

On the Movement of Vertex Fixed Points in the Simple GA

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ABSTRACT

The Vose dynamical system model of the simple genetic algorithm models the behavior of this algorithm for large population sizes and is the basis of the exact Markov chain model. Populations consisting of multiple copies of one individual correspond to vertices of the simplex. For zero mutation, these are fixed points of the dynamical system and absorbing states of the Markov chain. The stability of vertex fixed points is understood from previous work. We show that as mutation increases from zero, hyperbolic asymptotically stable fixed points move into the simplex, and hyperbolic asymptotically unstable fixed points move outside of the simplex. We calculate the derivative of local path of the fixed point with respect to the mutation rate. Simulation analysis shows how fixed points bifurcate with larger changes in the mutation rate and changes in the crossover rate.

Keywords

Genetic Algorithms, Theory, Crossover, Fixed Points

1. INTRODUCTION

Remark—Alden: I am not sure whether we need a separate introduction, or what it would contain. Perhaps we can just start with the next section.

But note the first paragraph of the Bistability section where an example is given of using the fixed points of an infinite population model to predict GA behavior. This could perhaps be moved to this introduction.

2. DYNAMICAL SYSTEM MODELS

2.1 The infinite population model

As the name suggests, the infinite population model (IPM) of the simple genetic algorithm (SGA) is a model that describes the behavior of the SGA as the population size goes

to infinity. It is also the basis for the exact mathematical description of the SGA, namely the exact Markov chain model. The infinite population model and the exact Markov chain model are primarily due to Michael Vose, but also to collaborators Gunar Liepins, Alden Wright, A. E. Nix, and others. See [11], [12], [15], [13], [5].

The SGA is a generational genetic algorithm over bit strings of length ℓ . As developed by Vose in [11], it includes any mask-based crossover, a very general model of mutation, and proportional, ranking, or tournament selection. (The model for ranking and tournament selection assumes that no two individuals have the same fitness.)

Populations are represented as vectors over the integers in half-open interval $[0, 2^\ell)$ where these integers correspond to length ℓ bit strings through their binary representation. A population vector x has the properties $\sum_i x_i = 1$ and $x_i \geq 0$ for all $i \in [0, 2^\ell)$. The relative frequency of the bit string i in the population is x_i . The space of all possible population vectors is the $(n-1)$ -simplex Δ in \mathbb{R}^n where $n = 2^\ell$. Thus, $\Delta = \{x \in \mathbb{R}^n : \sum_i x_i = 1 \text{ and } x_i \geq 0\}$. The vertices of the simplex are the unit vectors in \mathbb{R}^n ; the i^{th} unit vector e_i corresponds to a uniform population consisting only of individuals whose string representation is the binary string representation of i .

Following [11], we use $\mathbf{1}$ as a notation for a column vector of all ones of length ℓ , which corresponds to a string of all ones. In particular, if $i \in [0, n)$, then $\mathbf{1}^T i$ denotes the number of ones in the binary representation of i . We also use $\mathbf{1}$ as a notation for a column vector of all ones of length $n = 2^\ell$. The meaning of the $\mathbf{1}$ symbol should be clear from the context.

Population vectors in the simplex can be viewed either as populations of indeterminate size, or as sampling distributions for the next generation of the finite-population GA. (The formula for the exact Markov chain model is simply the application of the multinomial theorem to this sampling distribution.)

The infinite population model is a discrete-time dynamical system where time steps correspond to generations of the SGA. The model is described by a continuously differentiable (C^1) map $\mathcal{G} : \Delta \rightarrow \Delta$. If x is the current population of the SGA, then the next generation population is obtained by sampling from $\mathcal{G}(x)$. The IPM is deterministic with trajectory $x, \mathcal{G}(x), \mathcal{G}^2(x), \dots$. Vose [11] shows that the expected next finite population is $\mathcal{G}(x)$, he also has theorems that show that IPM is the limiting behavior of the SGA as the population size goes to infinity.

The \mathcal{G} map extends naturally to a neighborhood of the

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simplex in \mathbb{R}^n , and we will use \mathcal{G} to denote this extended map.

The map \mathcal{G} is the composition of a selection map \mathcal{F} and a mixing map \mathcal{M} : $\mathcal{G} = \mathcal{M} \circ \mathcal{F}$. Explicit formulas are given for each of these: see [11], [12], [15], [13], [5].

An important property of the mixing map is that when mutation is positive, \mathcal{M} maps the simplex into its interior [11]. Thus, \mathcal{G} also has this property. This is stated as theorem 4.7 of [11]. We will not give the precise definition of positive mutation, but bitwise mutation with a positive mutation rate is positive mutation.

2.2 A change of basis

In this subsection we show how to do an orthonormal change of basis so that we can work in the hyperplane containing the simplex. Recall that $\mathbf{1}$ is the vector of all ones. Note that $\{x \in \mathbb{R}^n : \mathbf{1}^T x = 1\}$ is the $(n-1)$ -dimensional hyperplane that contains the simplex, and $\mathbf{1}^\perp = \{x \in \mathbb{R}^n : \mathbf{1}^T x = 0\}$ is the translate of this hyperplane to the origin.

LEMMA 1. For proportional selection, $\mathbf{1}^T d\mathcal{G}_x = 0$.

Remark: Examples show that this is true for ranking and tournament selection, and the full paper will extend this result to those forms of selection.

PROOF. The differential of \mathcal{G} evaluated at x is given by

$$d\mathcal{G}_x = d\mathcal{M}_{\mathcal{F}(x)} d\mathcal{F}_x. \quad (1)$$

Vose shows (in theorem 6.13 of [11]) that

$$\mathbf{1}^T d\mathcal{M}_y = 2\left(\sum y_u\right)\mathbf{1}^T. \quad (2)$$

For proportional selection, let F denote the diagonal matrix whose diagonal entries are the elements of the fitness vector f . Then

$$\mathcal{F}(x) = \frac{Fx}{f^T x}$$

$$d\mathcal{F}_x = \frac{f^T x F - Fx f^T}{(f^T x)^2}.$$

Note that $\mathbf{1}^T F = f^T$. Thus,

$$\mathbf{1}^T d\mathcal{F}_x = \frac{f^T x f^T - f^T x f^T}{(f^T x)^2} = \frac{f^T - f^T}{f^T x} = 0. \quad (3)$$

Combining equations (1), (2), and (3) gives the result. \square

LEMMA 2. Let A be an $n \times n$ real matrix. Suppose that $\mathbf{1}^T A = \lambda \mathbf{1}^T$ (so that $\mathbf{1}$ is an eigenvector of A^T). Then there is an orthonormal change of basis with basis change matrix B where the first column is $\mathbf{1}$ rescaled to have unit length, and where

$$B^T A B = \begin{pmatrix} \lambda & 0 \\ * & C \end{pmatrix}. \quad (4)$$

(Here $*$ denotes possibly nonzero entries.) Then C represents the action of A on the hyperplane $\mathbf{1}^\perp = \{x \in \mathbb{R}^n : \mathbf{1}^T x = 0\}$. The eigenvalues of A in addition to λ are the same as the eigenvalues of C .

PROOF. This proof is adapted from the proof of theorem 6.12 of [11].

Since $\mathbf{1}^T A = \lambda \mathbf{1}^T$, it follows that $A : \mathbf{1}^\perp \rightarrow \mathbf{1}^\perp$. Let $\{b_0, b_1, \dots, b_{n-1}\}$ be an orthonormal basis with b_0 being $\mathbf{1}$

normalized to have unit length, and let B be the matrix whose columns are this basis. (The Walsh basis is such a basis.) Note that if $j > 0$, then

$$B^T A B e_j = B^{-1} A b_j \subseteq B^{-1}(\mathbf{1}^\perp) \subseteq e_0^\perp.$$

(Recall that e_j is the j^{th} unit vector.) Thus, $B^T A B$ satisfies equation 4.

Observe that $e_0^T B^T A B = (B^T A \mathbf{1})^T = \lambda (B^{-1} b_0)^T = \lambda e_0^T$. Thus, the upper left entry of $B^T A B$ is λ .

With respect to the above basis the elements of $\mathbf{1}^\perp$ have the form $\begin{pmatrix} 0 \\ * \end{pmatrix}$. Thus, C represents A on $\mathbf{1}^\perp$. The eigenvalues of a matrix are invariant under a change of basis. \square

2.3 Dynamical system fixed points

Let g be a map that defines a discrete-time dynamical system. A fixed point v of g is *asymptotically stable* if there is a neighborhood U of the fixed point such that $\lim_{k \rightarrow \infty} g^k(y) = v$ for all $y \in U$. The fixed point v is *unstable* if there is a neighborhood U of v , such that for all $\delta > 0$ there exists a point y with $|y - v| < \delta$ such that $g^k(y)$ is not in U for some k . **Tomas: There are two concepts of stability: Lyapunov stability and stronger one, asymptotic stability. What I wrote down for definition of unstable is the negation of Lyapunov stability. There are examples which are then neither asymptotically stable nor unstable, they are just Lyapunov stable., but this is a good definition for our purposes.**

A fixed point v is *hyperbolic* if no eigenvalue of the differential dg_v has an eigenvalue with modulus 1. Vose and Eberlein have shown that for proportional selection, the fixed points of \mathcal{G} are hyperbolic for a dense open set of fitness coefficients in the positive orthant [11]. Gedeon, et al. [3] show that for a “typical” mixing operator \mathcal{G} has finitely many fixed points, and Hayes and Gedeon have shown that the fixed points of \mathcal{G} are hyperbolic for a “typical” mixing operator [4].

For a hyperbolic fixed point v of g , the asymptotic stability of v is related to the differential dg_v at the fixed point. If all eigenvalues of dg_v have modulus less than 1, then v is *asymptotically stable*. And if any eigenvalue of dg_v has modulus greater than 1, then v is *asymptotically unstable*. We will define a hyperbolic fixed point to be a *saddle fixed point* if some eigenvalues have modulus less than 1 and some eigenvalues have modulus greater than 1. Clearly, a saddle fixed point is asymptotically unstable.

The stable Manifold theorem (see theorem 10.1 of [6]) characterizes the behavior of g in a sufficiently small neighborhood of a hyperbolic fixed point. If there are s eigenvalues whose modulus is less than 1, then there is a stable manifold of dimension s , and if there are u eigenvalues whose modulus is greater than 1, then there is an unstable manifold of dimension u . The stable manifold consists of points x such that $\lim_{k \rightarrow \infty} g^k(x) = v$ and the unstable manifold consists of points x such that $\lim_{k \rightarrow \infty} (g^{-1})^k(x) = v$ where g^{-1} denotes the inverse of g when the inverse exists. When g is not locally invertible, the unstable manifold can be defined in terms of the past history of its points. See [6] or other books on dynamical systems for details.

2.4 Fixed points of the SGA IPM

The Perron-Frobenius theorem states that there can exist only one fixed-point in the simplex for a linear system with positive irreducible transition matrix [2]. Further, this fixed

point is asymptotically stable.

This is exactly the situation for the SGA IPM with proportional selection, positive mutation, and zero crossover since the normalization of proportional selection can be ignored in determining the long-term behavior of the IPM. Thus, in this situation, \mathcal{G} has one stable fixed point in the interior of the simplex.

When the mutation rate is $1/2$, the mutation map takes all populations to the center of the simplex. Hence, \mathcal{G} with crossover, any selection method, and any fitness function has the same property.

Vose [11] conjectures that when started at a point in the simplex Δ , the iterates of \mathcal{G} converge to a fixed point. Wright and Bidwell [16] empirically tested this conjecture and found what appeared to be cyclic behavior. However, these examples used a non-standard mutation which is not bitwise mutation with a rate. Given the extensive experience with GAs, the conjecture seems very likely to be true for bitwise mutation by a rate where the rate is less than or equal to $1/2$.

2.5 Vertex fixed points

Mask-based crossover is *pure* in that crossing an individual with itself results only in that individual. Thus, when mutation is zero, the mixing map \mathcal{M} applied to a uniform population gives that population. Selection applied to a uniform population cannot produce any new individuals, and thus the selection map \mathcal{F} applied to a uniform population also gives that population. Thus, we have shown the following:

LEMMA 3. *Assume no mutation. If v is a vertex of the simplex Δ , $\mathcal{G}(v) = v$. In other words, v is a fixed point of \mathcal{G} .*

The SGA Markov chain model is absorbing when mutation is zero, and the vertex populations are the absorbing states.

For vertex fixed points of \mathcal{G} , there are some special results on stability [14], section 11.3 of [11]. The differential of \mathcal{G} is upper triangular, so the eigenvalues are the diagonal elements. In the case of proportional selection, there are simple formulas for the eigenvalues based on the fitness coefficients for one-point and uniform crossover [14]. These are given in the next theorem.

If $i \in (0, n)$, let $\text{hi}(i)$ and $\text{lo}(i)$ be the smallest and largest k such that $i \otimes 2^k \neq 0$. In other words, $\text{hi}(i)$ is the position of the leftmost one in the binary representation of i , and $\text{lo}(i)$ is the position of the rightmost one in the binary representation of i . Let $\delta(i) = \text{hi}(i) - \text{lo}(i) + 1$; $\delta(i)$ is commonly called the defining length of i .

THEOREM 4. *Assume proportional selection. Let χ denote the crossover rate for one-point or uniform crossover. For one-point crossover, the spectrum of $d\mathcal{G}_{e_k}$ is given by*

$$\text{spec}(d\mathcal{G}_{e_k}) = \left\{ \frac{f_{i \oplus k}}{f_k} \left(1 - \chi + \chi^\ell \frac{\ell - \delta(i)}{\ell - 1} \right) \right\} \cup \{0\}.$$

For uniform crossover, the spectrum of $d\mathcal{G}_{e_k}$ is given by

$$\text{spec}(d\mathcal{G}_{e_k}) = \left\{ \frac{f_{i \oplus k}}{f_k} (1 - \chi + \chi 2^{1-1^T i}) \right\} \cup \{0\}.$$

PROOF. This theorem is a restatement of theorem 3.4 and lemma 5.1 of [14]. \square

Remark by Neal: We should explicitly state here via equation/thm that stable fixed points have a $d\mathcal{G} > 1$.

Remark. In the full version of this paper, we should be able to extend this result to ranking and tournament selection.

Note that theorem 4 shows that each eigenvalue (except for 0) of the differential of \mathcal{G} at vertex fixed point e_k corresponds to the fitness of some other search space point $i \oplus k$. More precisely, it is the fitness ratio $\frac{f_{i \oplus k}}{f_k}$ times a factor that depends on i and on the crossover method.

For a crossover rate of zero (pure selection), only the vertices corresponding to global optima are stable fixed points. Global optima with no globally optimal neighbors are asymptotically stable. As the crossover rate increases, more vertices may become stable fixed points. But vertices corresponding to search space points with more fit neighbors can never be stable.

The following lemma shows that stability in \mathbb{R}^n for vertex fixed points is the same as stability in the simplex.

LEMMA 5. *If v is a vertex fixed point with the spectral radius (modulus of largest eigenvalue) of $d\mathcal{G}_v$ greater than 1, then v is an asymptotically unstable fixed point of \mathcal{G} considered as a map from the hyperplane containing the simplex to itself.*

PROOF. This is theorem 4.3 of [14]. Or lemma 2 can be used to prove this theorem. \square

2.6 Bistability

In dynamical systems theory, bistability refers to a situation where there are two stable fixed points with distinct domains of attraction. The fixed point that the system converges to depends on the initial conditions.

It is easy to construct fitness functions with multiple peaks (local maxima) so that the SGA IPM with no mutation has stable fixed points which are the uniform populations consisting only of multiple copies of the fitness peaks. See theorem 4 for details. (Note, however, that a local maximum of the fitness function does not necessarily correspond to a stable fixed point.) It is one of the main results of this paper (see theorem 19) that with a sufficiently small increase in mutation, these fixed points move inside the simplex.

This, it is easy to construct examples where the SGA IPM has dynamical systems bistability, and these examples are not surprising. However, there is a more restricted form of bistability that can happen in infinite population models which is surprising.

When the mutation rate is $1/2$, then there is a single stable fixed point of the SGA IPM at the center of the simplex. One might guess that if there was a single fitness peak, then as the mutation rate decreased from $1/2$ to zero, this stable fixed point would migrate from the center of the simplex to the uniform population corresponding to the fitness peak. However, something more complex can happen [19]: at a critical mutation rate, the stable fixed point can bifurcate into two stable fixed points and an unstable fixed point. One of the stable fixed points moves towards the fitness peak, and the other stays closer to the center of the simplex. For a range of mutation rates less than this critical mutation rate, there are two stable fixed points which is bistability in the sense defined above. But it is surprising since it is not caused by multiple fitness peaks, but is rather related

to the disruptiveness of the combination of mutation and crossover. This situation with two stable fixed points and one fitness peak was called *bistability* in [19].

As the mutation rate continues to decrease, at another smaller critical mutation rate, the center of the simplex stable fixed point disappears or stops being stable. As the mutation rate continues to decrease to zero, the other stable fixed point moves to the uniform population corresponding to the fitness peak. The above description is based on the gene pool model given in [19]. This model is similar to but not the same as the SGA IPM.

In practical terms, when there is bistability, a GA initialized with a random population is likely to be trapped close to the center of the simplex fixed point which prevents it from accumulating points of the optimal population. This is illustrated by the results of Suzuki and Iwasa [9] on the needle-in-the-haystack fitness (which they called a “babel-like fitness landscape”). They found that crossover accelerated time to convergence if the crossover rate was not too high, but over a critical crossover rate, the time to find the needle diverged. The discovery of the bistability phenomenon explained their results.

The phenomenon was discovered by Boerjlist et al [1] in a quasi species model of virus reproduction, and was analyzed for the needle-in-the-haystack and the bineedle fitness functions and proportional selection in [19]. These results were extended to truncation selection in [17] and to a “sloping plateau” fitness function in [18]. The model used in the latter three papers was a gene pool model where crossover always takes the population directly to linkage equilibrium. For this model, the fixed point equations reduce to a single equation in one variable and the existence of bistability can be rigorously proved. Iterating the SGA infinite population model demonstrates bistability for the infinite population SGA model.

Bistability (in the more restricted sense) is only known to occur in the presence of crossover, mutation, and selection. When bistability occurs, there is one fixed point “close” to the fitness peak, and one fixed point “close” to the center of the simplex. For the needle and bineedle fitness functions, the fitness peak is at a vertex of the simplex. Thus, when the GA infinite population model is initialized with a population corresponding to the center of the simplex, the GA model will converge to the center of the simplex fixed point, and when the model is initialized with a population corresponding to the fitness peak, the model will converge to the fitness peak fixed point. A finite population GA with the same parameters and fitness function, when initialized with a random population will likely be “trapped” for a long time by the center of the simplex fixed point, and while when initialized at the fitness peak, will likely be “trapped” for a long time by the fitness peak fixed point. (“A long time” is the best that we can say since the GA with mutation is an ergodic Markov chain, and all populations will be visited infinitely often.)

3. QUESTIONS

Remark. Should this be in a separate section (as is the case now), or should it be in the introduction, or a subsection of the Dynamical Systems Models section?

The dichotomy of many fixed points for crossover-selection GAs and one fixed point for mutation-selection GAs and for mutation rate $1/2$ suggests some questions:

- What happens to the vertex fixed points when mutation is increased slightly from zero? We answer this question for hyperbolic fixed points in the next section.
- What happens to the vertex fixed points when the mutation rate is increased from 0 to $1/2$? Recall that when the mutation rate is $1/2$, there is a single stable fixed point at the center of the simplex.
- What happens to the Perron-Frobenius fixed point as the crossover rate is increased from zero? Presumably, the fixed point must bifurcate when there are multiple stable fixed points under crossover. What kinds of bifurcations are possible?
- What happens to the fixed points if the crossover rate were varied to zero at the same time the mutation rate were varied to one? **Remark by Alden: I am dubious about this question. I added the second question above as a substitute. Tomas: I am not sure this will have a nice answer either. I prefer question 2**

Note that varying the mutation rate to one here is done only for abstract purposes for completeness, a mutation rate of one has no practical use in optimization. **Remark.** This sentence refers only to the last question.

4. THE MOVEMENT OF VERTEX FIXED POINTS UNDER SMALL POSITIVE MUTATION

In this section we investigate the behavior of hyperbolic vertex fixed points of \mathcal{G} as the mutation rate increases from zero. Let p denote the mutation rate, and let $\mathcal{G} : \Delta \times (-1, 1) \rightarrow \Delta$ denote the SGA map parametrized by the mutation rate p . (While a negative mutation rate is not meaningful in terms of a GA, the formulas for \mathcal{G} apply for a negative mutation rate, and this allows us to not consider one-sided derivatives.) Let $v = v_0$ be a hyperbolic vertex fixed point for $\mathcal{G}(x, 0)$. We will use the notation $\mathcal{G}_p(x)$ for $\mathcal{G}(x, p)$ when it is convenient.

While we are stating our results in term of the mutation rate, in fact all we need is that $\mathcal{G}(x, p)$ is continuously (i. e. C^1) differentiable in both x and p , and \mathcal{G}_p maps the simplex into its interior for $p > 0$.

In this section, we will be differentiating with respect to both x and p , so we will use a different notation for these derivatives. Let $\frac{\partial \mathcal{G}}{\partial x}(y, q)$ denote the derivative of \mathcal{G} with respect to $x \in \mathbb{R}^n$ evaluated at $(y, q) \in \mathbb{R}^n \times (-1, 1)$. (In the notation of the previous section, this was $d(\mathcal{G}_p)(y, p)$.) Let $\frac{\partial \mathcal{G}}{\partial p}$ denote the derivative of \mathcal{G} with respect to the mutation rate p .

Let $id : \mathbb{R}^n \rightarrow \mathbb{R}^n$ denote the identity map. Of course, the differential of id is the identity matrix.

LEMMA 6. *If $g : \mathbb{R}^n \rightarrow \mathbb{R}^n$ is differentiable at a point y with no eigenvalues equal to 1, then $g - id$ is differentiable with a nonsingular differential at y .*

PROOF. There is a similarity transformation P such that $P^{-1} \frac{dg}{dx}(y) P$ is in Jordan canonical form with the eigenvalues on the diagonal. Then $P^{-1} (\frac{dg}{dx}(y) - I) P$ is also in Jordan canonical form with eigenvalues on the diagonal. Thus, the eigenvalues of $\frac{dg}{dx}(y) - I$ are the eigenvalues of $\frac{dg}{dx}(y)$ minus

1, and by assumption these are nonzero. Thus, $\frac{dg}{dx}(y) - I$ is nonsingular. \square

Define $\mathcal{H} : \mathbb{R}^n \times (-1, 1) \rightarrow \mathbb{R}^n$ by $\mathcal{H} = \mathcal{G} - id$. Recall that we have assumed that v is a hyperbolic vertex fixed point of \mathcal{G} which means that $\frac{\partial \mathcal{G}}{\partial x}(p, 0)$ has no eigenvalues on the unit circle. Thus, $\mathcal{H}(v, 0) = 0$ and $\frac{\partial \mathcal{H}}{\partial x}(v, 0) = \frac{\partial \mathcal{G}}{\partial x}(v, 0) - I$ is non-singular by Lemma 6.

LEMMA 7. *There is a neighborhood V of v , an $\varepsilon > 0$, and a continuously differentiable function $h : [0, \varepsilon) \rightarrow V$ such that $\mathcal{H}(h(p), p) = 0$ and $h(0) = v$. If we define $v_p = h(p)$, then $\mathcal{G}(v_p, p) = v_p$, so v_p is a fixed point of \mathcal{G}_p . Furthermore, the derivative of h is given by*

$$\frac{\partial h}{\partial p}(p) = - \left(\frac{\partial \mathcal{H}}{\partial x}(h(p), p) \right)^{-1} \frac{\partial \mathcal{H}}{\partial p}(h(p), p). \quad (5)$$

PROOF. By the above argument our assumption of hyperbolicity of the vertex fixed point v implies that $\frac{\partial \mathcal{G}}{\partial x}(v, 0)$ is nonsingular. There is a neighborhood U of v and a $\delta > 0$ such that $\frac{\partial \mathcal{G}}{\partial x}(x, p)$ is nonsingular for $x \in U$ and $p \in (-\delta, \delta)$. The implicit function theorem shows that there is a neighborhood $V \subseteq U$ of v , an $\varepsilon > 0$, and a function h with the required properties. \square

We have now shown that as p increases from 0, there is a path of fixed points v_p of \mathcal{G}_p . This path can intersect the boundary of the simplex only at $v = v_0$ since \mathcal{G}_p maps the boundary of the simplex into the interior of the simplex for $p > 0$.

4.1 Asymptotically stable fixed vertex points

LEMMA 8. *Let v be a hyperbolic asymptotically stable vertex fixed point of \mathcal{G} . Then there is a neighborhood V of v in Δ and a $\delta > 0$ such that for all $p < \delta$, \mathcal{G}_p has a unique fixed point in V , and this fixed point is asymptotically stable.*

PROOF. Taking standard matrix norm in the eigenvector basis $\|\cdot\|$ we have $\|\frac{\partial \mathcal{G}}{\partial x}(v, 0)\| = \alpha < 1$. By continuity of the derivative, there exists a $\beta > \alpha$, a small neighborhood $U \subset \Delta$ of v , and a $\delta > 0$ such that for all $(x, p) \in U \times [0, \delta)$ we have

$$\left\| \frac{\partial \mathcal{G}}{\partial p} \right\| \leq \beta < 1.$$

By going to a smaller neighborhood $V \subseteq U$ if necessary, we have that for any $p \in [0, \delta)$ and any pair $x, y \in V$,

$$\begin{aligned} \|\mathcal{G}_p(x) - \mathcal{G}_p(y)\| &= \left\| \frac{\partial \mathcal{G}}{\partial p}(x) \right\| \|x - y\| + o(x - y) \\ &\leq \beta \|x - y\| + \frac{1 - \beta}{2} \|x - y\| \\ &\leq \frac{1 + \beta}{2} \|x - y\|. \end{aligned}$$

Thus, \mathcal{G}_p is a contraction on V for all $p \in [0, \delta)$. By the contraction mapping theorem (theorem 2.5 of [6]), there is a unique fixed point $v_p \in V$ for all $p \in [0, \delta)$. \square

4.2 Unstable fixed vertex points

THEOREM 9. *Let $v = v_0$ be a hyperbolic unstable vertex fixed point of \mathcal{G} . Then for sufficiently small $p > 0$, \mathcal{G}_p has no fixed point in Δ . ??*

PROOF. The domain of this proof is the $(n-1)$ -dimensional hyperplane $H = \{x \in \mathbb{R}^n : \mathbf{1}^T x = 1\}$. We can apply lemma 2 to represent $\frac{\partial \mathcal{G}}{\partial x}(v_0, 0)$ in this hyperplane, and when we refer to differentials in this proof, we are referring to their representation in this hyperplane.

The implicit function theorem argument of lemma 7 shows that there is a $\varepsilon > 0$ such that v_p is a hyperbolic fixed point of $\mathcal{G}(x, p)$ for $p \in (-\varepsilon, \varepsilon)$.

By applying the Center Manifold theorem [6] to the map $\mathcal{H} : H \times (-\varepsilon, \varepsilon) \rightarrow \mathbb{R}^n$ defined by $\mathcal{H}(x, p) = (\mathcal{G}(x, p), p)$, we conclude that the stable manifold $W^s(v_p, \mathcal{G}(x, p))$ and the unstable manifold $W^u(v_p, \mathcal{G}(x, p))$ depend C^1 jointly on both x and p . In other words, there exists a $\delta > 0$ with $\delta < \varepsilon$ such that for each such p the unstable manifold can be represented as a graph of a C^1 function

$$\sigma : E_{(v_0, 0)}^u \times (-\delta, \delta) \rightarrow E_{(v_0, 0)}^s$$

where $E_{(v_0, 0)}^u$ is a span of the eigenvectors that correspond to eigenvalues of $\frac{\partial \mathcal{G}}{\partial x}(v_0, 0)$ with modulus greater than 1 and where $E_{(v_0, 0)}^s$ is a span of the eigenvectors that correspond to eigenvalues of $\frac{\partial \mathcal{G}}{\partial x}(v_0, 0)$ with modulus less than 1. The graph consists of triples $(x, p, \sigma(x, p))$ where $x \in E_{(x_0, 0)}^u$, $p \in (-\delta, \delta)$ and $\sigma(x) \in E_{(x_0, 0)}^s$.

Suppose that v_p for $p \in (0, \delta)$ lies in the interior of Δ . Since v_0 hyperbolic and unstable, $\frac{\partial \mathcal{G}}{\partial x}(v_0, 0)$ has at least one eigenvalue with modulus greater than 1. Thus, the unstable manifold $W^u(v_0, \mathcal{G}(x, 0))$ is nonempty. The graphs of $W^u(v_0, \mathcal{G}(x, 0)) = \sigma(0)$ and $W^u(v_0, \mathcal{G}(x, p)) = \sigma(p)$ are C^1 close to each other and have the same dimension.

Let $B_r^u(v_0)$ be a ball of radius r in $E_{(v_0, 0)}^u$. For any $\varepsilon > 0$ (where ε will be chosen later), there exists an $r > 0$ and an η with $0 < \eta < \delta$ such that

$$\|\sigma(x, p) - \sigma(x, 0)\|_{C^1} < \varepsilon \quad \text{for all } x \in B_r^u(v_0), \quad p \in (0, \eta). \quad (6)$$

Since v_0 is a vertex of Δ and $E_{(v_0, 0)}^u$ is a linear space, we must have that

$$B_r^u(v_0) \cap \text{ext}(\Delta) \neq \emptyset, \quad \text{for all } r$$

where $\text{ext}(\Delta)$ is the exterior of Δ . Since $W_{(v_0, 0)}^u$ is tangent to $E_{(v_0, 0)}^u$ for sufficiently small r and $y \in B_r^u(v_0) \setminus \{v_0\}$, we must have

$$\text{graph}(\sigma(y, 0)) \cap \text{ext}(\Delta) \neq \emptyset.$$

Let $y_0 \in \text{graph}(\sigma(y, 0)) \cap \text{ext}(\Delta)$. Then there is a positive distance ϵ between the compact set $\text{graph}(\sigma(y_0, 0))$ and Δ . Therefore, by equation (6)

$$\text{graph}(\sigma(y_0, p)) \cap \text{ext}(\Delta) \neq \emptyset$$

for all $p \in (0, \eta)$. Let y_p be in this set.

The reverse iterates of y_p under \mathcal{G}_p must converge to v_p . Thus, there must be some reverse iterate of y_p that is in Δ but is mapped by \mathcal{G}_p to $\text{ext}(\Delta)$. But this contradicts that fact that \mathcal{G}_p must map Δ to the interior of Δ . Thus, our assumption that $v_p \in \Delta$ is not correct. \square

4.3 The direction of movement of fixed points as mutation increases from zero

Recall that the function h defined in lemma 7 defined the local path of fixed points as the mutation rate p increased from zero. In this section we calculate $\frac{dh}{dp}$ and discuss the implications of the result.

Throughout this section v will be a vertex fixed point of

\mathcal{G}_0 . Without loss of generality, we can rearrange the order of the coordinates of \mathbb{R}^n so that $v = e_0$ which is the first unit vector in \mathbb{R}^n .

LEMMA 10. *Let v be a vertex fixed point and assume that mutation is bitwise mutation with mutation rate p . Then*

$$\frac{\partial \mathcal{G}}{\partial p}(v, 0) = \begin{cases} -\ell & \text{if } i = 0 \\ 1 & \text{if } \mathbf{1}^T i = 1 \\ 0 & \text{otherwise} \end{cases} \quad (7)$$

Furthermore, the vector $\frac{\partial \mathcal{G}}{\partial p}(v, 0) - v$ is in the direction of the simplex.

PROOF. The GA map g can be written as a composition of a selection map, a crossover map, and a mutation map. Thus,

$$\mathcal{G}(p, x) = \mathcal{M}(\mathcal{C}(\mathcal{F}(x, p))).$$

Since the crossover map \mathcal{C} and the selection map \mathcal{F} don't depend on the mutation rate p , and since v is a fixed point of \mathcal{C} and \mathcal{F} , we have that $\frac{\partial \mathcal{G}}{\partial p}(v, 0) = \frac{d\mathcal{M}}{dp}(v, 0)$.

The definition of the mutation map is

$$\mathcal{M}(x, p) = Ax.$$

where A is the $n \times n$ matrix defined by

$$A_{i,j} = p^{\mathbf{1}^T(i \oplus j)}(1-p)^{\ell - \mathbf{1}^T(i \oplus j)}.$$

Thus,

$$\mathcal{M}(p, x)_i = \sum_j p^{\mathbf{1}^T(i \oplus j)}(1-p)^{\ell - \mathbf{1}^T(i \oplus j)} x_j.$$

Since v is the first unit vector in \mathbb{R}^n ,

$$\mathcal{M}(p, v)_i = p^{\mathbf{1}^T i}(1-p)^{\ell - \mathbf{1}^T i}.$$

Clearly, for $\mathbf{1}^T i \notin \{0, 1\}$, $\frac{\partial \mathcal{M}}{\partial p}(v, 0)_i = 0$, and it is easy to check that for $\mathbf{1}^T i = 1$, $\frac{\partial \mathcal{M}}{\partial p}(v, 0)_i = 1$ and $\frac{\partial \mathcal{M}}{\partial p}(v, 0)_0 = -\ell$. Thus, we have shown that equation (7) holds.

Define the change-of-basis matrix P to have columns $e_0, e_1 - e_0, e_2 - e_0, \dots, e_{n-1} - e_0$. Note that the columns of P , except for the first, are the directions from $v = e_0$ to the other vertices of the simplex. Multiplying by P transforms the standard basis into a basis whose elements are the columns of P . A vector from v points into the simplex if it lies in the plane of the simplex (i. e., the sum of the coordinates are zero) and if its coordinates after the first in this basis are nonnegative. Clearly, $\frac{\partial \mathcal{G}}{\partial p}(v, 0)$ satisfies these conditions. \square

Following [11] and [?], we define the *twist* A^* of an $n \times n$ matrix A to have i, j th entry $A_{i \oplus j, i}$. A matrix A is called *separative* if $A_{i,j} \neq 0$ implies that $i^T j = 0$.

Mixing (crossover and mutation) is defined through a *mixing matrix* $M(p)$ which we parametrize by the mutation rate p . See [11] or [?] for more details.

Example. For string length 2, the mixing matrix for one-point crossover with rate χ and no mutation is:

$$M(0) = \begin{pmatrix} 1 & 1/2 & 1/2 & 1/2 - 1/2\chi \\ 1/2 & 0 & 1/2\chi & 0 \\ 1/2 & 1/2\chi & 0 & 0 \\ 1/2 - 1/2\chi & 0 & 0 & 0 \end{pmatrix}.$$

The twist of this matrix is:

$$M(0)^* = \begin{pmatrix} 1 & 1/2 & 1/2 & 1/2 - 1/2\chi \\ 0 & 1/2 & 0 & 1/2\chi \\ 0 & 0 & 1/2 & 1/2\chi \\ 0 & 0 & 0 & 1/2 - 1/2\chi \end{pmatrix}.$$

LEMMA 11. *The mixing matrix $M(0)$ (for zero mutation) is separative.*

PROOF. Theorems 6.5 and 6.6 of [11] show that $M(0)$ is separative. \square

If matrix A is separative, then its twist A^* satisfies the condition

$$A_{i,j}^* \neq 0 \implies i = i \otimes j.$$

We will call a matrix satisfying this condition *twist separative*. Clearly, $M(0)^*$ in the example above is twist separative.

For example, suppose that $i = 6 = 110$ and $j = 3 = 011$. Then $i \otimes j = 010 \neq 110 = i$, so if A is twist separative, $A_{6,3} = 0$. So whenever there is a locus of j which is zero while the corresponding locus of i is one, the pair i, j does not satisfy $i = i \otimes j$, and thus $A_{i,j} = 0$.

LEMMA 12. *A twist separative matrix is upper triangular.*

PROOF. $i = i \otimes j \implies i \leq j$. \square

LEMMA 13. *The inverse of a twist separative matrix is twist separative.*

PROOF. The following is a ‘‘back-substitution’’ algorithm to compute the inverse of an upper triangular matrix:

INVERSEUPPERTRIANGULAR(A)

```

1   $B \leftarrow$  a square zero matrix of the same dimensions as  $A$ 
2  for  $r \leftarrow 0$  to  $n - 1$  do
3     $B[r, r] \leftarrow 1/A[r, r]$ 
4  for  $r \leftarrow 1$  to  $n - 1$  do
5    for  $i \leftarrow 0$  to  $n - r - 1$  do
6       $j \leftarrow i + r$ 
7       $B[i, j] \leftarrow -\frac{1}{A[i, i]} \sum_{k=i+1}^j A[i, k]B[k, j]$ 
8  return  $B$ 
```

Let i, j be such that $i \neq i \otimes j$. We need to show that $B[i, j] = 0$. As above, there must be a locus at which j has a zero bit while i has a one bit. Consider the possibilities for that locus of the summation index k in line 7 of the algorithm. If that locus of k is a one bit, then $k \neq k \otimes j$ which implies that $B[k, j] = 0$. If that locus of k is a zero bit, then $i \neq i \otimes k$ which implies that $A[i, k] = 0$. Thus, each term of the summation of line 7 is zero, which implies that $B[i, j] = 0$. \square

LEMMA 14. *If A is an $n \times n$ twist separative matrix and $B = A^{-1}$, then for j such that $\mathbf{1}^T j = 1$, $B_{0,j} = \frac{A_{0,j}}{A_{0,0}A_{j,j}}$.*

PROOF. Line 7 of the above algorithm applied to $B[0, i]$ is

$$B[0, j] \leftarrow -\frac{1}{A[0, 0]} \sum_{k=1}^j A[0, k]B[k, j].$$

Since B is twist separative, $B[k, j] = 0$ for $k = 1, 2, \dots, j-1$. Thus, the only nonzero term in the summation is $A[0, j]B[j, j] = A[0, j]/A[j, j]$. \square

LEMMA 15. *The product of twist separative matrices is twist separative.*

PROOF. The following is the algorithm to compute the product of upper triangular matrices:

```

PRODUCTUPPERTRIANGULAR( $A, B$ )
1   $C \rightarrow$  a square matrix of the same dimensions as  $A$  and  $B$ 
2  for  $i \leftarrow 0$  to  $n-1$  do
3      for  $j \leftarrow i$  to  $n-1$  do
4           $C[i, j] \leftarrow \sum_{k=i}^j A[i, k]B[k, j]$ 
5  return  $C$ 

```

The argument of the proof of Lemma 13 applies to line 4 of this algorithm to show that $i \neq i \otimes j \Rightarrow C[i, j] = 0$. \square

LEMMA 16. *The differential of \mathcal{G} at simplex vertex $v = e_0$ is given by*

$$\frac{\partial \mathcal{G}}{\partial x}(v, p) = \frac{\partial \mathcal{G}}{\partial x}(e_0, p) = 2M(p)^* \frac{d\mathcal{F}}{dx}(e_0).$$

where \mathcal{F} denotes the selection map. For proportional selection, $\frac{d\mathcal{F}}{dx}(e_0)$ is twist separative. The matrices $\frac{\partial \mathcal{H}}{\partial x}(v, 0)$ and $(\frac{\partial \mathcal{H}}{\partial x}(v, 0))^{-1}$ are also twist separative (where $\mathcal{H}(x, p) = \mathcal{G}(x, p) - x$).

Remark. This lemma depends on our rearrangement of coordinates so that $v = e_0$. Without this assumption, the rows and columns of the differential need to be permuted to be twist separative. See [14] or [11] for details on how this can be done.

Remark. Examples suggest that this lemma is also true for ranking and tournament selection. The full version of the paper will extend the lemma to these forms of selection.

PROOF. The proof of theorem 11.8 of [11] gives the formula for the differential. (Since we are taking the differential at e_0 , the σ permutation matrices in formula of [11] are the identity.)

$M(0)^*$ is twist separative by lemma 11. Let the fitness vector be $\langle f_0, f_1, \dots, f_{n-1} \rangle^T$. The proof of theorem 11.8 also shows that

$$\left(\frac{d\mathcal{F}}{dx}(e_0) \right)_{i,j} = \frac{\delta_{i,j} f_i - \delta_{i,0} f_j}{f_0}$$

when \mathcal{F} is defined by proportional selection. Thus $\frac{d\mathcal{F}}{dx}(e_0)$ is nonzero only on the diagonal and the first row which implies that it is twist separative. $\frac{\partial \mathcal{H}}{\partial x}(e_0, 0) = \frac{\partial \mathcal{G}}{\partial x}(e_0, 0) - I$ is clearly twist separative, and lemma 13 shows that $(\frac{\partial \mathcal{H}}{\partial x}(e_0, 0))^{-1}$ is twist separative. \square

LEMMA 17. *For proportional, ranking, and tournament selection, $\frac{\partial \mathcal{G}}{\partial x}(v, 0) = \frac{\partial \mathcal{G}}{\partial x}(e_0, 0)$ is upper triangular and its diagonal entries are its eigenvalues $\lambda_0, \lambda_1, \dots, \lambda_{n-1}$. For proportional selection, $\lambda_0 = 0$ and for j such that $\mathbf{1}^T j = 1$, $\frac{\partial \mathcal{G}}{\partial x}(v, 0)_{0,j} = -\lambda_j$.*

PROOF. Vose shows that $\frac{d\mathcal{F}}{dx}(e_0)$ is upper triangular for all three kinds of selection in the proof of theorem 11.8 of [11]. For proportional selection, lemma 1 shows that $\mathbf{1}^T \frac{d\mathcal{F}}{dx}(e_0) = 0$. Since $\frac{d\mathcal{F}}{dx}(e_0)$ is twist separative, the only nonzero entries

in column j where $\mathbf{1}^T j = 1$ are the row 0 entry and the diagonal entry. Thus, the row 0 entry must be the negative of the diagonal entry λ_j . \square

Since $\frac{\partial \mathcal{G}}{\partial x}(v, 0)$ is upper triangular, its diagonal entries are its eigenvalues $\lambda_0 = 0, \lambda_1, \dots, \lambda_{n-1}$.

THEOREM 18. *Assume proportional selection. Let v be a hyperbolic fixed point of \mathcal{G}_0 . Then*

$$\frac{dh}{dp}(0)_i = \begin{cases} -\sum_{j:\mathbf{1}^T j=1} \frac{1}{1-\lambda_j} & \text{if } i=0 \\ \frac{1}{1-\lambda_i} & \text{if } \mathbf{1}^T i=1 \\ 0 & \text{otherwise} \end{cases}$$

where λ_i is the i^{th} diagonal entry and eigenvalue of $\frac{\partial \mathcal{G}}{\partial x}(v, 0)$.

PROOF. Lemma 7 shows that

$$\frac{dh}{dp}(0) = -\left(\frac{\partial \mathcal{H}}{\partial x}(v, 0) \right)^{-1} \frac{\partial \mathcal{H}}{\partial p}(v, 0).$$

Since the identity map does not depend on p , $\frac{\partial \mathcal{H}}{\partial p}(v, 0) = \frac{\partial \mathcal{G}}{\partial p}(v, 0)$ which is given by equation (7). This shows that $\frac{dh}{dp}(0)_i = 0$ for i such that $i \neq 0$ and $\mathbf{1}^T i \neq 1$.

Let E denote the matrix $(\frac{\partial \mathcal{H}}{\partial x}(v, 0))^{-1}$. Note that the i^{th} diagonal entry of the upper triangular matrix $\frac{\partial \mathcal{H}}{\partial x}(v, 0)$ is $\lambda_i - 1$ and therefore the i^{th} diagonal entry of E is $\frac{1}{1-\lambda_i}$.

Lemma 16 shows that E is twist separative. Then

$$\frac{dh}{dp}(0)_i = \sum_j E_{i,j} \frac{\partial \mathcal{H}}{\partial p}(v, 0)_j. \quad (8)$$

First, we consider $i > 0$ and the j^{th} entry in this sum. By equation (7) $\frac{\partial \mathcal{H}}{\partial p}(v, 0)_j$ is nonzero only when $j = 0$ or $\mathbf{1}^T j = 1$, and in this latter case $\frac{\partial \mathcal{H}}{\partial p}(v, 0)_j = 1$. Since E is twist separative, $E_{i,j}$ is nonzero only when $i = i \otimes j$. Thus, the only j for which the j^{th} term in the summation of equation (8) is nonzero is when $i = j$. Thus, when $i > 0$, $\frac{dh}{dp}(0)_i = E_{i,i} = \frac{1}{1-\lambda_i}$.

Now we consider the j^{th} entry in the sum of equation (8) when $i = 0$.

Since $\frac{\partial \mathcal{H}}{\partial p}(v, 0)_j = 0$ except when $\mathbf{1}^T j = 1$ and $j = 0$, we only need to consider entries $E_{0,j}$ where $\mathbf{1}^T j = 1$ and $j = 0$.

Lemma 17 shows that $\frac{\partial \mathcal{G}}{\partial x}(v, 0)_{0,0} = 0$. Thus, 17 shows that $\frac{\partial \mathcal{H}}{\partial x}(v, 0)_{0,0} = E_{0,0} = -1$.

From lemma 14 and lemma 17 it follows that if $\mathbf{1}^T j = 1$, $E_{0,j} = \frac{\lambda_j}{-(\lambda_j - 1)} = \frac{\lambda_j}{1 - \lambda_j}$. Thus,

$$\left(\frac{dh}{dp} \right)_0 = \ell + \sum_{j:\mathbf{1}^T j=1} \frac{\lambda_j}{1 - \lambda_j} = \sum_{j:\mathbf{1}^T j=1} \frac{1}{1 - \lambda_j}.$$

\square

Let $B_\varepsilon(v) = \{x \in \mathbb{R}^n : \|x - v\| < \varepsilon\}$ be the ball of radius ε around v . The next theorem shows that as mutation increases, a hyperbolic asymptotically stable fixed point moves into the interior of the simplex.

THEOREM 19. *Assume that v is a hyperbolic asymptotically stable fixed point of \mathcal{G} , and h is the map defined in lemma 7. There is an $\varepsilon > 0$ and a $\gamma > 0$ such that for $p \in [0, \gamma]$, $h(p)$ is the unique fixed point of \mathcal{G}_p in $B_\varepsilon(v)$.*

Remark: I moved this theorem here so that I can use lemma 10 to show that $\frac{\partial \mathcal{G}}{\partial p}(v, 0) \neq 0$.

PROOF. Lemma 10 shows that $\frac{\partial \mathcal{G}}{\partial p}(v, 0) = \frac{\partial \mathcal{H}}{\partial p}(v, 0) \neq 0$. Thus, $\frac{dh}{dp}(0) \neq 0$. By the continuity of the derivative, there is a $\eta > 0$ such that for $0 \leq q \leq \eta$, $\frac{dh}{dp}(q)^T \frac{dh}{dp}(0) > 0$. We can also assume that $\eta < \delta$ for the δ of lemma 8. Let $\gamma = \|v - h(q)\|$. Then for such q , $\|h(q) - v\|$ is strictly monotonically increasing as q increases. Let $\varepsilon > 0$ be such that $\varepsilon \leq \|h(\eta) - v\|$ and $B_\varepsilon(v)$ gives the unique fixed point of lemma 8. Now choose $\gamma > 0$ to be sufficiently small that if $0 < p < \gamma < \delta$, then $h(p) \in B_\varepsilon$. Then $h(p)$ must be the unique fixed point of lemma 8. \square

Remark, Alden 6/22/10: I will add some comments about the meaning of these results. For example, if there is an i with $\mathbf{1}^T i = 1$ and $\lambda_i > 1$, then we have shown that the fixed point moves outside of the simplex. The closer the eigenvalues are to 1, the faster that the fixed point moves away from the vertex. I will also give at least one empirical example. **Not to be included in submitted version.**

4.4 Discussion

Let v be a hyperbolic vertex fixed point corresponding to a uniform population of k individuals, i. e., $v = e_k$. Theorem 4 shows that each eigenvalue of $\frac{\partial \mathcal{G}}{\partial x}(v, 0)$ (other than 0) is determined by the fitness and the properties of some other point $i \oplus k$ of the search space. Theorem 18 shows that these fitnesses for the Hamming distance 1 neighbors of k determine the direction of $\frac{dh}{dp}(0)$. If all Hamming distance 1 neighbors have fitness less than the fitness of k , then the vector from v to $\frac{dh}{dp}(0)$ points in the direction of the interior of the face of Δ determined by v and its Hamming distance 1 neighbors. If some Hamming distance 1 neighbor has greater fitness, then the vector from v to $\frac{dh}{dp}(0)$ points outside of the simplex (providing an alternate proof of theorem ?? in this special case).

If $v = e_k$ is unstable under no mutation, this means that at least one eigenvalue of $\frac{\partial \mathcal{G}}{\partial x}(v, 0)$ is greater than 1. Lemma 4 shows that each eigenvalue corresponds to some point in the search space other than k which has higher fitness than k . The instability of v means that when the SGA IPM is initialized a population which is both near to v , interior to the simplex, and not on the stable manifold of v , it will diverge away from v due to the influence of the higher fitness points just mentioned.

Any population vector interior to the simplex must contain a nonzero representation of every point in the search space, including those higher fitness points that caused v to be unstable. But in a finite GA population in a situation where the string length is realistically long, this won't happen since the size of the search space grows exponentially with the string length. If the search space points that make v unstable have a large Hamming distance from v , they are unlikely to be included in a finite population near v . And if there is mutation with a mutation rate that is $\Theta(1/n)$, such points are unlikely to be discovered in a realistic time period. Thus, from the point of view of finite populations, v is stable in that when a with-mutation GA is at a population near v , it is likely to remain there for a long time (namely, until the higher-fitness points that make v unstable are discovered by mutation). In the case of no-mutation, we would conjecture that the GA would be likely to be absorbed into the population corresponding to v .

We can also conjecture that when the search space points that make v unstable at at least Hamming distance j from v , then as the mutation rate p increases from 0, the fixed point corresponding to v is order $O(p^j)$ close to the face of the simplex determined by v and its Hamming distance 1 neighbors. In other words, it would be very close to the simplex. When a saddle-point fixed point is very close to but not in the simplex, the IPM will move very slowly when close to this fixed point [11], [10].

4.4.1 Examples

We give two examples of the situation just described. Both examples use 1-point crossover with crossover rate 7/8 and the following fitness function:

$$f(i) = \begin{cases} 20 & \text{if } \mathbf{1}^T i = 0 \\ 165 & \text{if } \mathbf{1}^T i = \ell \\ 1 & \text{otherwise} \end{cases}$$

For any string length and 1-point crossover with rate 7/8, the uniform population consisting of the all zeros string is an unstable vertex fixed point because the eigenvalue corresponding to the all ones string is $\frac{33}{32}$ by theorem 4.

In the first example the SGA IPM is started at the all zeros string (which has fitness 20). The string length is 7 and the mutation rate is $\frac{1}{100}$. The all ones string (which has fitness 165) has a frequency of 10^{-14} after one time step. This frequency gradually increases. After one time step the fitness is 18.71, and this decreases to 18.641164 after 6 time steps. For the next 145 time steps, the fitness is very gradually decreasing, but to 8 significant digits, it remains at 18.641164. After 369 time steps, the fitness reaches a minimum of 18.272 and then it increases rapidly reaching 153.71 at time step 376. The IPM converges to within a tolerance of 10^{-12} after 382 time steps with a fitness of 153.79.

In the second example, the SGA is run with the same fitness, string length 9, mutation rate $\frac{1}{10}$, and population size 1000. Initialization is with multiple copies of the all zeros string. The SGA was run until it found the optimum. With 100 runs, the average number of generations to find the optimum was 37,645 with a standard deviation of 34,767. The number of fitness evaluations was approximately 1000 times the number of generations. Clearly, while the all zeros uniform population is unstable as a fixed point, the GA takes a very long time to leave a neighborhood of this fixed point.

5. EXAMPLES OF VERTEX FIXED POINT MOVEMENT

For the Simple GA a system let n be the string length and $N = 2^n$ be the search space size. Let $n = 2$ and $N = 4$ and define the BINEEDLE function be defined below with $a = 1$. For now assume that the mutation-rate μ is zero.

$$BINEEDLE f(x) = \begin{cases} 1 + a & \text{all ones string} \\ 1 & \text{otherwise} \\ 1 + a & \text{all zeros string} \end{cases} \quad (9)$$

This system produces this set of possible strings and fitness values. The index of this state is given as well, where this is defined as the decimal value of the binary string.

bitstring	fitness	index
00	2	1
01	1	2
10	1	3
11	2	4

(10)

As before, the GA-map is described below and operates within a $N - 1$ dimensional simplex Λ .

$$\mathcal{G}(x) = \mathcal{M}(\mathcal{C}(\mathcal{F}(x))) \quad (11)$$

A population exists on the vertex of that simplex when it contains only copies of one bitstring. For example when the population consists only of copies of 00, it exists at the $\langle 1, 0, 0, 0 \rangle$ vertex of the simplex.

Vose and Wright [14] detailed the analysis of vertex fixed points. The key finding of their work that the stability of the vertex fixed points can be calculated using a relatively simple formula. Let the population $v_1 = \langle 1, 0, 0, 0 \rangle$ mean that it contains only copies of 00. This relationship holds for v_1 and all vertex fixed points:

$$v_1 = \mathcal{G}(v_1) \quad (12)$$

Each of the other vertexes are fixed points as well as the center of the simplex point $\langle 1/4, 1/4, 1/4, 1/4 \rangle$. This is easily verifiable by simply iterating the GA map on these points as the starting population distribution.

6. STABILITY ANALYSIS OF FIXED POINTS

The next crucial question is determining the stability of these fixed points. There are two states of concern, stable and unstable. In the language of fixed points (see for example Strogatz [8]) a fixed point x^* is (asymptotically) stable and attracting if trajectories that start near x^* both stay nearby for all time as well as approach x^* as $t \rightarrow \infty$. A fixed point x^* is unstable trajectories starting near x^* do not stay nearby for all time and trajectories are not approaching x^* as $t \rightarrow \infty$.

An unstable saddle fixed point x^* is more complicated, they contain stable and unstable manifolds. In the unstable manifold iterations move away from the fixed point. Saddle points also contain a (typically lower dimensional) stable manifold. This is defined to be the subset of initial conditions x_0 for which $x_t \rightarrow x^*$ as $t \rightarrow \infty$ when the system is iterated. It is not always possible to represent these stable manifolds within a digital computer.

Saddle points can contain trajectories within the unstable manifold that are *eventually repelling*. In loose language, there exist initial conditions for which iterations move towards the fixed-point for a time, only to then eventually begin to move away from the fixed-point. See van Nimwegen [10] for instances of this behavior in GAs, he calls them "meta-stable regions". See any dynamical systems book for generic examples of these effects.

How can the stability of the fixed points be directly calculated? Assuming the system is differentiable (the \mathcal{G} -map is differentiable) the basic procedure is to compute the derivative about the fixed point in question and then compute the eigenvalues of the derivative. For discrete dynamical systems if all eigenvalues are less than one, then the fixed point

Table 1: BINEEDLE vertex fixed points, one-point crossover $\chi = 1.0$ and $\mu = 0$.

population	eigenvalues	type
$\langle 1, 0, 0, 0 \rangle$	$[1/2, 1/2, 0, 0]$	Stable
$\langle 0, 1, 0, 0 \rangle$	$[2, 2, 0, 0]$	Saddle
$\langle 0, 0, 1, 0 \rangle$	$[2, 2, 0, 0]$	Saddle
$\langle 0, 0, 0, 1 \rangle$	$[1/2, 1/2, 0, 0]$	Stable
$\langle 1/4, 1/4, 1/4, 1/4 \rangle$	$[4/3, 2/3, 0, 0]$	Saddle

Table 2: BINEEDLE vertex fixed points, uniform crossover $\chi = 1.0$ and $\mu = 0$.

population	eigenvalues	type
$\langle 1, 0, 0, 0 \rangle$	$[1/2, 1/2, 1/2, 0]$	Stable
$\langle 0, 1, 0, 0 \rangle$	$[2, 2, 1/2, 0]$	Saddle
$\langle 0, 0, 1, 0 \rangle$	$[2, 2, 1/2, 0]$	Saddle
$\langle 0, 0, 0, 1 \rangle$	$[1/2, 1/2, 1/2, 0]$	Stable
$\langle 1/4, 1/4, 1/4, 1/4 \rangle$	$[4/3, 2/3, 4/9, 0]$	Saddle

is stable. If all are greater than 1, then it's an unstable fixed point. If there is a mix of values above and below 1, then the fixed point is a saddle point. The differential of \mathcal{G} is given in Eq 1.

Getting back to the BINEEDLE example above, one can calculate the the stability of the five fixed points in question. For the \mathcal{G} -map for one-point crossover (rate $\chi = 1.0$) and mutation $\mu = 0$:

Note the switching of the $\langle 0, 1, 0, 0 \rangle$ and $\langle 0, 0, 1, 0 \rangle$ vertices from unstable to saddle points with swapping of crossover methods. If the process is repeated for one-point crossover $\chi = 0.5$, then the results are the same as that of uniform crossover. It is conjectured that the stable manifolds for the saddle vertex fixed points of uniform crossover exist outside the simplex. These outcomes can be confirmed by simply iterating the \mathcal{G} .

For the center of the simplex population $\langle 1/4, 1/4, 1/4, 1/4 \rangle$ the iterates return the same population. However if it is perturbed slightly to $\langle 0.2499, 0.2500\bar{3}, 0.2500\bar{3}, 0.2500\bar{3} \rangle$, then the iterates converge to the $\langle 0, 0, 0, 1 \rangle$ stable fixed point. For $\langle 0.2500\bar{3}, 0.2500\bar{3}, 0.2500\bar{3}, 0.2499 \rangle$ it converges to the $\langle 1, 0, 0, 0 \rangle$. These are likely portions of the unstable manifolds, though the exact boundaries are not defined here.

The stable manifold contains the point $\langle 0, 1/2, 1/2, 0 \rangle$ which converges to $\langle 1/4, 1/4, 1/4, 1/4 \rangle$ in one step. Note that this is the Hardy-Weinberg effect kicking in and taking the population to linkage equilibrium in one step,

This process was repeated completed for string length $n = 4$, $N = 2^4 = 16$ for BINEEDLE with $a = 1$. For both one-point and uniform crossover the only stable fixed points are at the all-ones and all-zeros string vertices. All other vertex fixed points are saddle points. The uniform population fixed point in the center of the simplex is also a saddle point.

If this analysis is done for the NEEDLE function, with fitness 1 for all string values except the all-ones string with fitness 2, then all vertex fixed points are unstable except the uniform population of the all-ones string. The center of the simplex has complex eigenvalues and is not a fixed point

here.

Other examples can be constructed with fitness functions with equal (and maximal) fitness in two or more search space elements where these elements are Hamming neighbors. If a population were to be initialized with equal/uniform membership in only these elements, this situation with the no-mutation GA should devolve into a random walk on that Hamming surface of the simplex. Once a point hit a vertex it would stay there. This is an example of drift as studied in population genetics.

Example fitness function for $n = 4$, $N = 2^4 = 16$:

$$\text{CONCATNEEDLE} : \langle 2, 2, 1, \dots, 1 \rangle \quad (13)$$

For an initial population of $\langle 1/2, 1/2, 0, \dots, 0 \rangle$, or any population $\langle X, Y, 0, \dots, 0 \rangle$ such that $X + Y = 1$, the eigenvalues of the system here have a single entry of 1 and all other entries are less than 1. This means that the surface itself is stable while specific points are not. In this case the surface is a line-segment between the vertexes. Each point of the segment is stable, yet not asymptotically stable.

7. INTRODUCING EPSILON MUTATION

For the BINEEDLE the a computational study was done to attempt to attempt determine where the vertex fixed points moved to under epsilon mutation. Note solving the full \mathcal{G} -map for fixed points is infeasible, see Chapter 7 of Vose [11] for a discussion. He suggests iterating the map to find them.

Here map-iteration experiments were done with initial populations set at either of the two stable vertex fixed points or the simplex-center uniform populations. A range of mutation rates were chosen and one-point crossover is used with $\chi = 1.0$. The results are represented in the table below. Note that the experiment was explicitly done for both stable vertex-populations at all-ones and all-zeros. The symmetry of the fitness function means that results for either hold for both, it's merely an exchange of ones and zeros in the state space.

Let the symbol ϕ represent a number very close to zero, here $|\phi| < 10^{-6}$. As these fixed-points are vectors of length 16, compact abbreviations of the vectors are used as appropriate. For each chosen mutation and initial condition the \mathcal{G} -map was iterated until observed convergence or at least 300 iterations. The stability of each observed fixed-point was calculated. For fixed-points marked as saddle points, they converged to the listed point after 500 generations.

Figure 1 displays an interpolated version of the bifurcation diagram. Three initial populations were used, one at the all-zeros needle, one at a uniform population, and one with 1/2 the population at the all-zeros and all-ones population.

This bifurcation is an instance of the pitchfork bifurcation, where a stable fixed point bifurcates into two stable fixed points with an unstable fixed point between them. The upper curve of Figure 1 is displaying *both* stable fixed points as the y -axis represents fitness and these points have the same fitness by symmetry. The lower curve displays the unstable saddle point's average fitness. The critical point of bifurcation is 7.65

This is an interesting result in that the unstable saddle point has a stable manifold that is converged to. By the symmetry of the BINEEDLE and the initial conditions, these iterations are on the stable manifold and iterations will re-

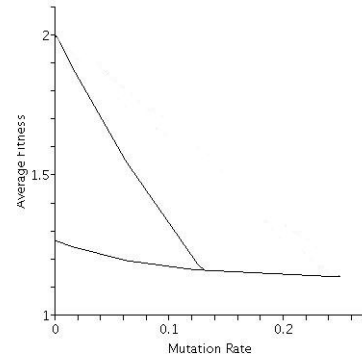


Figure 1: Epsilon mutation bifurcation of stable fixed points

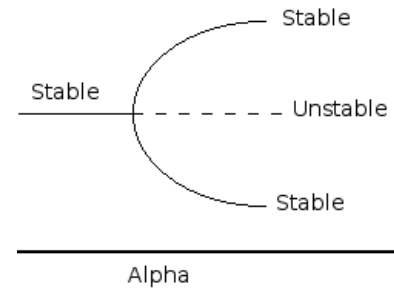


Figure 2: Typical pitchfork bifurcation

main there. This type of direct iterative observation of the lower-dimensional stable manifold is not always possible.

A typical pitchfork bifurcation is given in Figure 2 in pictorial form with alpha as the varied parameter.

The above results are by definition incomplete, they do not contain all fixed points. Many more initial populations would need to be tried, and unstable (non-saddle) fixed points are not observable via iteration. With small mutation rates, the overall dynamics have not changed much. There still exist three observable fixed points, two stable and one saddle point. Yet it's clearly observable that at approximately mutation rate 1/7.65 something interesting happens, a single stable fixed point splits into three fixed points for mutation rate 1/8.

However, for this \mathcal{G} -map one can not be certain of the locations and movement of unobserved fixed points. There could be other stable fixed points in the simplex, though this seems unlikely given the intuitive understanding of a GA with crossover and mutation operating on the BINEEDLE fitness function.

CONJECTURE 20. *For the GA with crossover and non-zero epsilon mutation, the stable vertex fixed-points of zero mutation GA move inside the simplex and the unstable vertex fixed-points of zero mutation GA move outside the simplex.*

8. INTRODUCING EPSILON CROSSOVER

A similar experiment was done with examining the effects of adding epsilon one-point crossover to a fixed mutation

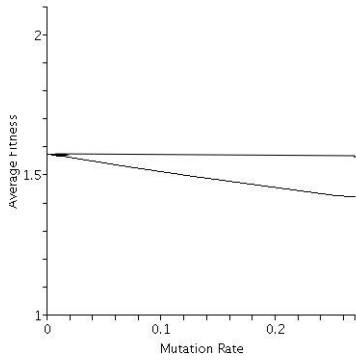


Figure 3: Epsilon crossover bifurcation of stable fixed points

rate \mathcal{G} -map. The mutation rate is set to $\mu = 1/N = 1/16$, and the crossover rate is varied over a range. Again note that with zero crossover there exists only a single stable fixed point in the interior of the simplex. Figure 3 displays an interpolated version of the bifurcation diagram.

These results are very interesting in that they indicate a critical (observable) bifurcation of a single stable fixed into a stable fixed point and a saddle point. This happens at approximately crossover rate $1/128$. Over 8,000 iterations of the \mathcal{G} -map were starting from the population uniformly at the all-zeros point. At this point that run was stopped, with the result being row 3 in the above table.

The leading eigenvalue of the derivative at this stopping point was 0.99960, meaning that the trajectory of iteration is very likely close to the stable manifold of the saddle point. The leading eigenvalue of the derivative at the fixed-point in row 4 was exactly 1. Note that these numbers are approximate and at these types of critical points the numerics of computation in binary computers can result in some inaccuracies.

Once the crossover rate grew to $1/64$ and above a clear separation of iterative convergence was established between the different starting populations. At crossover rate $63/64$ the interior saddle point's population distribution is such that it is approaching uniform frequency of 8% or $1/16$. This indicates that the crossover operator is being quite disruptive and has destroyed the GA's ability to maintain high membership in the fittest individuals.

9. REVISITING BISTABILITY

The study next revisited the sloping plateau function from Chapter ???. The sloping plateau functions are redefined below. Figure 4 duplicates Figure ??? with a plateau function with $\ell = 20, k = 5, a = 5, b = 5$. Remember that ℓ and n are interchangeable here to represent string length.

$$P_{a,b,k}(x) = \begin{cases} a + b + 1 & \text{if } |x| < k \\ b + (\ell - |x|)/\ell & \text{if } |x| \geq k \end{cases}$$

The previous chapter looked at the effects of bistability and did some varying of the mutation rate to establish the critical ranges of mutation for which bistability happens. This study chose instead to hold the mutation rate steady and vary the a in a range in an effort to discover a bifurcation

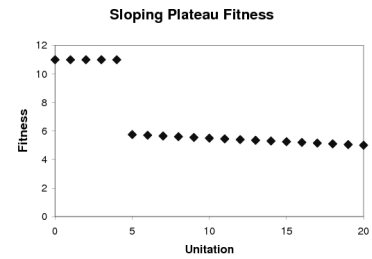


Figure 4: Sloping Plateau Fitness, $\ell = 20, k = 5, a = 5, b = 5$

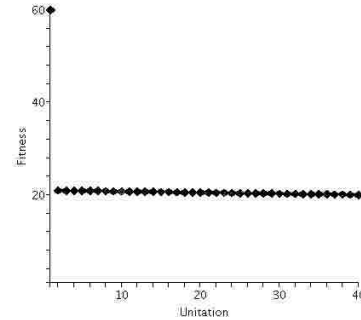


Figure 5: Sloping Needle Fitness, $\ell = 40, k = 1, a = 20, b = 20$

point. The parameters of the fitness function were changed as well to $\ell = 40, k = 1, b = 20$ and $a \in [1, 40]$. This forms a sloping needle and is shown in Figure 5.

A key point of this fitness function is that the *floor* area of the function slopes directly to the needle. To a simple hillclimber $(1 + 1)EA$ this function is indistinguishable from a function like ZEROMAX (the inverse of ONEMAX). In addition it is easily solvable by a non-crossover EA/GA with an arbitrary population size. Just as with the sloping plateau, the function is designed to deceive proportional selection. In general, any EA with a large population will be slower to optimize this function than one with a small population where the effects of 'weak selection' are muted.

The experiments were conducted as follows. At each value of $a \in [1, 40]$ the \mathcal{G} -map was iterated to convergence starting from two initial populations. The first is a uniform population while the second consists entirely of members from the needle at the all-zeros string. A mutation rate of $1/3\ell$ was used along with uniform crossover with rate = 1.0.

For values of $a < 21$ both initial population converged to the same center of the simplex point. At $a = 21$ a bifurcation point is reached. The stable fixed point splits into three stable fixed points. Recall that the system has symmetric fixed points near the all-ones and all-zeros strings. For increasing values of a , the average population fitness of these two fixed points climbs until it reaches approximately avg-fitness 41 and levels off. The fixed point for the initial uniform population remains at avg-fitness = 20.5 for all values of a tested.

The resulting bifurcation diagram is pictured below in Figure 6. The y-axis represents the average fitness of a fixed point and not the fixed point itself. Recall that visualiz-

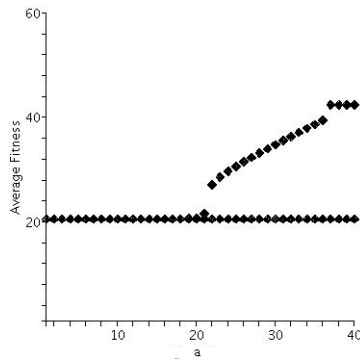


Figure 6: Sloping Needle fixed point bifurcation

ing the population distribution movement results in a 2-D surface graph like those seen in prior chapters.

No conclusions can be drawn on the movement of unobserved fixed points, yet presumably other likely unstable fixed points emerged from the bifurcation event as generally in dynamical systems a stable fixed point can not bifurcate into two without an unstable fixed point lying between them in space. See Strogatz [8], Brin and Stuck [2] or Seydel [7] for more information on bifurcations in dynamical systems.

10. CONCLUSIONS

TODO

place holder conclusions

The results here show multiple computational studies of the infinite population model \mathcal{G} -map in MapleTM. The first two were extensions of work on vertex fixed points by Vose and Wright [14]. Key questions were answered on where fixed points moved as mutation or crossover rate changed for the given fitness function. Stability analysis was also conducted. Not all fixed points are traceable in this way and these results say nothing about unobserved fixed points. The BINEEDLE was chosen due to its intuitive ease and optimization success with EAs, yet GAs with strong crossover fail in experiments.

The third study extended the results of Wright and Richter [18] to look at the sensitivity of the needle height in a sloping needle fitness function. This function is also deceptive to a GA with strong crossover due to the effects of weak selection and the disruptive effects of crossover's bit mixing. Interestingly, the height of the needle induces bistability in proportionate selection. Again, no conclusions can be drawn about the unobserved fixed points. A future direction would be to move to gene-pool crossover and reduce the \mathcal{G} -map to a system of equations and unknowns. This would allow the computation of all fixed-points and better exploration of the dynamics of high n gene-pool crossover GAs.

This is believed to be one of the few times an analysis has been done on the movement of fixed points of the \mathcal{G} -map with crossover.

11. ACKNOWLEDGMENTS

TODO

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