A Discipline of Evolutionary Programming

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Abstract

Genetic fitness optimization using small populations or small population updates across generations generally suffers from randomly diverging evolutions. We propose a notion of highly probable fitness optimization through feasible evolutionary computing runs on small size populations. Based on rapidly mixing Markov chains, the approach pertains to most types of evolutionary genetic algorithms, genetic programming and the like. We establish that for systems having associated rapidly mixing Markov chains and appropriate stationary distributions the new method finds optimal programs (individuals) with probability almost 1. To make the method useful would require a structured design methodology where the development of the program and the guarantee of the rapidly mixing property go hand in hand. We analyze a simple example to show that the method is implementable. More significant examples require theoretical advances, for example with respect to the Metropolis filter.

1 Introduction

Performance analysis of genetic computing using unbounded or exponential population sizes or population updates across generations [27,21,25,28,29,22,8] may not be directly applicable to real practical problems where we always have to deal with a bounded (small) population size [9,23,26].

Considering small population sizes it is at once obvious that the size and constitution of the population or population updates may have a major impact

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on the evolutionary development of the population. We aim to establish a fast feasible speed of convergence to a distribution of populations from which we can obtain by Monte Carlo sampling an optimal type individual with high probability. The method we propose clearly can be used by a wide range of genetic computing models which includes genetic algorithms on strings and genetic programming on trees, and so forth. Application of the method to problems is another matter; we have examples solving trivial problems but we don’t have an example solving a difficult problem. The main question for future research is to supply such an application.

The structure of the paper is as follows. In Section 2 we explain the finite Markov chain model for genetic processes. The states of the chain correspond to finite populations. The transition probability between two states is induced by the selection, reproduction, and fitness rules, as in [19,26,14].

Since the evolution from generation to generation is a random process, using finite populations different evolutions may diverge. This is not the case when we consider evolutions of probability density distributions. The idea is to view such processes as corresponding with infinite populations that are completely transformed in each generation. Or to view them as an approximation to very large populations with very large updates between generations or as an average of all possible evolutions from a finite population. Such evolutions considered by several authors as a convenient vehicle to analyze genetic processes are completely deterministic. In Section 3 we show that even if we view such a deterministic evolution as an “average” evolution, this average may behave very different from every particular real evolution. The crucial point here is how far a particular evolution (generally) strays from the average. We analyze the relation with the population size and the population update size.

Under mild conditions that guarantee ergodicity the Markov chain converges to a stationary distribution over the set of states (the set of reachable populations). From this stationary distribution we can sample a set of populations. If the total stationary probability concentrated on populations containing an individual of best fitness is large enough then this process finds such an individual with high probability. For this approach to be workable we must have small enough populations and the convergence to the stationary distribution has to be fast. Convergence to stationarity is fast enough in “rapidly mixing” Markov chains. Such chains have recently been the basis of spectacular randomized approximation algorithms, combinatorial counting, statistical physics, combinatorial optimization, and certain quadratic dynamic processes related to genetics of infinite populations, [20,4,7,22]. Section 4 introduces them in general genetic computing. The efficiency of our technique in applications depends crucially on the rate of convergence of the Markov chain. Since the number of states is typically very large, the chain should reach equilibrium after each particular evolution has only explored a tiny fraction of the state
space.

For the theory of genetic computing it is important that we demonstrate a formal method of genetic fitness optimization (applicable to restricted classes of GA, GP, and related optimization problems) together with a rigorous analysis demonstrating that this strategy is guaranteed to work with high probability, rather than intuitive heuristic or ad hoc arguments. For the application of genetic computing we find that because of the sampling from the stationary distribution the proposed process uses a large number of short runs as opposed to one long run.

Just to show that the method is meaningful we demonstrate it on a toy problem in Section 5 that in fact is trivially successful because of the abundance of optimal solutions. Really significant examples are currently much harder—and already beyond the scope of this exploration. Further along is the development of a structured methodology to set up the genetic system (selection, reproduction, fitness) such that the resulting Markov chain is rapidly mixing, and, moreover, such that the types with sufficiently high fitness will be obtained with sufficiently high probability from the (close to) final stationary state distribution. What we have in mind is a design methodology to develop a genetic system satisfying these requirements from the specifications of the problem statement.

2 The Model

Assume that \( r \) is an upper bound on the number of different possible types of individuals, say a set \( \Omega = \{0, \ldots, r - 1\} \). Such individuals can be strings, trees or whatever—our discussion is so general that the precise objects don’t matter. Even if the set of types can grow (such as trees) then practically speaking there will still be an upper bound \( r \). The genetic system tries to solve an optimization problem in the following sense. Each individual in \( \Omega \) is graded in terms of how well it solves the problem the genetic system is supposed to solve, expressed as a function \( f \) which maps \( \Omega \) to some grading set \( G \). For example, \( G \) can be the real interval \([0, 1]\). Let \( f(u) \) be the fitness of type \( u \). Then, the normalized fitness of individual \( u \) is

\[
\hat{f}(u) = \frac{f(u)}{\sum_{v \in \Omega} f(v)}.
\]

\(^3\) From a more applied perspective several researchers observed earlier that it pays to restart on a new population when the evolution takes a unpromising direction, for example [13,9]. Also J. Koza and L.J. Eshelman have algorithms that specifically restart automatically (GP, CHC, respectively), as do many others.
To fix thoughts, we use fitness proportional selection where selection of individuals from a population is according to probability related to the product of frequency of occurrence and fitness. That is, in a population $P = (P(1), \ldots, P(r))$ of size $n$, where type $u$ occurs with frequency $P(u) \geq 0$ with $\sum_{u \in \Omega} P(u) = n$, we have probability $p(u)$ to select individual $u$ (with replacement) for the cross-over defined by

$$p(u) = \frac{f(u)P(u)}{\sum_{v \in \Omega} f(v)P(v)}.$$

It is convenient to formulate the generation of one population from another one as a Markov chain. Formally:

**Definition 1** A sequence of random variables $(X_t)_{t=0}^\infty$ with outcomes in a finite state space $T = \{0, \ldots, N-1\}$ is a finite state time-homogeneous Markov chain if for every ordered pair $i, j$ of states the quantity $q_{i,j} = \Pr(X_{t+1} = j | X_t = i)$ called the transition probability from state $i$ to state $j$, is independent of $t$. If $M$ is a Markov chain then its associated transition matrix $Q$ is defined as $Q := (q_{i,j})_{i,j=0}^{N-1}$. The matrix $Q$ is non-negative and stochastic, its row sums are all unity.

Now let the Markov chain $M$ have states consisting of nonnegative integer $r$-vectors of which the individual entries sum up to the population size exactly $n$ and let $P$ denote the set of states of $M$. The number of states $N := \#P$ is given by [19]

$$N = \binom{n+r-1}{r-1}. \quad (1)$$

(This is the number of ways we can select $r-1$ elements from $n+r-1$ elements. If the elements constitute a linear list and the $r$ intervals marked by the selected elements—exclusive the selected elements—represents the elements of the $r$ types the result follows directly.) The associated transition matrix $Q = (q_{i,j})$ is a $N \times N$ matrix where the entry $q_{i,j}$ is the probability that the $k$th generation will be $P_j$ given that the $(k-1)$st generation is $P_i$ ($P_i, P_j \in P$).

A general closed form expression for transition probabilities for simple GA’s is derived in [19] and its asymptotics to steady state distributions as population size increases is determined. In [14] it is observed that the mentioned closed form expression allows expression of ‘expected waiting time until global optimum is encountered for the first time’, ‘expected waiting time for first optimum within some error tolerance of global optimum’, and ‘variance in such measures from run to run’, and so on, but no further analysis is provided. Instead, initial experimental work is reported. Here we are interested in quantitative estimates of such expressions.
Example 1 Consider a process where the generation of a next population $P'$ from the current population $P$ consists of sampling two individuals $u, v$ from $P$, removing these two individuals from $P$ ($P'' := P - \{u, v\}$), producing two new offspring $w, z$ and inserting them in the population resulting in a population $P' := P'' \cup \{w, z\}$.

The transition probability $q_{P,P'}$ of 

\[ P \rightarrow P' \]

where $P'$ results from sequentially executing the program \( P(u) := P(u) - 1; \) \( P(v) := P(v) - 1; \) \( P(w) := P(w) + 1; \) \( P(z) := P(z) + 1; \) \( P' := P, \) replacing the pair of individuals $u, v$ by $w, z$ with $\{u, v\} \cap \{w, z\} = \emptyset$, is given by

\[ q_{P,P'} := 2p(u)p(v)b(u, v, w, z), \tag{2} \]

where the local transition probability $b(u, v, w, z)$ is the probability of producing the pair $w, z$ from the selected pair $u, v$, incorporating both the mutation probability and the cross-over probability. The $r \times r \times r \times r$ matrix $B = (b(u, v, w, z))$ is called the local transition matrix. We can generally obtain such transition probabilities between states $P \rightarrow P'$ of the Markov chain. 

3 Evolutionary Trajectories

Small population size or sample size may cause evolutionary trajectories to drift apart. Without loss of generality, this can be illustrated in a simplified setting ignoring fitness selection.

3.1 Transformation of Distributions

Some approaches use the expedient to simply ignore the actual populations and deal with the probability density $p(\cdot)$ of types rather than with the number of occurrences $P(\cdot)$ of types in a population $P$. We show that the idea that the deterministic evolution is some sort of “average” of all evolutions of underlying populations has problems. Given a distribution density $p$ and a local transition matrix $B = (b(u, v, w, z))$, let the transformation $p' = g(p)$ be defined by

\[ p'(z) := \sum_{u,v} \left( p(u)p(v) \sum_w b(u, v, w, z) \right), \tag{3} \]
where $B$ is such that $p'$ is again a probability distribution. Consider a (not necessarily finite) population of individuals, each individual being of some type $u \in \{0, \ldots, r-1\}$. Let $p(u)$ be the probability of selecting an individual of type $u$. When a pair of individuals of types $u, v$ mate then they produce a pair of individuals of types $w, z$ with probability $b(u, v, w, z)$. Assuming that a mating of a pair must result in a pair of offspring means that $\sum_{w,z} b(u, v, w, z) = 1$. The resulting probability of $z$ is $p'(z)$ in Equation 3. Then,

$$\sum_{u,v} p(u)p(v)b(u, v, w, z) = p'(w)p'(z)$$
$$\sum_{u,v} p'(w)p'(z) = 1.$$ 

Probability density evolution has particular nice properties that can be demonstrated not to hold for population evolutions. In particular, probability density evolution converges. A distribution $\rho$ is called an equilibrium distribution (with respect to transformation $g$) if $g(\rho) = \rho$. In [3,19] for simple GA with fitness selection, and [21] for more general quadratic dynamical systems but without fitness selection, the following convergence property is derived.

**Theorem 1** The sequence $p^0, p^1, \ldots$ with $p^t = g^t(p^0)$ ($t \geq 0$) converges to an equilibrium distribution $\lim_{t \to \infty} p^t = \rho$.

In certain infinite evolutionary models equivalent to the above transformation of probability densities the evolution develops deterministically according to Equation 3. But in practice things are different. Namely, the single evolution of the probability density may be very different from every evolution of a represented population.

If the populations are small, or the population updates across successive generations are small, then we are dealing with a random process and chance selections can cause great divergence of evolution of populations. In the practice of evolutionary computing this is always the case. We would like to quantify this. Primarily considering probability densities, neither [19] nor [21] explores in an explicit quantitative manner the divergence of trajectories of individual runs based on population sizes. They rather focus on the issue that as the population size grows, the divergence of possible trajectories gets progressively smaller. In the limit, for infinite populations, the generations in the run converge to the expected trajectory for smaller populations. Clearly, if all trajectories are in a small envelope around the expected trajectory, then the expected trajectory is a good predictor for what happens with an individual run. If moreover the expected trajectory corresponds to the trajectory of Equation 3, as in the system analyzed in [19], then the analysis of transformation $g$ tells us what to expect from our individual bounded population.
However, the expected trajectory can be completely different from all individual trajectories; and if the individual trajectories of bounded populations diverge wildly, then the expected trajectory may not predict anything about what happens to an individual run. Analysis like in [19,21] do not deal with an individual run of a genetic algorithm, but rather with the sequence of expectations over all individual runs of the system. Such an expectation may not say anything about what actually happens.

To see this, consider a dictatorial coin which gives a first outcome 0 or 1 with fair odds. However, afterwards it always gives the same outcome. So it either produces an all 0 run or an all 1 run with equal probabilities. The expectation of obtaining a 0 at the \( t \)th trial is \( \frac{1}{2} \). However, in actual fact at the \( t \)th \(( t > 1)\) trial we have either probability 1 or probability 0 for outcome 0. In terms of the above formalism, initially, \( p(0) = p(1) = \frac{1}{2} \). To express the “dictatorial coin” in terms of evolutionary processes and to analyze what happens we continue the above Markov chain terminology.

For \( s \in \mathcal{N} \), the \( s \)-step transition matrix is the power \( Q^s = (q_{i,j}^s) \) with \( q_{i,j}^s = \Pr(X_{t+s} = j|X_t = i) \), independent of \( t \). Denote the distribution of \( X_t \) by the row vector \( \pi^t = (\pi^t_0, \ldots, \pi^t_{N-1}) \) with \( \pi^t_i = \Pr(X_t = i) \). If \( \pi^0 \) denotes the initial distribution then \( \pi^t = \pi^0 Q^t \) for all \( t \in \mathcal{N} \). Often we have \( \pi^0_i = 1 \) for some \( i \) (and 0 elsewhere) in which case \( i \) is called the initial state.

**Definition 2** The chain is ergodic if there exists a distribution \( \pi \) over \( \mathcal{P} \) with strictly positive probabilities such that

\[
\lim_{s \to \infty} p_{i,j}^s = \pi_j,
\]

for all \( P_i, P_j \in \mathcal{P} \). In this case we have that \( \pi^t = \pi^0 Q^t \to \pi \) pointwise as \( t \to \infty \), and the limit is independent of \( \pi^0 \). The stationary distribution \( \pi \) is the unique vector satisfying \( \pi Q = \pi \), where \( \sum_i \pi_i = 1 \); that is, the unique normalized left eigenvector of \( Q \) with eigenvalue 1. Necessary and sufficient conditions for ergodicity are that the chain should be irreducible, for each pair of states \( P_i, P_j \in \mathcal{P} \) there is an \( s \in \mathcal{N} \) such that \( p_{i,j}^s > 0 \) \((P_j \text{ can be reached from } P_i \text{ in a finite number of steps})\); and aperiodic, the gcd\( \{s : p_{i,j}^s > 0\} = 1 \) for all \( P_i, P_j \in \mathcal{P} \).

An ergodic Markov chain is (time-)reversible iff either (and hence both) of the following equivalent conditions hold.

- For all \( P_i, P_j \in \mathcal{P} \) we have \( p_{i,j} \pi_i = p_{j,i} \pi_j \). That is, in the stationary distribution, the expected number of transitions per unit time from state \( P_i \) to state \( P_j \) and from state \( P_j \) to state \( P_i \) are equal. For an ergodic chain, if \( \pi \) is a
positive vector satisfying above condition and the normalization condition
$\sum_i \pi_i = 1$, then the chain is reversible and $\pi$ is its stationary distribution.

- The matrix $D^{1/2}QD^{-1/2}$ is symmetric, where $D^{1/2}$ is the diagonal matrix
diag($\pi_0^{1/2}, \ldots, \pi_N^{1/2}$) and $D^{-1/2}$ is its inverse.

**Example 2** We can formulate a “dictatorial coin” example in the evolutionary format of Equation 3. Let the $B$ transformation be given by Figure 1 where $0 < \epsilon \leq \frac{1}{8}$. The evolution of the probability densities by transformation of the distributions according to Equation 3 gives

$$p \rightarrow p' \rightarrow p'' \rightarrow \cdots$$

with $p'(0) = p'(1) = 1/2$ (= $p(0) = p(1)$) by symmetry between “0” and “1.”

But if we look at what the system does in actual evolutions then the following happens. Consider a state space $P$ consisting of the two-element populations: $P_0 = \{0, 1\}$, $P_1 = \{0, 0\}$ and $P_2 = \{1, 1\}$. To pass from one generation to the next one, with uniform probability and with replacement draw two elements from the current population. Subsequently, execute a cross-over according to the $B$ matrix. The resulting two individuals form the next generation. For example, from a population $P_0 = \{0, 1\}$ we obtain as the next generation

- with probability 1/4 a population $P_1 = \{0, 0\}$ with $p_1(0) = 1, p_1(1) = 0$;
- with probability 1/4 a population $P_2 = \{1, 1\}$ with $p_2(0) = 0, p_2(1) = 1$; and
- with probability 1/2 a population $P_3 = \{0, 1\}(= P_0)$ with $p_3(0) = 1/2, p_3(1) = 1/2$.

This $B$ gives rise to an ergodic Markov chain, has strictly positive entries, and it satisfies $b(u, v, w, z) = b(v, u, w, z) = b(u, v, z, w) = b(v, u, z, w)$ and hence is symmetric in the sense of [21].

| $u$ $v$ $w$ $z$ | $b(u, v, w, z)$ | $u$ $v$ $w$ $z$ | $b(u, v, w, z)$ |
|----------------|----------------|----------------|----------------|
| 0 0 0 0        | $1 - 4\epsilon$ | 1 0 0 1        | $\frac{1}{2} - \epsilon$ |
| 0 0 1 0        | $\epsilon$     | 1 0 1 0        | $\frac{1}{2} - \epsilon$ |
| 0 0 0 1        | $\epsilon$     | 1 0 1 1        | $\epsilon$     |
| 0 0 1 1        | $2\epsilon$    | 1 0 0 0        | $\epsilon$     |
| 0 1 1 0        | $\frac{1}{2} - \epsilon$ | 1 1 1 1 | $1 - 4\epsilon$ |
| 0 1 0 1        | $\frac{1}{2} - \epsilon$ | 1 1 0 1 | $\epsilon$ |
| 0 1 0 0        | $\epsilon$     | 1 1 1 0        | $\epsilon$     |
| 0 1 1 1        | $\epsilon$     | 1 1 0 0        | $2\epsilon$    |

Fig. 1. Dictatorial $B$-transformation
The associated Markov chain of this process is given by the matrix

\[
Q := \begin{pmatrix}
\frac{1}{2} & \frac{1}{4} & \frac{1}{4} \\
2\epsilon & 1 - 4\epsilon & 2\epsilon \\
2\epsilon & 2\epsilon & 1 - 4\epsilon
\end{pmatrix}
\]

where the entry \(q_{i,j}\) gives the transition probability of going from state (population) \(P_i\) to \(P_j\), \(0 \leq i, j \leq 2\).

Denote the probability of being in state \(P_i\) after \(t\) steps by \(\pi_t^i\), and \(\pi_t = (\pi_t^0, \pi_t^1, \pi_t^2)\). Since the Markov chain is ergodic (or by simple inspection) the pointwise limit \(\lim_{t \to \infty} \pi_t^i \to \pi\) exists where \(\pi\) is the stationary distribution. Solving \(\pi Q = \pi\) gives

\[
\begin{align*}
\pi_0 &= \frac{4\epsilon}{1 + 4\epsilon} \to 0 \text{ for } \epsilon \to 0 \\
\pi_1 &= \frac{1}{2 + 8\epsilon} \to \frac{1}{2} \text{ for } \epsilon \to 0 \\
\pi_2 &= \frac{1}{2 + 8\epsilon} \to \frac{1}{2} \text{ for } \epsilon \to 0
\end{align*}
\]

In fact, starting from population \(P_0\) after \(t\) steps and with \(\epsilon\) small enough to satisfy \(t \ll -\log \epsilon\) we will be in population \(P_0\) with probability \(\approx 1/2^t\), and in both population \(P_1\) and population \(P_2\) with probability \(\approx 1/2(1 - 1/2^t)\). Once we are in population \(P_1\) or \(P_2\) we stay in that population at the next generation with probability \(1 - 4\epsilon\), for small \(\epsilon > 0\) this is almost surely. Therefore, the evolution from \(P_0\) will quickly settle in either \(P_1\) or \(P_2\) and henceforth remain there for a long time.

Additionally we observe that for \(\epsilon = 1/8\) we have that \(Q\) is equal to its transpose \(Q^T\) and the stationary distribution \(\pi = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})\) and therefore the chain is reversible.

3.2 Finite Population: Large Sample

Assume that we have a finite population \(P\) with probability density \(p(u)\) of drawing individual \(u\) in the selection phase. Assume furthermore that in the selection phase we draw a sample of cardinality \(s\). The larger \(s\) is the better we can approximate \(p\) by the resulting frequencies. Quantitatively this works out as follows.

Let there be \(r\) types of individuals in \(\Omega\) and let \(s(u, v)\) be an outcome of the
random variable measuring the number of outcomes of the pair \((u, v)\) in \(s\) trials. By Chernoff’s bound, see for example [15],

\[
\Pr \{ \left| s(u, v) - p(u)p(v)s \right| > \varepsilon s \} < \frac{2}{e^\alpha} \text{ with } \alpha = \frac{e^2s}{3p(u)p(v)}.
\]

Let \(p'(\cdot)\) be the next probability distribution as defined in Equation 3, and let \(\hat{p}'(\cdot)\) be the frequency distribution we obtain on the basis of the outcome \(s(u, v)\) in drawing \(s\) examples. For our further considerations the dependence of \(\alpha\) on \(u, v\) is problematic. It is convenient to replace \(\alpha = \alpha(u, v)\) by an \(\alpha'\) independent of \(u, v\) and \(\alpha' \leq \varepsilon^2s/3 \leq \alpha(u, v)\). Then,

\[
\Pr \{ \left| s(u, v) - p(u)p(v)s \right| > \varepsilon s \} < \frac{2}{e^{\alpha'}}
\]

for every \(u, v \in \Omega\). This gives the probability that we exceed the value \(\varepsilon s\) for one pair \((u, v)\). The probability that we exceed the value \(\varepsilon s\) for some pair \((u, v)\) is upper bounded by \(2r^2/e^{\alpha'}\). Hence the probability that we do not exceed the value \(\varepsilon s\) for any pair \((u, v)\) is at least \(1 - (2r^2/e^{\alpha'})\). We can now conclude that for every \(z \in \Omega\), the absolute error of the estimate \(\hat{p}'(z)\) is

\[
|p'(z) - \hat{p}'(z)| \leq \sum_{u,v} \left( \left| \frac{s(u, v)}{s} - p(u)p(v) \right| \sum_{w} b(u, v, w, z) \right)
\]

\[
\leq \varepsilon \sum_{u,v,w} b(u, v, w, z) = er,
\]

with probability at least \(1 - 2r^2/e^{\alpha'}\). For example, choose \(\varepsilon = 1/s^{1/4}\) and sample size \(s\) with \(s^{1/4} > 3p(u)p(v)\) to ensure that \(\varepsilon^2s/3 \geq \alpha' > s^{1/4}\), for all \(u, v \in \Omega\). (The upper bound of \(\alpha'\) was required by the relation between \(\alpha'\) and \(\alpha\).)

Then, for all types \(z \in \Omega\), for \(s^{1/8} \geq r\)

\[
\Pr \left\{ \left| p'(z) - \hat{p}'(z) \right| < \frac{1}{s^{1/8}} \right\} > 1 - \frac{2r^2}{e^{s^{1/4}}} \left( \geq 1 - \frac{2s^{3/4}}{e^{s^{1/4}}} \right).
\]

That is, for growing \(s\) the probability that the estimator \(\hat{p}'(z)\) differs from the real \(p'(z)\) by more than \(1/s^{1/8}\) decreases as \(e^{-s^{1/4}}\). We call such a sample large because it is polynomial in the number of types \(r\) which typically means that the sample is exponential in the problem parameter \(l\) (as when \(\Omega = \{0, 1\}^l\)).

\[\text{It is possible to estimate a boundary envelope on the evolution trajectories.}\]

\[\text{Cubic results appearing in [10,9] are cubic in the population size } n \text{ and refer to different issues.}\]
around the single evolution trajectory determined by Equation 3 as a function of the sample size. This may be the subject of a future paper. 

3.3 Finite Population: Small Sample

Consider a population $P$ with types out of $\Omega$ with associated probability density $p(\cdot)$ of types over $\Omega$ and local transition matrix $B = (b(u, v, w, z))$. We generate the next population by drawing a small sample consisting of one pair $u, v$ of individuals from $P$ (without replacement) according to probability density $p$ and replace $u, v$ in $P$ by a pair $w, z$ with probability $b(u, v, w, z)$ to obtain population $P'$ with associated probability density $p'(\cdot)$.

In a concrete computational run of a genetic algorithm this means that given a population $P$ with associated density distribution $p(\cdot)$ we obtain with probability $p(u)p(v)b(u, v, w, z)$ a distribution $p'(\cdot)$ being the associated probability density of the population $P'$ resulting from eliminating a pair of individuals $u, v$ from $P$ and adding a pair of individuals $w, z$ as in Example 1. Start with a population of size $n$ containing $\Omega(n)$ different types and let each types have positive probability to be selected to produce the next generation. Then there are $\Omega(n^4)$ different distributions that can be obtained from $p(\cdot)$ this way (by Equation 3).

Repeating this procedure, we potentially obtain in $t$ steps up to $n^4t$ distributions. For example, if $B = (b(u, v, w, z))$ is strictly positive and the associated Markov chain is ergodic then this means that in

$$t_0 \approx \frac{\log N}{4 \log n}$$

generations we can possibly realize the total range of all $N$ different populations and therefore all distributions $p'(\cdot)$. Every population $P \in \mathcal{P}$ is obtained with some probability in $t_0$ generations. The single deterministic evolution of $t_0$ generations of probability distributions

$$p = p^0 \rightarrow p^1 \rightarrow \ldots \rightarrow p^{t_0}$$

according to Equation 3 gives the expectation $p^{t_0}(z)$ of an individual of type $z$ in

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\[ In a more restricted setting of a quadratic cross-over system with $\Omega = \{0, 1\}^l$ reference \[22\] shows that the probability distribution of an infinite quadratic cross-over system (without fitness selection) stays for the duration of an evolution of $t$ generations in an appropriate sense close to that of a population of size $O(n^2t)$ initially drawn randomly from the infinite population. \]
the $t_0$th generation, but it does not say anything about the actual probability density $\hat{p}^{t_0}(h)$ in the $t_0$th generation of an actual evolution.

4 Towards a Discipline of Evolutionary Programming

The upshot of the considerations so far is that with limited size populations and population updates the variation in evolutions is very great. In practice we always deal with very limited size populations such as, say, 500 individuals. The question arises how to overcome the problem that an individual evolution can become trapped in an undesirable niche—as in Example 2—for example a niche consisting of populations with non-optimal individuals. The answer is that we need to randomize over the evolutions. Inspecting the populations in such a random sample of evolutions we want to find, almost surely, an individual of best fitness. The latter is easy if the set of inspected evolutions is so large that it covers almost all populations. But this is infeasible in general. Let us look at two easy tricks that point the way we have to go.

Example 3 (Using the Law of Large Numbers) Consider an ergodic Markov chain associated with an evolutionary process. Using the law of large numbers, $c_t(P)/t \to \pi(P)$ as $t \to \infty$ almost surely, where $c_t(P)$ is the number of occurrences of population $P$ in the first $t$ generations, and $\pi(P)$ is the stationary probability of $P$. Therefore, in the same manner, it is easy to show $\sum_{P \in \mathcal{P}^*} \frac{c_t(P)}{t} \to \pi(\mathcal{P}^*)$ almost surely where $\mathcal{P}^*$ is the set of populations that include an individual $i^*$ with the best fitness value, and $\pi(\mathcal{P}^*)$ is the stationary probability that a population includes $i^*$.

But this approach doesn’t give a speed of convergence guarantee. What we actually want is an approach that the expected time for an element of $\mathcal{P}^*$ to show up is polynomial. One way to formulate a sufficient condition for this is that we guarantee that for all parameters $\epsilon, \delta > 0$ the probability

$$\Pr \left\{ \frac{\left| \sum_{P \in \mathcal{P}^*} \frac{c_t(P)}{t} \pi(\mathcal{P}^*) \right|}{\epsilon} < \delta \right\} < \delta,$$

with $t$ polynomial in the problem parameter $l$ (like the length of the individuals), $1/\epsilon$ and $1/\delta$. Roughly speaking, this is achieved by “rapidly mixing” processes below.

Example 4 (Probability Boosting) As M.O. Rabin and others have observed, the power of randomization over deterministic algorithms is that it can solve problems with probability almost 1 by repeated independent runs of the algorithm, provided each single run has probability of error appropriately less
than 1 (see the text [18]). A direct application of probability boosting to evolutionary computing, [24], is as follows. Let $T$ be a random variable defined as the first-case hit for an optimal solution by a randomized algorithm like a GA. Let the expectation satisfy $\mathbb{E}(T) \leq \hat{T}$, where the upper bound $\hat{T}$ is a polynomial in the problem dimension $l$ (like the length of the individuals). Now if the randomized algorithm is stopped after $t \geq 2\hat{T}$ steps then the best solution found so far may not be the globally optimal solution. The probability that it is not is $P(T > t)$ which by Markov’s inequality satisfies

$$P(T > t) \leq \frac{\mathbb{E}(T)}{t} \leq \frac{1}{2}.$$ 

After $k$ independent runs (with independently random initial conditions) the probability that the global solution is found at least once is greater or equal to $1 - 1/2^k$.

For this observation to be useful we must show that in the case of interest the expected running time up to first-case hitting time of an optimal solution (or approximately optimal solution) is polynomial in the problem dimension. In fact, it suffices if this is the case with respect to only a subset of the computations of appropriate positive probability, like in Equation 4.

### 4.1 Rapidly Mixing Markov Chains

We follow the exposition in [20]. Given an ergodic Markov chain, consider the problem of sampling elements from the state space, assumed very large, according to the stationary distribution $\pi$. The desired distribution can be realized by picking an arbitrary initial state and simulating the transitions of the Markov chain according to probabilities $p_{i,j}$, which we assume can be computed locally as required. As the number $t$ of simulated steps increases, the distribution of the random variable $X_t$ will approach $\pi$. The rate of approach to stationarity can be expressed in the following time-dependent measure of deviation from the limit. For every non-empty subset $U \subseteq \mathcal{P}$, the relative pointwise distance (r.p.d.) over $U$ after $t$ steps is given by

$$\Delta_U(t) = \max_{i,j \in U} \left| \frac{p_{i,j}^t - \pi_j}{\pi_j} \right|.$$ 

This way, $\Delta_U(t)$ is the largest relative distance between $\pi^t$ and $\pi$ at a state $P_j \in U$, maximized over all possible states in $U$. The parameter $U$ allows us to specify relevant portions of the state space. In case $U = \mathcal{P}$ we will omit the subscript and write $\Delta$ instead of $\Delta_U$. 

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The stationary distribution $\pi$ of an ergodic chain is the left eigenvector of $Q$ with associated eigenvalue $\lambda_0 = 1$. Let $\lambda_1, \ldots, \lambda_{N-1}$ with $\lambda_i \in \mathbb{C}$ (the complex numbers) be the remaining eigenvalues (not necessarily distinct) of $Q$. By the standard Perron-Frobenius theory for non-negative matrices these satisfy $|\lambda_i| < 1$ for $1 \leq i \leq N - 1$. The transient behavior of the chain, and hence its rate of convergence, is governed by the magnitude of the eigenvalues $\lambda_i$. In the reversible case, the second characterization above implies that the eigenvalues of $Q$ are those of the symmetric matrix $D^{1/2}QD^{-1/2}$ and so are all real. This leads to the following clean formulation of above dependence:

**Lemma 1** Let $Q$ be the transition matrix of an ergodic reversible Markov chain, $\pi$ is stationary distribution, and $\lambda_0 = 1, \ldots, \lambda_{N-1}$ its (necessarily real) eigenvalues. Then, for every nonempty subset $U \subseteq \mathcal{P}$ and all $t \in \mathbb{N}$ the relative pointwise distance over $U$ satisfies

$$\Delta_U(t) \leq \frac{\lambda_{\text{max}}^t}{\min_{P \in U} \pi_i},$$

where $\lambda_{\text{max}}$ is the largest value in $|\lambda_1|, \ldots, |\lambda_{N-1}|$.

**Lemma 2** With the notation of Lemma 1 the relative pointwise distance over $\mathcal{P}$ satisfies

$$\Delta(t) \geq \lambda_{\text{max}}^t$$

for every even $t \in \mathcal{N}$. Moreover, if all eigenvalues of $Q$ are non-negative, then the bound holds for all $t \in \mathcal{N}$.

Therefore, provided $\pi$ is not extremely small in some state of interest, the convergence of the reversible chain will be rapid iff $\lambda_{\text{max}}$ is suitably bounded away from 1. Such a chain is called rapid mixing.

If we order the eigenvalues $1 = \lambda_0 > \lambda_1 \geq \cdots \geq \lambda_{N-1} > -1$ then $\lambda_{\text{max}} = \max\{\lambda_1, |\lambda_{N-1}|\}$ and the value of $\lambda_{N-1}$ is significant only if some eigenvalues are negative. The oscillatory behavior associated with negative eigenvalues cannot occur if each state is equipped with sufficiently large self-loop probability. It is enough to have $\min_j q_{j,j} \geq 1/2$. To see this, let $I_N$ denote the $N \times N$ identity matrix and consider the non-negative matrix $2Q - I_N$, whose eigenvalues are $\mu_i = 2\lambda_i - 1$. By Perron-Frobenius, $\mu_i \geq -1$ for all $i \in \mathcal{P}$ which implies that $\lambda_{N-1} \geq 0$.

What do we do when we have negative eigenvalues? To be able to apply Lemma 2 without oscillations we require all eigenvalues to be positive. It turns out that we there is a simple modification of the chain with negative eigenvalues that turns it into a chain with only positive eigenvalues without
slowing down the convergence to stationarity too much. We simply increase the self-loop probability of every state by $\frac{1}{2}$ after halving it first:

**Lemma 3** With the notation of Lemma 1, let the eigenvalues of $Q$ be ordered $1 = \lambda_0 > \lambda_1 \geq \cdots \geq \lambda_{N-1} > -1$. Then the modified chain with transition matrix $Q' = \frac{1}{2}(I_N + Q)$, with $I_N$ as above, is also ergodic and reversible with the same stationary distribution, and its eigenvalues $\lambda'_i$ similarly ordered satisfy $\lambda'_{N-1} > 0$ and $\lambda'_{max} = \lambda'_1 = \frac{1}{2}(1 + \lambda_1)$.

Following [20] we define rapid mixing.

**Definition 3** Given a family of ergodic Markov chains $M(x)$ parametrized on strings $x$ over a given alphabet. For each such $x$, let $\Delta^{(x)}(t)$ denote the r.p.d. of $M(x)$ over its entire state space after $t$ steps, and define the function $\tau^{(x)}(\epsilon)$ from the positive reals to the natural numbers by

$$
\tau^{(x)}(\epsilon) = \min\{t : \Delta^{(x)}(t') \leq \epsilon \text{ for all } t' \geq t\}.
$$

We call such a family rapidly mixing iff there exist a polynomial bounded function $q$ such that $\tau^{(x)}(\epsilon) \leq q(|x|, \log \epsilon^{-1})$ for all $x$ and $0 < \epsilon \leq 1$.

In the applications to evolutionary programming, $x$ will be a problem instance and the state space of $M(x)$ will include solution sets $R(x)$ of some relation $R$.

The question arises whether the approach to rapidly mixing Markov chains can be generalized from reversible chains to non-reversible chains. This was affirmatively settled in [17] and another treatment was later given in [7]. See the short discussion in [20].

**Example 5** To compute the permanent of a dense matrix is $\#P$-complete. The permanent of an $n \times n$ matrix $A$ with 0-1 entries $a_{i,j}$ is defined by

$$
\text{per}A := \sum_{\sigma} \prod_{i=0}^{n-1} a_{i,\sigma(i)},
$$

where the sum is over all permutations of the set $\{0, \ldots, n\}$. Since the class of $\#P$-complete decision problems includes the class of NP-complete decision problems, computing the permanent is at least NP-hard.

A celebrated result of Jerrum and Sinclair [11] shows how to use rapidly mixing Markov chains to obtain a randomized algorithm that approximates the value of the permanent of a matrix $A$ within ratio $1 + \epsilon$ with probability at least $3/4$ in time polynomial in $|A|$ and $|1/\epsilon|$ where $|\cdot|$ denotes the length of the binary representation. By probability boosting, we can by $O(\log \delta)$ iterations boost the success probability to at least $1 - \delta$. This breakthrough result has led
to a “Markov Chain Renaissance” to employ rapidly mixing Markov chains to obtain such “fully polynomial randomized approximation schemes (fpras)” to hard problems in computer science [5,20,1]. These applications generate a uniform stationary distribution from which the approximation is obtained by Monte Carlo sampling of the states and determining the proportion of the successful states. In our application to genetic computing we proceed differently: with high probability we sample states containing a best fit individual (or an approximately best fit individual). We illustrate the idea by example in Section 5.

4.2 Optimization by Rapidly Mixing Evolutionary Algorithms

To optimize by rapidly mixing evolutionary algorithms we require two properties:

(1) The stationary distribution $\pi$ of populations $P$ of the associated Markov chain of the evolutionary process converges to concentrate a sufficient amount of probability on populations containing maximally fit individuals, or on populations containing individuals that enable us to compute the required solutions. That is,

$$\sum_{P_i \in P^*} \pi_i \geq \epsilon,$$

where $P^*$ is the set of populations containing at least one solution of best fitness (or a solution that approximates the global optimum, or solutions that enable us to compute the required solution or approximation) and $\pi_i$ is the stationary probability of population $P_i$. To ensure feasibility of the algorithm we customarily require that $1/\epsilon$ is polynomial in the problem parameter.

(2) The Markov chain of the evolutionary process converges sufficiently fast to the stationary distribution: it is rapidly mixing as in Section 4.1.

The rapid mixing property (2) can be satisfied by having the evolutionary system satisfy some structural properties. Such properties can, at least in principle (if not in practice), always be taken care of while implementing the evolutionary system by choosing the selection rules, cross-over operator, and mutation rules appropriately. These requirements are covered in Section 4.3.

The question of probability concentration, property (1), is more subtle, and it is not yet clear how to generally go about it, even in principle. In many if not most cases we are satisfied to obtain an approximately globally optimal solution.
4.3 A Discipline of Evolutionary Programming

For a structural discipline of evolutionary programming we need to develop a methodology that given a problem specification guides us to construct an evolutionary system such that the associated Markov chain satisfies the following requirements:

**Property 1** the second largest eigenvalue\(^7\) \(\lambda_{\text{max}}\) is suitably bounded away far enough from 1 so that the Markov chain is rapidly mixing (Definition 3 of Section 4.1); and

**Property 2** the stationary distribution \(\pi\) gives probability greater than \(\epsilon\), where \(1/\epsilon\) is polynomial in the problem parameter, to the set of states that contain individuals of best fitness.

For Property 1 it is required that the matrices are (i) irreducible, and (ii) have nonnegative entries. Since the only matrices we consider are stochastic where the entries are transition probabilities, (ii) is in our case easy to satisfy up to the ‘suitable’ condition in Property 1. Since we only deal with ergodic matrices, and (i) is required for ergodicity, Property 1 is always satisfied in our case. Ergodicity is immediate if we have a positive mutation probability of transforming \(i\) into \(j\) for each pair of types \(i, j\). Hence by proper choice of the genetic system leading to suitable transition probabilities inducing a rapidly mixing Markov chain one can satisfy Property 1 in construction of an evolutionary system. It is perhaps less easy to see whether it is feasible to satisfy Property 2 in each particular case, or indeed without knowing the optimal individual a priori. However, as discussed above a similar approach for approximating very hard combinatorial optimization problems, [20], worked out fine.

Assume that we have defined our evolutionary system satisfying Properties 1, 2. The program we use is then as follows. Repeat a polynomial number of times:

**Step 1:** From a start state evolve through a polynomial number of generations;

**Step 2:** From the final population vector select the fittest individual.

**Paradigm.** Running the program longer than a polynomial number of generations will not significantly change the closeness of the state distribution to the stationary distribution in the Markov chain. We can only guarantee that we find a state (vector) containing an optimal fit individual with probability

\(^7\) The second largest eigenvalue was used earlier in genetic computing to advantage for another purpose in [26].
say inversely polynomial in the problem parameter. However, polynomially repeating this procedure implies Monte Carlo sampling which almost surely discovers the individual with optimal fitness.

5 A Toy Rapidly Mixing Genetic Algorithm

Consider a toy evolutionary problem as follows. We consider a population of size $\sqrt{l}$ and very simple crossover only and some mutation. This example already illustrates adequately the rapid mixing phenomenon. The genetic algorithm $G$ is defined as follows. The set of all program types is $\Omega = \{0, 1\}^l$ with $l$ fixed, even, and large enough for the following analysis to hold. The fitness of a program $\omega \in \Omega$ with $\omega = \omega_1\omega_2 \ldots \omega_l$ is given by the function

$$f(\omega) = 1 \text{ if } \sum_{i=1}^{l} \omega_i = l/2, \text{ and } 1/2 \text{ otherwise}.$$ 

The starting population $P^0$ at time $t_0 = 0$ contains $\sqrt{l}$ copies of the individual $00 \ldots 0$; its cardinality (number of elements in $P^0$) is $\sqrt{l}$. We express the frequency of a string $\omega$ in a population $P$ by $\#_\omega(P)$. That is, $\#_{00 \ldots 0}(P^0) = \sqrt{l}$ and $\#_{\omega}(P^0) = 0$ for $\omega \neq 00 \ldots 0$

The transition of one population to the next generation (population) is as follows. To avoid problems of periodicity, we add self-loop probability of $1/2$ to each state (that is, population). Note that this also dispenses with the problem of negative eigenvalues. Consequently, there is probability $1/2$ that the state changes using crossover and mutation, and there is probability $1/2$ that it stays the same. The probability $p(\omega)$ of selecting a string $\omega$ from a population $P$ is

$$p(\omega) = \frac{\#_\omega(P)f(\omega)}{\sum_{\omega \in \Omega} \#_\omega(P)f(\omega)}.$$ (5)

In the selection phase we select two individuals in $P$, say $\omega^i, \omega^j$, according to these probabilities, and with probability $1/2$ we perform a crossover and mutation on each (and with probability $1/2$ we do nothing). The crossover operator interchanges a single bit of $\omega^i$ with the corresponding bit of $\omega^j$. It selects the single bit position with uniform probability $1/l$. Subsequently, we mutate each offspring by flipping a single bit with uniform probability $1/l$ chosen from the positions 1 through $l$. (If $i = j$ then the cross-over doesn’t do anything and the two mutations may result in 0,1, or 2 bit flips of $\omega_i$.) We first prove that $G$ is rapid mixing by showing that if the following system $G'$ is rapidly mixing then so is $G$. 

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Let $G'$ be a system where the initial state is a binary $l$-vector. At each step uniformly at random select a bit position of the current $l$-vector and flip that bit with fifty-fifty probability to produce the next $l$-vector. Then $G'$ is a Markov chain where the states are the binary $l$-vectors.

**Lemma 4** The chain $G'$ is rapid mixing with r.p.d. at most $\epsilon$ within $O(l^2(l + \log(1/\epsilon)))$ steps.

For a proof see [20], pp. 63–66. This system is an almost uniform generator for $\Omega$, using singleton populations, where it suffices to use an arbitrary starting singleton population. In terms of GA’s it is single-bit mutation. Our example involves single-bit mutation, single-bit cross-over, and selection. The reader is advised that this is only a cosmetic change to make the example look more like a ‘realistic’ GA. Our toy example $G$ is essentially the example $G'$ as in Lemma 4. To see this, consider the vectors in successive generations $P^0, P^1, \ldots$ of $G$ to maintain their identity. If $P^t = \{\omega^{t,1}, \ldots, \omega^{t,\sqrt{l}}\}$ for $t > 0$ and in the selection phase we select indices $i, j$, then $\omega^{t+1,k} = \omega^{t,k}$ for $0 \leq k \leq \sqrt{l}$ and $k \neq i, j$, or $\omega^{t+1,h}$ results from $\omega^{t,h}$ (the ‘same vector’) by at most two bit flips for $h = i, j$.

**Lemma 5** Let $\epsilon > 0$ and $T(l) = O(l^{5/2}(l + \log(1/\epsilon)))$. For each $t \geq T(l)$, with probability at least $1 - 1/T(l)$ and for each $l$-vector $\omega$, every $l$-vector $\omega^{0,j} \in P^0$ has probability $(1 \pm \epsilon)/2l$ of being changed into $\omega^{t,j} = \omega$ in $t$ generations of $G$.

**Proof.** For a fraction of at least $1 - 1/t$ of all runs of $t > \sqrt{l}$ steps of a population of $\sqrt{l}$ elements, then each element $j$ out of $1, \ldots, \sqrt{l}$ (representing the vector $\omega^{j}$) is selected with frequency of at least

\[
\frac{t}{2\sqrt{l}} \pm O\left(\sqrt{\frac{t \log t}{\sqrt{l}}}\right) \tag{6}
\]

in the selection phases of the generating process. This is shown similar to the statistical analysis of ‘block frequencies’ of high Kolmogorov complexity strings in [15], Theorem 2.15.

Namely, consider $t$ throws of a $\sqrt{l}$-sided coin, each pair of throws constituting the selection of the index of the two individuals mated to produce the next generation. There are $2^{(t \log l)/2}$ possible sequences $x$ of $t$ outcomes. Hence, the maximal Kolmogorov complexity is given by $C(x|t, l) \leq (t \log l)/2 + O(1)$. Moreover, since there are only $2^{(t \log l)/2}/t$ binary descriptions of length $< (t \log l)/2 - \log t + O(1)$, there is a fraction of at least $1 - 1/t$th part of all sequences $x$ which has $C(x|t, l) \geq (t \log l)/2 - \log t + O(1)$. Consider each such $x$ as a binary string consisting of blocks of length $\log \sqrt{l}$, each block encoding one of the $\sqrt{l}$ types. Let $\#j(x)$ denote the number of occurrences of each of
the \( \sqrt{l} \) blocks \( j \) (elementary outcomes) in \( x \). Then, by [15] p. 163,

\[
|\#j(x) - t/\sqrt{l}| \leq \sqrt{\log \sqrt{l} + \log \log \sqrt{l} + \log t + O(1) \log e}.
\]

Since individuals have fitness 1/2 or 1, some indexes may at various times have as low as half the probability of being selected than other individuals. Repeating the same argument for an \( 2\sqrt{l} \)-sided coin and represent by the first \( \sqrt{l} \) outcomes for indexes 1 through \( \sqrt{l} \) and the remaining outcomes represent dummy indexes (possibly the original ones) we obtain the lower bound of Equation 6.

Following the same vector in the successive generations, consider each time it is selected. At such times, with fifty-fifty probability either nothing is done or the vector incurs (i) a bit flip in a position which was selected uniformly at random because of the cross-over (or no bit flip if the bits in that position of the two parents happened to be the same), followed by (ii) a bit flip in a position selected uniformly at random because of the mutation. From the viewpoint of the individual vector and the mutation operations alone it simply emulates a trajectory of the singleton \( l \)-vector in Lemma 4 of length as given in Equation 6. The extra random bit flips due to the cross-over only increase the length of the emulation.

Substitute \( t \) in Equation 6 by \( T(l) \) as in the statement of the lemma. By Lemma 4 the lemma is proven.

Let \( \omega \) be an \( l \)-vector. For every \( \epsilon > 0 \) and \( t \geq T(l) \), every \( l \)-vector in the initial population \( P_0 \) turns into \( \omega \) in exactly \( t \) steps with probability at least \( (1 - 1/t)(1 \pm \epsilon)/2^l \). Therefore, \( P_0 \) generates in \( t \) steps every particular population \( P \) of \( \sqrt{l} \) individuals with probability

\[
(1 - \frac{1}{t}(1 \pm \epsilon))/N,
\]

where \( N \) is the number of \( \sqrt{l} \)-size populations. Then, the r.p.d. of \( G \) to the uniform stationary distribution \( \pi \) \( (\pi(P) = 1/N \text{ for all } P \in \{0, 1\}^l \) with \( \#(P) = \sqrt{l} \) after \( t > T(l) \) steps is bounded above by \( \frac{1}{t}(1 + \epsilon) \). Choosing \( t > \max\{T(l), 1/\epsilon\} + 1 \) the r.p.d. is upper bounded by \( \epsilon \).

**Corollary 1** It follows that \( G \) is a rapidly mixing Markov Chain with a uniform stationary distribution.

**Lemma 6** The probability of finding a population with an optimally fit element in \( t \) runs is at least \( 1 - 2e^{-\alpha t} \) with \( \alpha = c/(16(1 - c)) \), for the fixed constant \( c \)
Proof. There are \( \binom{l}{l/2} \approx 2^l/\sqrt{\pi l/2} \) strings with fitness 1. Hence a fraction of at most
\[
(1 - 1/\sqrt{\pi l/2})^{\sqrt{l}} < e^{-\sqrt{2/\pi}}
\]
populations of size \( \sqrt{l} \) contain no such strings. This means that a constant fraction of at least
\[
c = 1 - e^{-\sqrt{2/\pi}},
\]
of the populations of size \( \sqrt{l} \) contain at least one string of fitness 1.

Consider each run of \( T(l) \) generations an experiment with a success outcome if the final population contains an individual with fitness 1. Let the number of successes in \( t \) trials be \( s(t) \). Then, with \( \beta \) defined as
\[
\beta = \Pr\{|s(t) - ct| > \delta t\}
\]
we have
\[
\beta < 2e^{-\delta^2 t/(3c)},
\]
by Chernoff’s bound. For \( \delta = c/2 \) we know that the number of successes \( s(t) > 0 \) with probability at least \( 1 - \beta \). \( \square \)

**Theorem 2 ((Rapidly Mixing GA Algorithm))** Let \( \epsilon \) and \( T(l) \) be as in Lemma 5 and let \( \alpha \) be as in Lemma 6. Repeat \( t \) times: run \( G \) for \( T(l) \) generations. This procedure uses \( O(T(l) \cdot t) \) elementary steps consisting of the generation from one population to the next population. (With \( t = l \) this is a low degree polynomial in \( l \) and \( \epsilon \)). The probability of finding an optimal element exceeds
\[
1 - 2e^{-\alpha t},
\]
where \( \alpha > 0 \), that is, with probability of failure which vanishes exponentially fast with rising \( t \).

**Proof.** By Lemmas 5, 6. \( \square \)

### 6 Non-uniform Stationary Distributions

In the above example the stationary distribution is uniform and success of the method depends on the abundance of populations containing an optimal
individual. However, we want the stationary distribution of populations to heavily concentrate probability on populations containing optimal or near-optimal individuals even if those populations are scarce. For example, if our fitness function is \( f : \Omega \rightarrow \mathbb{N} \) and we extend \( f \) to populations \( P \) with \( f(P) = \max_{\omega \in P} \{f(\omega)\} \) then we want to generate a random element from a distribution concentrated on the set of optimum solutions. This is similar to generating a random \( P \) from a distribution \( \pi \) where \( \pi(P) = \Theta(2^{f(P)/\alpha}) \) with \( \alpha \) a small positive number. Then, with large probability a random \( P \) will maximize \( f \). A general method to modify a random walk so that it converges to an arbitrary prescribed probability distribution is the Metropolis filter, [16]. Let’s explain a simple example of this. Suppose \( \Omega = \{0, 1\}^l \), we are dealing with singleton populations, and our fitness function is \( f \). We describe a random walk on \( \Omega \) by single bit-flips and “filtered” by the function \( f \). The next population is generated from the current population \( \{\omega\} \) as follows. First select a random bit position in \( \omega \). Let \( \omega' \) be the string resulting from flipping that bit of \( \omega \) If \( f(\omega') > f(\omega) \) then the next generation is \( \{\omega'\} \); otherwise the next population is \( \{\omega'\} \) with probability \( f(\omega')/f(\omega) \) and the next population is \( \omega \) with probability \( 1 - f(\omega')/f(\omega) \). Clearly this modified random walk is a Markov chain (and it is also time-reversible). The stationary distribution \( \pi^f \) is

\[
\pi^f(\omega) = \frac{f(\omega)}{\sum_{\omega' \in \Omega} f(\omega')}.
\]

For example, with \( f(\omega) = 2^i \) where \( i \) is the number of 1’s in \( \omega \) the optimal individual is \( 11 \ldots 1 \) which is sampled from the stationary distribution with high probability. Unfortunately, it is not in general known how to estimate the mixing time of a Metropolis-filtered random walk. On the positive side, in [2] they compute a volume in \( n \)-space using this method and they show that the filtered walk mixes essentially as fast as the corresponding unfiltered walk. A similar approach to combinatorial optimization using the Markov chain Monte Carlo method in the sense of a Metropolis process-type Markov chain having a stationary distribution that concentrates high probability on the optimal (or approximately optimal) solutions is surveyed in [12]. They give a polynomial time Metropolis process to find an approximate maximum matching in arbitrary graphs with high probability. More precisely, if \( G \) is an arbitrary graph on \( n \) vertices then the algorithm finds a matching in \( G \) of size at least \( \lceil (1 - \epsilon)k_0 \rceil \) where \( k_0 \) is the size of the maximal matching and \( \epsilon \) is an accuracy parameter which is assumed to be constant—the running time is actually exponential in \( 1/\epsilon \). However, these successes are scarce. For the current status and references on Metropolis algorithms see [6].
7 Conclusion and Further Research

We have suggested a theoretical possibility of constructing genetic processes that provably optimize an objective function with high probability in polynomial time. We have given a simple example that, however, succeeds because of the abundance of optimal solutions. Altogether it seems difficult at this time to even construct an example of a genetic process that is both rapidly mixing and also has a nonuniform stationary distribution that heavily concentrates probability on populations containing optimal individuals in case such populations are scarce. An example of this would give evidence of the power of the proposed method.

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