straightforward to establish an upper bound of 1.21 for the average price of anarchy, which is independent of w as well as the size of the star.

Corollary 6.19. *The average price of anarchy for the class of star w-coordination games (with $n+1$ agents) is at most* 1.21.

Proof. There are exactly two possible outcomes with positive probability; all the agents choose strategy A and all choose strategy B. Assume we take one sample at random $(x_1, ..., x_n, y)$ from $\times_{i=1}^{n+1} \Delta_2$ where $n+1$ are the number of players. It turns out from the oracle above on the star-graph (see also discussion above) game that if $\sum_i x_i < n\frac{w}{w+1}$ and $y < \frac{w}{w+1}$ then the dynamics eventually converge to all agents choose B. Hence the region of attraction of the outcome all agents choose B will be at least the probability p that a sample at random satisfies $\sum_i x_i < n\frac{w}{w+1}$ and $y < \frac{w}{w+1}$. Since the optimal is $w(n+1)$, we get that the average price of anarchy is at most $\frac{w(n+1)}{pw(n+1)+(1-p)(n+1)} = \frac{w}{pw+1-p}$. Using properties of IrwinHall distribution (sum of uniform random variables follows Irwin-Hall) we see that the probability is increasing in n (for fixed w). Hence the average price of anarchy is decreasing in n (since $w \geq 1$, and so an upper bound for the average price of anarchy of this class of games can be achieved for $n = 1$, case which we have already analyzed (see Corollary 6.13. From Corollary 6.13 the claim follows. □

6.7 APoA in linear, symmetric load balancing games

6.7.1 Linear symmetric load balancing games

In this section, we prove the following bounds on the average price of anarchy of linear, symmetric load balancing games. In symmetric load balancing games, each agent[14] chooses a distribution over machines selfishly and we assume that the cost of machine γ is a linear function of γ's load.

Theorem 6.20 (APoA for linear load balancing). *The average price of anarchy in terms of makespan of symmetric, linear load balancing games is at most* $3/2$.

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[14]Agents have same cost functions.

Moreover, generically, the average price of anarchy of symmetric, linear load balancing games is 1. *Specifically, given any number of agents and machines, the set of linear latency functions such that the average price of anarchy of the resulting game is greater than* 1 *is a zero measure set within the set of all linear latency functions.*

We will break down the proof of theorem 6.20 into several technical lemmas. The next definition encodes Nash equilibria where randomizing agents do not "interact" with each other.

Definition 24 (**Almost pure NE**)**.** *We call a mixed Nash equilibrium of a load balancing game to be almost pure, if the intersection of the supports of the strategies of any two randomizing agents contains only edges whose latency functions are constant functions.*

Lemma 6.21. *The average price of anarchy of a symmetric, linear load balancing games is at most equal to the ratio of the cost of the worst almost pure Nash equilibrium divided by the cost of the optimal outcome.*

Proof. By corollary 6.5 we have that for all but a zero measure of initial conditions replicator dynamics converges to weakly stable equilibria. By definition, weakly stable equilibria have the property that given any two agents with mixed strategies if one agent deviates to one the strategies in his support and plays it with probability one then the second agent should still stay indifferent between the strategies in his support. If there exists two agents with mixed strategies such that the intersection of their supports contains machines with strictly increasing latency functions then if one agent deviates to playing that machine with probability one, he will strictly increase the cost experienced by the second agent on that machine, whereas by this deviation he can only decrease the cost of all other machines in the support of the second agent. The second agent is no longer indifferent between the strategies in his support and thus the initial equilibrium was not weakly stable. In the worst case average price

of anarchy places all of the probability mass of initial conditions to the worst almost pure Nash equilibrium. In this case the average price of anarchy would be equal to the ratio of the cost of the worst almost pure Nash equilibrium divided by the cost of the optimal outcome. □

Lemma 6.22 (**Pure NE are optimal**). *In symmetric linear load balancing games all pure Nash equilibria have optimal makespan.*

Proof. Suppose not, that is, suppose that there exists a pure Nash equilibrium whose makespan, *i.e.,* the load of the most congested machine, is not optimal amongst all outcomes/configurations. That means that its most loaded machine must be a machine with a strictly increasing cost function that has higher load than its load at the optimal outcome[15]. Hence, there must be another machine whose load is strictly less than its load at the optimal configuration. If we move one agent from the first to the second machine we claim that its cost will strictly decrease. Indeed, its new latency is at most the latency of the second machine in the optimal configuration, which is less or equal to the optimal makespan, which by hypothesis is strictly less than the makespan of the first configuration, which was its original cost. Hence, the original configuration cannot be a Nash equilibrium and we have reached a contradiction. □

Lemma 6.23. *In any symmetric, linear load balancing games the ratio of the cost of the worst almost pure Nash equilibrium divided by the cost of the optimal outcome is at most $3/2$. Furthermore, this bound is tight.*

Proof. First, we create the lower bound. We have a load balancing game with two agents and three machines. The latency function for the first machine is $3x$ whereas for the other two machines is $2x$. It is straightforward to check that the strategy outcome where the first agent chooses the first machine and the second agent chooses

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[15]If there exist more than one outcomes with minimal makespan, we just arbitrary focus on one of the optimal configurations.

one of the remaining two machines uniformly at random is a Nash equilibrium and, in fact, a weakly stable one. The makespan of this equilibrium is 3, whereas the optimal state has each of the two agents choosing deterministically one of the last two machines and using it by themselves. The makespan of that outcome is 2, which results in a lower bound of $3/2$.[16]

Next, we will show that this bound is tight. First, we will establish that it suffices to examine Nash equilibria where the intersection between the supports of the mixed strategies of any two randomizing agents is empty. Indeed, suppose that we have two randomizing agents where the intersection of their supports contains some machines with constant latency functions. If we force one of the two agents to deviate and choose deterministically the strategy of constant latency in his support then the makespan of the state remains constant and furthermore the outcome is still a weakly stable Nash. The reason that it remains a Nash is that if an agent wished to deviate to some strategy used by the deviating agent originally, then when deviating to that machine he would experience exactly the same cost as when using the machine with the constant cost function. Thus, he could have profitably deviated in the initial configuration. This is impossible since that configuration was a Nash equilibrium. Trivially, this new Nash equilibrium is weakly stable since we have only decreased the number of randomizing agents and the supports of the remaining randomizing agents remained the same. We can keep performing these deviations up until there no longer randomizing agents for which the intersection of the supports contains any machine (of constant latency function). Hence, in terms of identifying the almost pure Nash equilibrium with the worst makespan it suffices to focus on the set of almost mixed NE where the intersection of the supports of any two randomizing agents is empty.

We have established that if suffices to focus on mixed Nash equilibria where each machine has at most one randomizing agent. We will establish that the makespan of

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[16]This construction is due to Bobby Kleinberg,

each such equilibrium is within a ³/₂ factor of the makespan of a pure Nash equilibrium, which by lemma 6.22 implies that it is within a ³/₂ factor of the optimal makespan. The argument is as follows: We will start from the mixed Nash and will proceed by fixing the randomizing agents to playing strategies in their support with probability one. We start from the randomizing agent i that experiences minimum cost amongst all randomizing agents. We fix him to playing the strategy in his support that he chose with minimal probability in the original mixed Nash. We also fix the rest of the randomizing agents to arbitrary strategies in their support. Next, we repeatedly go through all agents in decreasing cost order and we allow each agent to move and migrate to the least expensive (available) path if it is strictly cheaper than his current path. Due to symmetry once we find one agent who does not wish deviate all of the rest of the agents do not wish to deviate either due to symmetry of the available paths. This process will terminate at equilibrium since this is a potential game. Furthermore, agent i (nor of any of the other agents in his machine) will ever move during this process. If he did move then there would exist at some point a profitable deviating move from him. However, immediately after fixing the randomizing agents to choosing something in their current support, agent i did not have any improving deviations since his experienced cost was minimal amongst all randomizing agents and hence at least as small as the cost of any deviation. In fact, the cheapest available deviations are exactly the strategies that belonged in his support. As we allow costly agents to move greedily from their current strategy to the best available strategy the cost of the best available deviation cannot decrease with time. Thus, agent i will not deviate. Hence, the makespan at the resulting pure Nash equilibrium will be at least equal the cost of agent i when his was fixed to the strategy that he played with minimal probability. If we denote that edge as e and its load (excluding agent i) as x_e then this implies that the makespan at the resulting Nash and thus the optimal makespan is at least $a_e(x_e + 1) + b_e$. However, the original mixed state was

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an equilibrium and if agent i played strategy e with probability p then no agent in the original Nash equilibrium would experience cost more than $a_e(x_e + p + 1) + b_e$.[17] But since e was chosen to be the strategy played with minimal probability in his original support $p \leq 1/2$ and hence no agent can experience cost more than $a_e(x_e + 3/2) + b_e$. So, the original makespan is at most $a_e(x_e + 3/2) + b_e$ and the optimal makespan is at least $a_e(x_e + 1) + b_e$. The ratio between these two terms becomes maximal (and equal to $3/2$) for $b_e = 0$ and $x_e = 0$, which is exactly satisfied by our tight lower bound. $\square$

Remark 16. *If we slightly perturb the above tight example so that the latency function for the first machine is $3x$ whereas for the other two machines is $2x + \epsilon$ then the continuum of equilibria with the bad makespan will have a non-negligible region of attraction resulting in an average price of anarchy which is strictly greater than one.*

Lemma 6.24. *In generic symmetric linear load balancing games the set of almost pure Nash equilibria coincides with the set of pure Nash equilibria. Specifically, the set of linear latency functions such the set of almost pure Nash equilibria is a strict superset of the set of pure Nash equilibria is of measure zero within the set of all linear latency functions.*

Proof. We will show that if a linear symmetric load balancing game has an almost pure Nash equilibrium that is not pure, *i.e.*, that has at least one agent using a randomized strategy, then the coefficients of the linear latency functions belong to a zero measure set. Indeed, let's focus on one of the randomizing agents. Since this agent is indifferent between (at least) two machines/edges e, e' and he is the only randomizing agent using these machines (or some of these machines have a constant latency function) then there exist integer numbers k, k', so that the cost of these two machines are equal under loads k, k'. This implies that $a_e \cdot k + b_e = a_{e'} \cdot k' + b'_{e'}$. However, for any fixed k, k' the set of coefficients $a_e, a_{e'}, b_e, b_{e'}$ that satisfy this linear

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[17]If he did we would strictly prefer to deviate to edge e.

equation is a zero measure set. Hence, given any number of agents and machines the set of functions that have almost pure Nash equilibria that are not pure can be expressed as a countable union of zero-measure sets, which is a zero-measure set. □

By combining the lemmas of this section, Theorem 6.20 follows immediately.

6.7.2   Better APoA in N balls N bins

In the classic game of N identical balls, with N identical bins, each ball chooses a distribution over the bins selfishly and we assume that the cost of bin γ is equal to γ's load. We know for this game that the PoA is $\Omega(\frac{\log N}{\log \log N})$ [35]. We prove that the Average PoA is 1.

Theorem 6.25 (APoA in N balls N bins). *The average price of anarchy in terms of makespan for the (identical) N-balls N-bins is 1.*

This is derived via Corollary 6.5 and by showing that in this case the set of weakly stable Nash equilibria coincides with the set of pure equilibria.

Claim 6.26 (Every weakly stable NE is pure). *In the problem of N identical balls and N identical bins every weakly stable Nash equilibrium is pure.*

Proof. Assume we have a weakly Nash equilibrium **p**. From corollary 6.5, we have the following facts:

- Fact 1: For every bin γ, if a player i chooses γ with probability $1 > p_{i\gamma} > 0$, he must be the only player that chooses that bin with nonzero probability. Let i, j two players that choose bin γ with nonzero probabilities and also $p_{i\gamma}, p_{j\gamma} < 1$. Clearly if player i changes his strategy and chooses bin γ with probability one, then player j doesn't stay indifferent (his cost $c_{i\gamma}$ increases).

- Fact 2: If player i chooses bin γ with probability one, then he is the only player that chooses bin γ with nonzero probability. This is true because every player $j \neq i$ can find a bin with load less than 1 to choose.

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From Facts 1,2 and since the number of balls is equal to the number of bins we get that **p** must be pure. □

Proof of Theorem 6.25. Hence from Lemma 6.26 and 6.5 we get that for all but measure zero starting points of $g(\Delta)$, the replicator converges to pure Nash Equilibria. Every pure Nash equilibrium (each ball chooses a distinct bin) has social cost (makespan) 1 which is also the optimal. Hence the Average PoA is 1. □

Remark 17. *The lemma below shows how crucial is Lindelöf's lemma A.1(essentially separability of $\mathbb{R}^m$ for all m) in the proof of Theorem 6.4. Even simple instances of games with constant number of agents and strategies may have uncountably many equilibria. In such games, naive union bound arguments do not suffice since we cannot argue about the measure of an uncountable union of measure zero sets.*

Lemma 6.27. *For $N \geq 4$ the set of NE of the N balls N bins game is uncountable.*

Proof. We will prove it for $N = 4$ and then the generalization is easy, *i.e.*, if $N > 4$ then the first 4 players will play as shown below in the first 4 bins and each of the remaining $N - 4$ players will choose a distinct remaining bin. Below we give matrix A where $A_{i\gamma} = p_{i\gamma}$. Observe that for any $x \in [\frac{1}{4}, \frac{3}{4}]$ we have a Nash equilibrium.

$$
A = \begin{pmatrix}
x & 1-x & 0 & 0 \\
1/2 & 0 & 1/2 & 0 \\
0 & 1/2 & 0 & 1/2 \\
0 & 0 & x & 1-x
\end{pmatrix}.
$$

□

6.8 Conclusion and remarks

The results of this chapter appear in [102] and it is joint work with Georgios Piliouras. We show that replicator dynamics converges point-wise to fixed points for linear congestion and network coordination games. Moreover, we define an average

case analysis notion in dynamical systems focusing on games and replicator dynamics. We call this notion average price of anarchy (APoA) and provide upper and lower bounds for APoA in different classes of games. Several questions arise:

- **Other settings/games/mechanisms.** In recent followup work, [127] applies our approach to peer prediction mechanisms where the size of the basin of attraction of the truthful equilibrium is used as a proxy for the robustness of truthful play. The replicator model predicts/confirms the significant improvement in robustness of recent mechanisms over earlier approaches. It would be interesting to test the robustness of other (approximately) truthful, differentially private mechanisms in a similar manner.

- **Other dynamics.** Perform average case analysis for other dynamics and compare them against replicator dynamics.

- **Generalization of APoA.** Generalize the notion of APoA to dynamics that do not necessarily converge. In particular, it would be intriguing to define an APoA notion for chain recurrent sets (see [106]).

- **Point-wise convergence.** Generalize the point-wise convergence result to a larger class of congestion games, (*e.g.,* for polynomial cost functions).

- **Volumes of regions of attraction as a function.** Given a prior distribution over initial conditions (*e.g.,* uniform), every point-wise convergent dynamical system with isolated fixed points induces a probability distribution over these fixed points. By approximating this function (from priors over initial conditions to posteriors over equilibria), we can predict the average case (long-term) behavior of the system (without having the equations of the dynamics). Nontrivial distributions will result to a (unique) distribution/prediction that puts positive measure on several equilibria. It would be interesting to see a formal theory along these lines.

CHAPTER VII

GRADIENT DESCENT AND SADDLE POINTS

7.1   Introduction

The interplay between the structure of saddle points and the performance of gradient descent dynamics is a critical and not well understood aspect of non-convex optimization. Despite our incomplete theoretical understanding, in practice, the intuitive nature of the gradient descent method (and more generally gradient-like algorithms) make it a basic tool for attacking non-convex optimization problems for which we have very little understanding of the geometry of their saddle points. In fact, these techniques become particularly useful as the equilibrium structure becomes increasingly complicated, *e.g.,* such as in the cases of nonnegative matrix factorization [73] or congestion/potential games [122] (see Chapter 6), where symmetries in the nature of non-convex optimization problems give rise to continuums of saddle points with complex geometry. In these cases, particularly, the simplistic, greedy attitude of the gradient descent method, which is by design agnostic towards the global geometry of the cost function to be minimized, comes rather handy. As we move forward in time, the cost keeps decreasing and convergence is guaranteed.

This simplicity, however, comes at least seemingly at a significant cost. For example, it is well known that there exist instances where bad initialization of gradient descent converges to saddle points [95]. Despite the existence of such worst case instances in theory, practitioners have been rather successful at applying these techniques across a wide variety of problems [117]. Lee *et al.* [74] have given a very clear justification of the effectiveness of gradient descent methods in terms of circumventing the saddle equilibrium problem using tools from dynamical systems. At a glance,

the paper argues the following intuitively clear message: The instability of (locally unstable) saddle points translates to a global phenomenon and the probability of converging to such a saddle point given a randomly chosen (random not over a local neighborhood but over the whole state space) initial condition is zero. We have seen the analogue of this in Theorems 2.9, 3.15, 3.13.

Formally, Lee *et al.* define a cost function f as satisfying the "strict saddle" property if each critical point $\mathbf{x}$ of f is either a local minimizer, or a strict saddle, *i.e.*, $\nabla^2 f(\mathbf{x})$ has at least one strictly negative eigenvalue (for formal definitions see Definition 25). They argue that if $f : \mathbb{R}^N \to \mathbb{R}$ is a twice continuously differentiable function then gradient descent with constant step-size α (defined by $\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha \nabla f(\mathbf{x}_k)$) with a random initialization and sufficiently small constant step-size converges to a local minimizer or negative infinity almost surely.

Critically, for this result to apply, f is required to have isolated saddle points, ∇f is assumed to be globally L-Lipschitz[1] and the step-size α is taken to be less than $1/L$. These regularity conditions soften somewhat the impact of the statement both theoretically as well as in practice. First, although the assumption of isolated fixed points is indeed generic for abstract classes of cost functions, in several special cases of practical interest where the cost function has some degree of symmetry (*e.g.,* due to scaling invariance) this assumption is not satisfied. For this reason, the important question of *whether the assumption of isolated equilibria is indeed necessary* was explicitly raised in [74]. Moreover, the assumption of *global Lipschitz continuity for* ∇f is not satisfied even by low degree polynomials (*e.g.,* cubic). Finally, a natural question is *how tight is the assumption on the step-size?*

Our contribution. In this chapter we provide answers to all the above questions. We show that the assumption of isolated saddle points is indeed not necessary to argue generic convergence to local minima. To argue this, we need to combine tools

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[1]That is, f satisfies $\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\|_2 \leq L \|\mathbf{x} - \mathbf{y}\|_2$.

that we essentially used in previous chapters when we argued about measure zero set of initial conditions, *e.g.,* we make use of Center-Stable Manifold Theorem 1.3 (see Theorem 7.1). Moreover, we show that the globally Lipschitz assumption can be circumvented as long as the domain is convex and forward invariant with respect to gradient descent (see Theorem 7.2). This technique makes our results easily applicable to many standard settings. Finally, using linear algebra and eigenvalue analysis we provide an upper bound on the allowable step-size (see 7.3). Our work shows that the high level message of [74] is practically always binding. Saddle points are indeed of little concern for the gradient descent method in practice, but it takes some theory to argue so.

7.2 Related work

First-order descent methods can indeed escape strict saddle points when assisted by near isotropic noise. [108] establishes convergence of the Robbins-Monro stochastic approximation to local minimizers for strict saddle functions, whereas [70] establishes convergence to local minima for perturbed versions of multiplicative weights algorithm in generic potential games. Recently, [58] quantified the convergence rate of perturbed stochastic gradient descent to local minima. The addition of isotropic noise can significantly slow down the convergence rate. Our setting is deterministic and corresponds to the simplest possible discrete-time implementation of gradient descent.

Numerous curvature-based optimization techniques have been developed in order to circumvent saddle points (*e.g.,* trust-region methods [33, 130], modified Newton's method with curvilinear line search [90], cubic regularized Newton's method [96], and saddle-free Newton methods [38]). Unlike gradient descent, these methods have superlinear per iteration implementation costs, making them impractical for high dimensional settings.

Gradient descent with carefully chosen initial conditions can bypass the problem

of local minima altogether and converge to the global minimum for many practical non-convex optimization settings (*e.g.,* dictionary learning [6], latent-variable models [144], matrix completion [68], and phase retrieval [21]). In contrast, we focus on the performance of gradient descent under generic initial conditions. Finally, some recent work has been focusing on the connections between stability and efficiency of fixed points in non-convex optimization (*e.g.,* Gaussian random fields [28]).

7.3 Preliminaries and formal statement of results

Assume a minimization problem of the form $\min_{\mathbf{x} \in \mathbb{R}^N} f(\mathbf{x})$ where $f : \mathbb{R}^N \to \mathbb{R}$ is a twice continuously differentiable function. Gradient descent is one of the most well-known algorithms (discrete dynamical system) to attack this generic optimization problem. It is defined by the equations below:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha \nabla f(\mathbf{x}_k),$$

or equivalently $\mathbf{x}_{k+1} = g(\mathbf{x}_k)$ with $g(\mathbf{x}) = \mathbf{x} - \alpha \nabla f(\mathbf{x})$, $g : \mathbb{R}^N \to \mathbb{R}^N$ and $\alpha > 0$.

It is easy to see that the fixed points of the dynamical system $\mathbf{x}_{k+1} = g(\mathbf{x}_k)$ are exactly the points $\mathbf{x}$ so that $\nabla f(\mathbf{x}) = \mathbf{0}$, called *critical points or equilibria.* The set of local minima of f is a subset of the set of critical points of f. These two sets do not coincide and this poses a serious obstacle for proving strong theoretical guarantees for gradient descent, since the dynamics may converge to a critical point which is not a local minimum, called a *saddle point.*

Lee *et al.* [74] argue, under technical conditions which include the assumption of isolated critical points, that the set of initial conditions that converge to *strict saddle points* is a zero measure set (for definition of strict saddle, see Definition 25). The paper leaves as an open question whether the condition of isolated equilibria was necessary. We prove that the set of initial conditions that converge to a strict saddle point is a zero measure set even in the case of non-isolated critical points[2].

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[2]Our arguments hence allow for cost functions f's with uncountably many critical points.

Furthermore, one of the conditions for f is that ∇f is globally Lipschitz, which implies that the second derivative of f is bounded, *i.e.*, there exists a $\beta > 0$ such that for all $\mathbf{x}$ we have $\|\nabla^2 f(\mathbf{x})\|_2 \leq \beta$. However, even third degree polynomial functions are not globally Lipschitz. We provide a theorem which can circumvent this assumption as long as the domain $\mathcal{S}$ is *forward or positively invariant* with respect to g, *i.e.*, $g(\mathcal{S}) \subseteq \mathcal{S}$. Finally, we provide an easy upper bound on the step-size α, via eigenvalue analysis of the Jacobian of g, *i.e.*, $I - \alpha \nabla^2 f(\mathbf{x})$.

Below we give some necessary definitions for the rest of this chapter.

Definition 25.

- *A point $\mathbf{x}^*$ is a critical point of f if $\nabla f(\mathbf{x}^*) = \mathbf{0}$. We denote by $C = \{\mathbf{x} : \nabla f(\mathbf{x}) = \mathbf{0}\}$ the set of critical points (can be uncountably many).*

- *A critical point $\mathbf{x}^*$ is isolated if there is a neighborhood U around $\mathbf{x}^*$ and $\mathbf{x}^*$ is the only critical point in U [3]. Otherwise is called non-isolated.*

- *A critical point $\mathbf{x}^*$ of f is a saddle point if for all neighborhoods U around $\mathbf{x}^*$ there are $\mathbf{y}, \mathbf{z} \in U$ such that $f(\mathbf{z}) \leq f(\mathbf{x}^*) \leq f(\mathbf{y})$.*

- *A critical point $\mathbf{x}^*$ of f is strict saddle if $\lambda_{\min}(\nabla^2 f(\mathbf{x}^*)) < 0$ (minimum eigenvalue of matrix $\nabla^2 f(\mathbf{x}^*)$ is negative).*

- *A set $\mathcal{S}$ is called forward or positively invariant with respect to some function $h : \mathcal{E} \to \mathbb{R}^N$ with $\mathcal{S} \subseteq \mathcal{E} \subseteq \mathbb{R}^N$ if $h(\mathcal{S}) \subseteq \mathcal{S}$.*

7.3.1 Main theorems

In [74], the steps of the proof of their result are the following: Under the regularity assumption that ∇f is globally Lipschitz with some Lipschitz constant L, Lee *et al.* are able to show that $g(\mathbf{x}) = \mathbf{x} - \alpha \nabla f(\mathbf{x})$ is a diffeomorphism for $\alpha < 1/L$.

---

[3] *If the critical points are isolated, then they are countably many or finite.*

Afterwards, using the Center-Stable Manifold Theorem 1.3, they show that the set of initial conditions so that g converges to saddle points has measure zero, under the assumption that the critical points are isolated. We generalize their result for non-isolated critical points, answering one of their open questions (see also the example in Section 7.5.1, where there is a line of critical points).

Theorem 7.1 (Non-isolated). *Let $f : \mathbb{R}^N \to \mathbb{R}$ be twice continuously differentiable and $\sup_{\mathbf{x} \in \mathbb{R}^N} \|\nabla^2 f(\mathbf{x})\|_2 \leq L < \infty$. The set of initial conditions $\mathbf{x} \in \mathbb{R}^N$ so that gradient descent with step-size $0 < \alpha < 1/L$ converges to a strict saddle point is of measure zero, without the assumption that critical points are isolated.*

We can prove a stronger version of the theorem above, circumventing the globally Lipschitz condition for domains which are forward invariant (see also the example in Section 7.5.2).

Theorem 7.2 (Non-isolated, forward invariant). *Let $f : \mathcal{S} \to \mathbb{R}^N$ be twice continuously differentiable in an open convex set $\mathcal{S} \subseteq \mathbb{R}^N$ and $\sup_{\mathbf{x} \in \mathcal{S}} \|\nabla^2 f(\mathbf{x})\|_2 \leq L < \infty$. If $g(\mathcal{S}) \subseteq \mathcal{S}$ (where $g(\mathbf{x}) = \mathbf{x} - \alpha \nabla f(\mathbf{x})$) then the set of initial conditions $\mathbf{x} \in \mathcal{S}$ so that gradient descent with step-size $0 < \alpha < 1/L$ converges to a strict saddle point is of measure zero, without the assumption that critical points are isolated.*

Finally, via eigenvalue analysis of $I - \alpha \nabla^2 f(\mathbf{x})$, we can find upper bounds on the step-size of gradient descent. A straightforward theorem is the following:

Theorem 7.3 (Upper bound on step-size). *Let f be a twice continuously differentiable function in an open set $\mathcal{S} \subseteq \mathbb{R}^N$ and $\mathcal{C}^*$ be the set of local minima. Assume also that $\gamma < \inf_{\mathbf{x} \in \mathcal{C}^*} \|\nabla^2 f(\mathbf{x})\|_2 < \infty$. A necessary condition so that gradient descent converges to local minima for all but (Lebesgue) measure zero initial conditions in $\mathcal{S}$ is that the step-size satisfies $\alpha < \frac{2}{\gamma}$.*

7.4 Proving the theorems

Before we proceed with the proofs, let us argue that Theorem 7.2 is a generalization of Theorem 7.1. This can be checked easily by setting $\mathcal{S} := \mathbb{R}^N$ and observing that $g(\mathbb{R}^N) \subseteq \mathbb{R}^N$. We continue with the proofs of Theorems 7.2 and 7.3.

7.4.1 Proof of Theorem 7.2

In this section, we prove Theorem 7.2. We start by showing that the assumptions of Theorem 7.2 imply that $\nabla f(\mathbf{x})$ is Lipschitz in $\mathcal{S}$.

Lemma 7.4 (Bounded second derivative implies Lipschitz condition). *Let $f : \mathcal{S} \to \mathbb{R}^N$ where $\mathcal{S}$ is an open convex set and f be twice continuously differentiable in $\mathcal{S}$. Also assume that $\sup_{\mathbf{x} \in \mathcal{S}} \|\nabla^2 f(\mathbf{x})\|_2 \leq L < \infty$. Then ∇f satisfies the Lipschitz condition in $\mathcal{S}$ with Lipschitz constant L.*

Proof. Let $\mathbf{x}, \mathbf{y} \in \mathcal{S}$ (column vectors) and define the function $H : [0,1] \to \mathbb{R}^N$ as $H(t) = \nabla f(\mathbf{x} + t(\mathbf{y} - \mathbf{x}))$. By the chain rule we get that $H'(t) := \frac{dH}{dt} = (\nabla^2 f(\mathbf{x} + t(\mathbf{y} - \mathbf{x}))) \cdot (\mathbf{y} - \mathbf{x})$. It holds that

$$
\begin{aligned}
\|\nabla f(\mathbf{y}) - \nabla f(\mathbf{x})\|_2 = \left\| \int_0^1 H'(t) dt \right\|_2 &\leq \int_0^1 \|H'(t)\|_2 \, dt \\
&= \int_0^1 \left\| (\nabla^2 f(\mathbf{x} + t(\mathbf{y} - \mathbf{x})))(\mathbf{y} - \mathbf{x}) \right\|_2 dt \\
&\leq \int_0^1 \left\| \nabla^2 f(\mathbf{x} + t(\mathbf{y} - \mathbf{x})) \right\|_2 \|\mathbf{y} - \mathbf{x}\|_2 \, dt \\
&\leq \int_0^1 L \|\mathbf{y} - \mathbf{x}\|_2 \, dt = L \|\mathbf{y} - \mathbf{x}\|_2 .
\end{aligned}
$$

$\square$

Remark 18. *From Schwarz's theorem we get that $\nabla^2 f(\mathbf{x})$ is symmetric for $\mathbf{x} \in \mathcal{S}$, hence $\|\nabla^2 f(\mathbf{x})\|_2 = \mathrm{sp}\,(\nabla^2 f(\mathbf{x}))$.*

The assumption that $\sup_{\mathbf{x} \in \mathcal{S}} \|\nabla^2 f(\mathbf{x})\|_2 \leq L < \infty$ implies that $\nabla f(x)$ is Lipschitz with constant L in the convex set $\mathcal{S}$, as stated by Lemma 7.4. We show that the

converse holds as well, *i.e.*, the Lipschitz condition for $\nabla f(\mathbf{x})$ with constant L in the main theorem in Lee *et al.* implies $\|\nabla^2 f(\mathbf{x})\|_2 \leq L$ for all $\mathbf{x} \in \mathcal{S}$ and hence the assumption in Theorems 7.1, 7.2 that $\sup_{\mathbf{x} \in \mathcal{S}} \|\nabla^2 f(\mathbf{x})\|_2 \leq L$ is satisfied.

Lemma 7.5 (Lipschitz condition implies bounded second derivative). *Let $f :$ $\mathcal{S} \to \mathbb{R}^N$ where $\mathcal{S}$ is an open convex set and f is twice continuously differentiable in $\mathcal{S}$. Assume $\nabla f(\mathbf{x})$ is Lipschitz with constant L in $\mathcal{S}$, then it holds $\sup_{\mathbf{x} \in \mathcal{S}} \|\nabla^2 f(\mathbf{x})\|_2 \leq L$.*

Proof. Fix an $\epsilon > 0$. By Taylor's theorem since f is twice differentiable with respect to some point $\mathbf{x}$ it holds that

$$\|\nabla f(\mathbf{y}) - \nabla f(\mathbf{x})\|_2 \geq \left\|(\nabla^2 f(\mathbf{x}))(\mathbf{y} - \mathbf{x})\right\|_2 - o(\|\mathbf{y} - \mathbf{x}\|_2)$$

$$\geq \left\|(\nabla^2 f(\mathbf{x}))(\mathbf{y} - \mathbf{x})\right\|_2 - \epsilon \|\mathbf{y} - \mathbf{x}\|_2$$

for $\mathbf{y}$ sufficiently close to $\mathbf{x}$ (depends on ϵ). Therefore under the Lipschitz assumption we get that there exists a closed neighborhood $U(\epsilon)$ of $\mathbf{x}$ so that for all $\mathbf{y} \in U$ we get

$$\left\|(\nabla^2 f(\mathbf{x}))(\mathbf{x} - \mathbf{y})\right\|_2 \leq \|\nabla f(\mathbf{x}) - \nabla f(\mathbf{y})\|_2 + \epsilon \|\mathbf{y} - \mathbf{x}\|_2 \leq (L + \epsilon) \|\mathbf{x} - \mathbf{y}\|_2. \quad (82)$$

We consider a closed ball B subset of U, with center $\mathbf{x}$ and radius r (in ℓ_2) and set $\mathbf{z} = \mathbf{x} - \mathbf{y}$. It is true that $\|\nabla^2 f(\mathbf{x})\|_2 = \sup_{\|\mathbf{z}\|_2 = r} \frac{\|(\nabla^2 f(\mathbf{x}))\mathbf{z}\|_2}{\|\mathbf{z}\|_2}$ by definition of spectral norm, scaled so that the length of the vectors are at most r. Using 82 we get that $\|\nabla^2 f(\mathbf{x})\|_2 \leq L + \epsilon$. Since ϵ is arbitrary, we get that $\|\nabla^2 f(\mathbf{x})\|_2 \leq L$. We conclude that $\sup_{\mathbf{x} \in \mathcal{S}} \|\nabla^2 f(\mathbf{x})\|_2 \leq L$. $\qquad\square$

Lemmas 7.4 and 7.5 show that the smoothness assumptions in Lee *et al.* paper are equivalent to ours. We use the condition on the spectral norm of the matrix $\nabla^2 f(\mathbf{x})$ so that we can work with the eigenvalues in our theorems (*e.g.*, in Remark 18 the spectral norm coincides with spectral radius for $\nabla^2 f(\mathbf{x})$). Below we prove that the update rule of gradient descent, *i.e.*, function g is a diffeomorphism under the assumptions of Theorem 7.2 (similar approach appeared in [74]).

Lemma 7.6 (Diffeomorphism). *Under the assumptions of Theorem 7.2, function g is a diffeomorphism in $\mathcal{S}$.*

Proof. First we prove that g is a injective. We follow the same argument as in [74]. Suppose $g(\mathbf{y}) = g(\mathbf{x})$, thus $\mathbf{y} - \mathbf{x} = \alpha(\nabla f(\mathbf{y}) - \nabla f(\mathbf{x}))$. We assume that $\mathbf{x} \neq \mathbf{y}$ and we will reach contradiction. From Lemma 7.4 we get $\|\nabla f(\mathbf{y}) - \nabla f(\mathbf{x})\|_2 \leq L \|\mathbf{y} - \mathbf{x}\|_2$ and hence $\|\mathbf{x} - \mathbf{y}\|_2 \leq \alpha L \|\mathbf{y} - \mathbf{x}\|_2 < \|\mathbf{y} - \mathbf{x}\|_2$ since $\alpha L < 1$ (contradiction).

We continue by showing that g is a local diffeomorphism. Observe that the Jacobian of g is $I - \alpha \nabla^2 f(\mathbf{x})$. It suffices to show that $\alpha \nabla^2 f(\mathbf{x})$ has no eigenvalue which is 1, because this implies matrix $I - \alpha \nabla^2 f(\mathbf{x})$ is invertible. As long as $I - \alpha \nabla^2 f(\mathbf{x})$ is invertible, from Inverse Function Theorem (see [129]) follows that g is a local diffeomorphism. Finally, since g is injective, the inverse g^{-1} is well defined and since g is a local diffeomorphism in $\mathcal{S}$, it follows that g^{-1} is smooth in $\mathcal{S}$. Therefore g is a diffeomorphism.

Let λ be an eigenvalue of $\nabla^2 f(\mathbf{x})$. Then $|\lambda| \leq \mathrm{sp}\left(\nabla^2 f(\mathbf{x})\right) = \|\nabla^2 f(\mathbf{x})\|_2 \leq L$ where the equality comes from Remark 18 and first and last inequalities are satisfied by assumption. Therefore $\alpha \nabla^2 f(\mathbf{x})$ has as eigenvalue $\alpha\lambda$ and $|\alpha\lambda| \leq \alpha L < 1$. Thus all eigenvalues of $\alpha \nabla^2 f(\mathbf{x})$ are less than 1 in absolute value and the proof is complete. $\square$

To finish the proof of 7.2 we use the Center-Stable Manifold Theorem 1.3 since $g(\mathbf{x}) = \mathbf{x} - \alpha \nabla f(\mathbf{x})$ is a diffeomorphism, where $\sup_{\mathbf{x} \in \mathcal{S}} \|\nabla^2 f(\mathbf{x})\|_2 \leq L$ and $\alpha < 1/L$.

Our approach deviates a lot from that of [74] from this point until the end of the proof. Let $\mathbf{r}$ be a critical point of function $f(\mathbf{x})$ and $B_{\mathbf{r}}$ be the (open) ball that is derived from Theorem 1.3. We consider the union of these balls

$$A = \cup_{\mathbf{r}} B_{\mathbf{r}}.$$

Due to Lindelöf's Lemma A.1, we can find a countable subcover for A, *i.e.,* there exists fixed-points $\mathbf{r}_1, \mathbf{r}_2, \ldots$ such that $A = \cup_{m=1}^{\infty} B_{\mathbf{r}_m}$. If the dynamics of gradient descent converges to a strict saddle point, starting from a point $\mathbf{v} \in \mathcal{S}$, there must

exist a t_0 and m so that $g^t(\mathbf{v}) \in B_{\mathbf{r}_m}$ for all $t \geq t_0$. From Theorem 1.3 we get that $g^t(\mathbf{v}) \in W^{sc}_{loc}(\mathbf{r}_m) \cap \mathcal{S}$ where we used the fact that $g(\mathcal{S}) \subseteq \mathcal{S}$ (from assumption forward invariant), namely the trajectory remains in $\mathcal{S}$ for all times [4]. By setting $D_1(\mathbf{r}_m) = g^{-1}(W^{sc}_{loc}(\mathbf{r}_m) \cap \mathcal{S})$ and $D_{i+1}(\mathbf{r}_m) = g^{-1}(D_i(\mathbf{r}_m) \cap \mathcal{S})$ we get that $\mathbf{v} \in D_t(\mathbf{r}_m)$ for all $t \geq t_0$.

Hence the set of initial points in $\mathcal{S}$ so that gradient descent converges to a strict saddle point is a subset of

$$P = \cup_{m=1}^{\infty} \cup_{t=0}^{\infty} D_t(\mathbf{r}_m)). \tag{83}$$

Since $\mathbf{r}_m$ is strict saddle point, the Jacobian $I - \alpha \nabla^2 f(\mathbf{x})$ has an eigenvalue greater than 1, namely the dimension of the unstable eigenspace satisfies $dim(E^u) \geq 1$, and therefore dimension of $W^{sc}_{loc}(\mathbf{r}_m)$ is at most $N-1$. Thus, the set $W^{sc}_{loc}(\mathbf{r}_m) \cap \mathcal{S}$ has Lebesgue measure zero in $\mathbb{R}^N$ and so does $D_1(\mathbf{r}_m)$. Finally since g is a diffeomorphism (from Lemma 7.6), g^{-1} is continuously differentiable and thus it is locally Lipschitz (see [110] p.71). Therefore using Lemma A.2 below, g^{-1} preserves the null-sets and hence by induction $D_i(\mathbf{r}_m)$ has measure zero. Thereby we get that P is a countable union of measure zero sets, *i.e.*, is measure zero and the claim of Theorem 7.2 follows.

A straightforward application of the Theorem 7.2 is the following:

Corollary 7.7 (Gradient descent only converges to minimizers). *Assume that the conditions of Theorem 7.2 are satisfied and all saddle points of f are strict. Additionally, let ν be a prior measure with support $\mathcal{S}$ which is absolutely continuous with respect to Lebesgue measure, and assume $\lim_{k \to \infty} g^k(x)$ exists[5] for all $\mathbf{x}$ in $\mathcal{S}$. Then*

$$\mathbb{P}_\nu[\lim_k g^k(\mathbf{x}) = \mathbf{x}^*] = 1,$$

where $\mathbf{x}^*$ is a local minimum.

---

[4]$W^{sc}_{loc}(\mathbf{r}_m)$ denotes the center-stable manifold of fixed point $\mathbf{r}_m$
[5]g^k *denotes the composition of g with itself k times.*

Proof. Since the set of initial conditions whose limit point is a (strict) saddle point is a measure zero set and we have assumed $\lim_{k\to\infty} g^k(x)$ exists for all initial conditions in $\mathcal{S}$ then the probability of converging to a local minimizer is 1. $\qquad\square$

Remark 19. *Arguing that $\lim_k g^k(\mathbf{x})$ exists follows from standard arguments in several settings of interest (e.g., for analytic functions f that satisfy Lojasiewicz Gradient Inequality), see papers [74], [1] and references therein.*

The importance of Theorem 7.2 will become clear in the examples that appear in Section 7.5. In the example of Section 7.5.2, the function is not globally Lipschitz (we use the example that appears in [74]), nevertheless Theorem 7.2 applies and thus we have convergence to local minimizers with probability 1. In the example of Section 7.5.1 we see that the function has non-isolated critical points.

7.4.2 Proof of Theorem 7.3

We proceed by contradiction. Consider any local minimum $\mathbf{x}^*$, and by assumption we get that $\mathrm{sp}\left(\nabla^2 f(\mathbf{x}^*)\right) > \gamma$. Let $\alpha \geq \frac{2}{\gamma}$. Therefore the Jacobian $I - \alpha \nabla^2 f(\mathbf{x}^*)$ of g at $\mathbf{x}^*$ has spectral radius greater than 1 since $\mathrm{sp}\left(I - \alpha\nabla^2 f(\mathbf{x}^*)\right) \geq \mathrm{sp}\left(\alpha\nabla^2 f(\mathbf{x}^*)\right) - 1 > \alpha\gamma - 1 \geq 1$. This implies that the fixed point $\mathbf{x}^*$ of g is (Lyapunov) unstable. Since this is true for every local minimum, it cannot be true that gradient descent converges with probability 1 to local minima.

7.5 Examples

7.5.1 Example for non-isolated critical points

Consider the simple example of the cost function $f : \mathbb{R}^3 \to \mathbb{R}$ with $f(x, y, z) = 2xy + 2xz - 2x - y - z$. Its gradient is $\nabla(f) = (2y + 2z - 2, 2x - 1, 2x - 1)$. Naturally, its saddle points correspond exactly to the line $(1/2, w, 1 - w)$ for $w \in \mathbb{R}$ and by computing their (common) eigenvalues we establish that they are all strict saddles (their minimum eigenvalue is $-2\sqrt{2}$). As we expect from our analysis effectively no

trajectories converge to them (instead the value of practically all trajectories goes to $-\infty$). We plot in red some sample trajectories for small enough step sizes, starting in the local neighborhood of the equilibrium set.
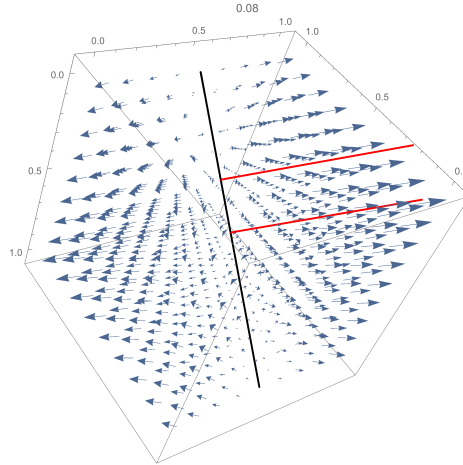
Figure 13: Example that satisfies the assumptions of Theorem 7.1. The black line represent critical points of f, all of which are strict. The red lines correspond to diverging trajectories of gradient descent with small step size.

### 7.5.2   Example for forward invariant set

We use the same function as in Lee *et al.* $f(x, y) = \frac{x^2}{2} + \frac{y^4}{4} - \frac{y^2}{2}$. As argued in previous sections, f is not globally Lipschitz so the main result in [74] cannot be applied here. We will use our Theorem 7.2 which talks about forward invariant domains.

The critical points of f are $(0, 0)$, $(0, 1)$, $(0, -1)$. $(0, 0)$ is a strict saddle point and the other two are local minima. Observe that the Hessian $\nabla^2 f(x, y)$ is

$$J = \begin{pmatrix} 1 & 0 \\ 0 & 3y^2 - 1 \end{pmatrix}.$$

For $\mathcal{S} = (-1, 1) \times (-2, 2)$, so we get that $\sup_{(x,y) \in \mathcal{S}} \|\nabla^2 f(x, y)\|_2 \le 11$ (for $y = 2$ gets the maximum value). We choose $\alpha = \frac{1}{12} < \frac{1}{11}$, and we have $g(x, y) = ((1 - \alpha)x, (1 + \alpha)y - \alpha y^3) = (\frac{11x}{12}, \frac{13y}{12} - \frac{y^3}{12})$. It is not difficult to see that $g(\mathcal{S}) \subseteq \mathcal{S}$ (easy

calculations). The assumptions of Theorem 7.2 are satisfied, hence it is true that the set of initial conditions in $\mathcal{S}$ so that gradient descent converges to $(0,0)$ has measure zero. Moreover, by Corollary 7.7 it holds that if the initial condition is taken (say) uniformly at random in $\mathcal{S}$, then gradient descent converges to $(0,1)$, $(0,-1)$ with probability 1. The figure below makes the claim clear, *i.e.,* the set of initial conditions so that gradient descent converges to $(0,0)$ lie on the axis $y = 0$, which is of measure zero in $\mathbb{R}^2$. For all other starting points, gradient descent converges to local minima. Finally, from the figure one can see that $\mathcal{S}$ is forward invariant.
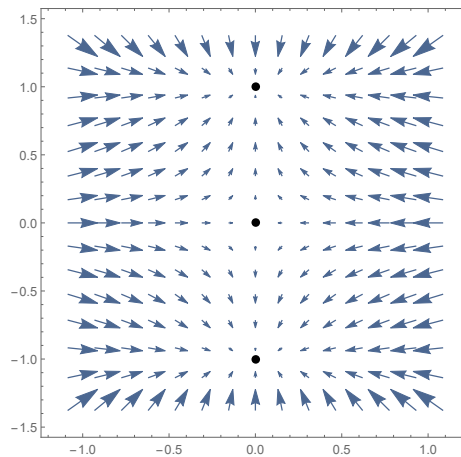
Figure 14: Example that satisfies the assumptions of Theorem 7.2. The three black dots represent the critical points. Function f is not Lipschitz.

7.5.3 Example for step-size

We use the same function as in the previous example. Observe that for $(0,0)$, $(0,1)$, $(0,-1)$ we have that the spectral radius of $\nabla^2 f$ is $1, 2, 2$ respectively (so the minimum of all is 1). We choose $\alpha \geq 2$ and we get that $g(x,y) = (-x, 3y - 2y^3)$. It is not hard to see that gradient descent does not converge (in the first coordinate function g cycles between x and $-x$).

7.6 Conclusion and remarks

The results of this chapter appear in [103] and it is joint work with Georgios Piliouras. Our work argues that saddle points are indeed of little concern for the gradient descent method in practice under rather weak assumptions for f which allow for non-isolated critical points. In some sense, this is the strongest positive result possible without making explicit assumptions on the structure of the cost function f nor using beneficial random noise/well chosen initial conditions. Naturally, all these directions are of key interest and are the object of recent work (see Section 7.2). Keeping up with this simplest, deterministic implementation of gradient descent a natural hypothesis is that (in settings of practical interest) it converges not only to local minimizers but moreover the size of the region of attraction of each local minimizer is in a sense directly proportional to its quality. Formalizing such statements and analyzing the average case performance of gradient descent given random initial conditions is a fascinating question that could shed more light into the in-many-cases surprising efficiency of the gradient descent method.

APPENDIX A

MISSING TERMS, LEMMAS AND PROOFS

A.1 Terms Used in Biology

We provide brief non-technical definitions of a few biological terms that we use in this thesis.

Gene. A unit that determines some characteristic of the organism, and passes traits to offsprings. All organisms have genes corresponding to various biological traits, some of which are instantly visible, such as eye color or number of limbs, and some of which are not, such as blood type.

Allele. Allele is one of a number of alternative forms of the same gene, found at the same place on a chromosome, Different alleles can result in different observable traits, such as different pigmentation.

Genotype. The genetic constitution of an individual organism.

Phenotype. The set of observable characteristics of an individual resulting from the interaction of its genotype with the environment.

Locus. A locus (plural loci) is the specific location of a gene, DNA sequence, or position on a chromosome. Each chromosome carries many genes; humans' estimated 'haploid' protein coding genes are 20,000-25,000, on the 23 different chromosomes.

Diploid. Diploid means having two copies of each chromosome. Almost all of the cells in the human body are diploid.

Haploid. A cell or nucleus having a single set of unpaired chromosomes. Our sex cells (sperm and eggs) are haploid cells that are produced by meiosis. When sex cells unite during fertilization, the haploid cells become a diploid cell.

A.1.1 Heterozygote Advantage (Overdominance)

Heterozygote Advantage describes the case when heterozygote genotype has a higher relative fitness than homozygote genotype. Cases of heterozygote advantage have been demonstrated in several organisms. The first confirmation of heterozygote advantage was with a fruit fly, Drosophila melanogaster. Kalmus demonstrated in a classic paper [64] how polymorphism can persist in a population through heterozygote advantage. In humans, sickle-cell anemia is a genetic disorder caused by the presence of two recessive alleles. Where malaria is common, carrying a single sickle-cell allele (trait) confers a selective advantage, *i.e.,* being a heterozygote is advantageous. Specifically, humans with one of the two alleles of sickle-cell disease exhibit less severe symptoms when infected with malaria. Theorems 3.13 and 3.17 are related to that phenomenon.

A.2 Statements and Proofs

A.2.1 Lindelöf's lemma

The following theorem holds for every separable metric space, *i.e.,* every metric space that contains a countable, dense subset. In particular, we use this theorem for $\mathbb{R}^n$ extensively in this thesis (in Theorems 2.8, 3.6 and 6.4).

Theorem A.1 (Lindelöf's lemma [67]). *For every open cover there is a countable subcover.*

A.2.2 Locally Lipschitz are null-set preserving

The following lemma is used in Chapters 2, 3, 6, 7 when we argue that the set of initial conditions so that the dynamics converges to fixed points with an unstable direction, has measure zero. It roughly states that if a function f is locally Lipschitz then it preserves the measure zero sets (measure zero sets are mapped to measure zero sets).

Lemma A.2 (Null-set preserving). *Let $h : \mathcal{S} \to \mathbb{R}^m$ be a locally Lipschitz function with $\mathcal{S} \subseteq \mathbb{R}^m$, then h is null-set preserving, i.e., for $E \subset \mathcal{S}$ if E has measure zero then $h(E)$ has also measure zero.*

Proof. The lemma is well-known, but we give a proof for completeness. Let B_γ be an open ball such that $\|h(\mathbf{y}) - h(\mathbf{x})\| \leq K_\gamma \|\mathbf{y} - \mathbf{x}\|$ for all $\mathbf{x}, \mathbf{y} \in B_\gamma$. We consider the union $\cup_\gamma B_\gamma$ which cover $\mathbb{R}^m$ by the assumption that h is locally Lipschitz. By Lindelőf's lemma A.1 we have a countable subcover, *i.e.,* $\cup_{i=1}^\infty B_i$. Let $E_i = E \cap B_i$. We will prove that $h(E_i)$ has measure zero. Fix an $\epsilon > 0$. Since $E_i \subset E$, we have that E_i has measure zero, hence we can find a countable cover of open balls $C_1, C_2, ...$ for E_i, namely $E_i \subset \cup_{j=1}^\infty C_j$ so that $C_j \subset B_i$ for all j and also $\sum_{j=1}^\infty \mu(C_j) < \frac{\epsilon}{K_i^m}$. Since $E_i \subset \cup_{j=1}^\infty C_j$ we get that $h(E_i) \subset \cup_{j=1}^\infty h(C_j)$, namely $h(C_1), h(C_2), ...$ cover $h(E_i)$ and also $h(C_j) \subset h(B_i)$ for all j. Assuming that ball $C_j := B(\mathbf{x}, r)$ (center $\mathbf{x}$ and radius r) then it is clear that $h(C_j) \subset B(h(\mathbf{x}), K_i r)$ (h maps the center $\mathbf{x}$ to $h(\mathbf{x})$ and the radius r to $K_i r$ because of Lipschitz assumption). But $\mu(B(h(\mathbf{x}), K_i r)) = K_i^m \mu(B(\mathbf{x}, r)) = K_i^m \mu(C_j)$, therefore $\mu(h(C_j)) \leq K_i^m \mu(C_j)$ and so we conclude that

$$\mu(h(E_i)) \leq \sum_{j=1}^\infty \mu(h(C_j)) \leq K_i^m \sum_{j=1}^\infty \mu(C_j) < \epsilon$$

Since ϵ was arbitrary, it follows that $\mu(h(E_i)) = 0$. To finish the proof, observe that $h(E) = \cup_{i=1}^\infty h(E_i)$ therefore $\mu(h(E)) \leq \sum_{i=1}^\infty \mu(h(E_i)) = 0$. □

A.2.3 Point-wise convergence for network coordination games

Theorem A.3 (Point-wise convergence in network coordination). *Given any initial condition replicator dynamics converges to a fixed point (point-wise convergence) in all network coordination games.*

Proof. We denote by $\hat{u}_i$ the expected utility of agent i under mixed strategy profile $\mathbf{p}$ and by $u_{i\gamma}$ his expected utility when he deviates to strategy γ and all other agents

still play according to **p**. We observe that

$$\Psi(\mathbf{p}) = \sum_i \hat{u}_i = \sum_{i,\gamma} p_{i\gamma} \sum_{j \in N(i)} \sum_\delta A_{ij}^{\gamma\delta} p_{j\delta}$$

is a Lyapunov function for our game since (strict increasing along the trajectories)

$$\frac{\partial \Psi}{\partial p_{i\gamma}} = u_{i\gamma} + \sum_{j \in N(i)} \sum_\delta A_{ji}^{\delta\gamma} p_{j\delta} = 2u_{i\gamma} \text{ since } A_{ij} = A_{ji}^T$$

and hence

$$\frac{d\Psi}{dt} = \sum_{i,\gamma} \frac{\partial \Psi}{\partial p_{i\gamma}} \frac{dp_{i\gamma}}{dt}$$

$$= \sum_{i,\gamma,\gamma'} p_{i\gamma} p_{i\gamma'} (u_{i\gamma} - u_{i\gamma'})^2 \geq 0,$$

with equality at fixed points. Hence (as in [70]) we have convergence to equilibria sets (compact connected sets consisting of fixed points). We address the fact that this doesn't suffice for point-wise convergence. To be exact it suffices only in the case the equilibria are isolated (which is not the case for network coordination games - see Figure 12).

Let **q** be a limit point of the trajectory **p**(t) where **p**(t) is in the interior of Δ for all $t \in \mathbb{R}$ (since we started from an initial condition inside Δ) then we have that $\Psi(\mathbf{q}) > \Psi(\mathbf{p}(t))$. We define the relative entropy.

$$I(\mathbf{p}) = -\sum_i \sum_{\gamma : q_{i\gamma} > 0} q_{i\gamma} \ln(p_{i\gamma}/q_{i\gamma}) \geq 0 \text{ (Jensen's inequality)}$$

and $I(\mathbf{p}) = 0$ iff $\mathbf{p} = \mathbf{q}$. We get that

$$
\begin{aligned}
\frac{dI}{dt} &= -\sum_i \sum_{\gamma:q_{i\gamma}>0} q_{i\gamma}(u_{i\gamma} - \hat{u}_i) \\
&= \sum_i \hat{u}_i - \sum_{i,\gamma} \sum_{j\in N(i)} \sum_\delta A_{ij}^{\gamma\delta} p_{j\delta} q_{i\gamma} \\
&= \sum_i \hat{u}_i - \sum_{j,\delta} \sum_{i\in N(j)} \sum_\gamma A_{ij}^{\gamma\delta} p_{j\delta} q_{i\gamma} \quad \text{(since } A_{ij} = A_{ji}^T) \\
&= \sum_i \hat{u}_i - \sum_{j,\delta} p_{j\delta} d_{j\delta} \\
&= \sum_i \hat{u}_i - \sum_i \hat{d}_i - \sum_{j,\delta} p_{j\delta}(d_{j\delta} - \hat{d}_j) \\
&= \Psi(\mathbf{p}) - \Psi(\mathbf{q}) - \sum_{i,\gamma} p_{i\gamma}(d_{i\gamma} - \hat{d}_i),
\end{aligned}
$$

where $d_{i\gamma}, \hat{d}_i$ correspond to the payoff of player i if he chooses strategy γ and his expected payoff respectively at point $\mathbf{q}$. The rest of the proof follows in a similar way to Losert and Akin [82].

We break the term $\sum_{i,\gamma} p_{i\gamma}(d_{i\gamma} - \hat{d}_i)$ to positive and negative terms (we ignore zero terms), *i.e.*, $\sum_{i,\gamma} p_{i\gamma}(d_{i\gamma} - \hat{d}_i) = \sum_{i,\gamma:\hat{d}_i>d_{i\gamma}} p_{i\gamma}(d_{i\gamma} - \hat{d}_i) + \sum_{i,\gamma:\hat{d}_i<d_{i\gamma}} p_{i\gamma}(d_{i\gamma} - \hat{d}_i)$.

Claim A.4. *There exists an $\epsilon > 0$ so that the function $Z(\mathbf{p}) = I(\mathbf{p}) + 2\sum_{i,\gamma:\hat{d}_i>d_{i\gamma}} p_{i,\gamma}$ has $\frac{dZ}{dt} < 0$ for $\|\mathbf{p} - \mathbf{q}\|_1 < \epsilon$ and $\Psi(\mathbf{q}) > \Psi(\mathbf{p})$.*

Proof of Claim. Assuming that $\mathbf{p} \to \mathbf{q}$, we get $u_{i\gamma} - \hat{u}_i \to d_{i\gamma} - \hat{d}_i$ for all i, γ. Hence for small enough $\epsilon > 0$ with $\|\mathbf{p} - \mathbf{q}\|_1 < \epsilon$, we have that $u_{i\gamma} - \hat{u}_i \le \frac{3}{4}(d_{i\gamma} - \hat{d}_i)$ for the terms which $d_{i\gamma} - \hat{d}_i < 0$. Therefore

$$
\begin{aligned}
\frac{dZ}{dt} &= \Psi(\mathbf{p}) - \Psi(\mathbf{q}) - \sum_{i,\gamma:\hat{d}_i<d_{i\gamma}} p_{i\gamma}(d_{i\gamma} - \hat{d}_i) - \sum_{i,\gamma:\hat{d}_i>d_{i\gamma}} p_{i\gamma}(d_{i\gamma} - \hat{d}_i) + 2\sum_{i,\gamma:\hat{d}_i>d_{i\gamma}} p_{i\gamma}(u_{i\gamma} - \hat{u}_i) \\
&\le \Psi(\mathbf{p}) - \Psi(\mathbf{q}) - \sum_{i,\gamma:\hat{d}_i<d_{i\gamma}} p_{i\gamma}(d_{i\gamma} - \hat{d}_i) - \sum_{i,\gamma:\hat{d}_i>d_{i\gamma}} p_{i\gamma}(d_{i\gamma} - \hat{d}_i) + 3/2\sum_{i,\gamma:\hat{d}_i>d_{i\gamma}} p_{i\gamma}(d_{i\gamma} - \hat{d}_i) \\
&= \underbrace{\Psi(\mathbf{p}) - \Psi(\mathbf{q})}_{<0} + \underbrace{\sum_{i,\gamma:\hat{d}_i<d_{i\gamma}} -p_{i\gamma}(d_{i\gamma} - \hat{d}_i)}_{\le 0} + \underbrace{1/2\sum_{i,\gamma:\hat{d}_i>d_{i\gamma}} p_{i\gamma}(d_{i\gamma} - \hat{d}_i)}_{\le 0} < 0,
\end{aligned}
$$

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where we substitute $\frac{p_{i\gamma}}{dt} = p_{i\gamma}(u_{i\gamma} - \hat{u}_i)$ (replicator), and the claim is proved. Notice that $Z(\mathbf{p}) \geq 0$ (sum of positive terms and $I(\mathbf{p}) \geq 0$) and is zero iff $\mathbf{p} = \mathbf{q}$. (i) $\qquad\square$

To finish the proof of the theorem, if $\mathbf{q}$ is a limit point of $\mathbf{p}(t)$, there exists an increasing sequence of times t_i, with $t_n \to \infty$ and $\mathbf{p}(t_n) \to \mathbf{q}$. We consider ϵ' such that the set $C = \{\mathbf{p} : Z(\mathbf{p}) < \epsilon'\}$ is inside $B = \|\mathbf{p} - \mathbf{q}\|_1 < \epsilon$ where ϵ is from claim above. Since $\mathbf{p}(t_n) \to \mathbf{q}$, consider a time t_N where $\mathbf{p}(t_N)$ is inside C. From claim above we get that $Z(\mathbf{p})$ is decreasing inside B (and hence inside C), thus $Z(\mathbf{p}(t)) \leq Z(\mathbf{p}(t_N)) < \epsilon'$ for all $t \geq t_N$, hence the orbit will remain in C. By the fact that $Z(\mathbf{p}(t))$ is decreasing in C (claim above) and also $Z(\mathbf{p}(t_n)) \to Z(\mathbf{q}) = 0$ it follows that $Z(\mathbf{p}(t)) \to 0$ as $t \to \infty$. Hence $\mathbf{p}(t) \to \mathbf{q}$ as $t \to \infty$ using (i). $\qquad\square$

A.3 Mathematica code

A.3.1 Mathematica code for proving Lemma 5.35

```
Reduce[((1-k*x)/(m - k))/(b + (1 - b)*(x + (1 - k*x)/(m - k)))
       <((1 - (k + 1)* x) /(m - k - 1))/(b + (1 - b)*(x + (1 -
       (k + 1)*x)/(m - k - 1))) && 1 > b > 0 && 1 > x > 0 &&
       1/(k + 1) > x > 1/m && m >= 3 && m >= k + 2 && k >= 1]


False
```

A.3.2 Mathematica code for proving Lemma 5.38

First inequality in Lemma 5.38:

```
Reduce[1 > b > 0 && m >= 3 && -(m - 2) (1 - b) s^2 - 2 s (1 + b
       (m - 2)) + 1 + b (m - 2) == 0 && 0 < s < x < 1 && y ==
       (1 - x)/(m - 1) && t == (x*y*(1 - b))/(b + (1 - b)*
       (x + y)) && t <= 1/m && (1 - m*t)*(y + b + (1 - 2*b)*y)/
       (b + (1 - b)*x^2 + (1 - b)*(m - 1)*y^2) >= 1]
```

```
False
```

Second inequality in Lemma 5.38:

```
Reduce[1 > b > 0 && m >= 3 && -(m - 2) (1 - b) s^2 - 2 s (1 + b
    (m - 2)) + 1 + b (m - 2) == 0 && 0 < s < x < 1 && y ==
    (1 - x)/(m - 1) && 1/m >= t && t == (x*y*(1 - b))/(b +
    (1 - b)*(x + y)) && ((1 - m*t)*((2*(x + y) + b*(2 - x +
    (m - 3)*y)))/(b + (1 - b)*x^2 + (1 - b)*(m - 1)*y^2) -
    (2*x*(b + (1 - b)*x)^2 + 2*(m - 1)*y*(b + (1 - b)*y)^2)/
    ((b + (1 - b)*x^2 + (1 - b)*(m - 1)*y^2)^2)) >= 1)]
```

```
False
```

A.3.3 Mathematica code for proving $\tau_c > \tau_u$ when $m > 2$

```
Reduce[1 > b > 0 && m >= 3 && -(m - 2) (1 - b) s^2 - 2 s (1 + b
    (m - 2)) + 1 + b (m - 2) == 0 && 0 < s < 1 && (s*(1 - s)
    *(1 - b))/((m - 1)*b + (1 - b)*(1 + (m - 2)*s)) <=
    (1 - b)/(m*(2 - 2*b + m*b))]
```

```
False
```

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