

GEOMETRIC CONVERGENCE OF GENETIC ALGORITHMS UNDER TEMPERED RANDOM RESTART

F. MENDIVIL,* *Acadia University*

R. SHONKWILER, AND M. C. SPRUILL,** *Georgia Tech*

Abstract

Geometric convergence to 0 of the probability the goal has not been encountered by the n th generation is established for a class of genetic algorithms. These algorithms employ a quickly decreasing mutation rate and a crossover which restarts the algorithm in a controlled way depending on the current population and restricts execution of this crossover to occasions when progress of the algorithm is too slow. It is shown that without the crossover studied here, which amounts to a tempered restart of the algorithm, the asserted geometric convergence need not hold.

Keywords: non-stationary Markov chain, hitting time, Perron-Frobenius, decreasing mutation rate

2000 Mathematics Subject Classification: Primary 60J20

Secondary 65C05

1. Introduction

This paper reports part of a continuing investigation initiated by the authors in [2] and [4] of the properties of restarted stochastic search algorithms. In the former paper, deterministic search, like steepest gradient is addressed and in the latter simulated annealing. In both, restarting is initiated when lack of improvement in the objective is observed. Here, a similar strategy is investigated in the context of genetic algorithms. Just as in the two former cases, geometric convergence toward the goal is established rigorously and the lack of this property is proven for the ordinary non-restarted version.

* Postal address: Mathematics Department, Acadia University, Wolfville, Nova Scotia, Canada

** Postal address: School of Mathematics, Georgia Institute of Technology, Atlanta, GA 30332-0160, USA

In the spirit of the technique of [5] used in the study of parallelization, the Perron-Frobenius theory of positive operators is utilized in [2] to prove geometric convergence; in [4], although renewal theory is employed, a result which extends the usual Perron-Frobenius theory is established and is used here to establish the rapid convergence of the restarted GA under both constant probability of application and under random restarting based upon progress of the algorithm towards the goal.

In all these papers, including this one, there is a substantial departure from the classical question of convergence of the distribution of states to an asymptotic distribution which has support on the goal states to one involving whether or not the goal state has been observed up to the present time. Thus instead of asking whether or not the rules lead to an asymptotic distribution (of the chain) on goal states, the question is one of whether the goal state appears among the states visited and the rate of convergence to 0 of the probability of the complement of this event. It is shown here, as in [2] and [4], that the rate of convergence to 0 is geometric even though the mutation rate is being driven to 0 geometrically fast. Slow convergence of the mutation rate to 0 can result in jumping away from good solutions prematurely while rapid convergence to 0 can result, without an appropriate crossover rule, to getting hung up at local extrema. Here, a crossover called *wrong side of the tracks*, yields geometric convergence to 0 as $n \rightarrow \infty$ of the probability the goal has not been encountered by epoch n . Wrong side of the tracks crossover means that a member of the current population mates with some (randomly chosen) member of the state space, and is called, for obvious reasons, “tempered restart.” A general feature of all three investigations is that the algorithms preferred are those which cycle through good states rapidly rather than settle down predictably to a prescribed set.

Although the classical focus of studies on convergence of genetic algorithms has been on asymptotic distributions over states, hitting times have been considered. In Löwe [3], for example, an upper bound on the tail probabilities (the probability the goal has not yet been encountered by time t) of the form Kt^{-c} is proven while in our case the bound is shown to be of the form Ke^{-ct} , where the generic constants K, c are positive. Löwe’s bounds on hitting times are proven for a family of GA’s which differ from the ones considered in this paper; there mutation rates and crossover schemes remain constant over time and selection probabilities evolve in a manner reminiscent

of simulated annealing rather than staying fixed as ours do. The applicability of Löwe's bounds depends upon a "logarithmic schedule" of selection probability change.

Details of our method are provided below, but informally, it consists of evolving a population of fixed size using the three mechanisms of random selection, crossover, and mutation. Given a current population, the next population is the outcome of

1. (roulette wheel selection) a multinomial experiment in which the probabilities are determined by the fitness of the current population,
2. (crossover) the possible mating of a member of the current population with a member of the population at large, and
3. (mutation) random mutation of the current members by flipping bits in a binary representation of the population members.

Of interest is whether or not the history of populations has ever, up to that point, included a member of the goal state in which an objective function achieves its maximum value. Since the fitnesses of the population members are calculated at each new generation the realization of such an event means that the maximum of the objective has been identified. It is important to distinguish our use of the word convergence and the common use in the area of GA; convergence of the tail probability to zero is studied here while the word convergence in typical GA-parlance refers to the distribution of the members of the population itself. So rather than asking about the asymptotic form of the population, whether it is concentrated on goal states or places positive probability on goal states, our emphasis is on cycling through states. It is clear that one would like the algorithm to head for maxima of the objective as quickly as possible and not to get trapped.

This is a shared goal with the classical analysis typified in the statement from Wikipedia, "A very small mutation rate may lead to genetic drift (which is non-ergodic in nature) or premature convergence of the genetic algorithm in a local optimum. A mutation rate that is too high may lead to loss of good solutions. There are theoretical but not yet practical upper and lower bounds for these parameters that can help guide selection." It will be shown here that one can send the mutation rate to zero quickly and still not have premature convergence, as long as the crossover described above is

employed. It is also shown that without this crossover, sending the rate to zero even much more slowly results in premature convergence with positive probability; thus the tail probabilities need not even converge to 0 even keeping the mutation rate much higher.

2. Notation

The underlying space on which the strictly positive function R is to be maximized is $S = \{0, 1\}^L$. We refer to the components, or bits, of $i \in S$ by i_k , $0 \leq k \leq L$. Let M , the population size, be a positive integer fixed throughout. Denote by Ξ the collection of probability distributions $\xi(\cdot)$ on S and by Ξ_0 the subset thereof for which $M\xi(i) = m(i) \geq 0$ are integers for all $i \in S$. The set Ξ_0 is in one to one correspondance with the state space of the GA, the ‘‘populations’’ of the algorithm, and is denoted in [1] as

$$S' = \{\bar{m} = (m(0), m(1), \dots, m(2^L - 1)) : \sum_{j=0}^{N-1} m(j) = M, m(j) \geq 0\},$$

where $N = 2^L$.

For $\xi \in \Xi$, $\nu \in \Xi$, and $\alpha \in [0, 1]$ consider the operator $\tau_{\alpha, \nu} : \Xi \rightarrow \Xi$ defined by

$$\tau_{\alpha, \nu}\xi(k) = \alpha \sum_i \sum_j E[I(i, j, k, W)]\xi(i)\nu(j) + (1 - \alpha)\xi(k). \quad (1)$$

This is the *crossover operator* and for the choice $\nu = \xi$ agrees in essence with that defined in [1] between their equations (6) and (7). The random variable W , the crossover point, is uniformly distributed on $\{0, 1, \dots, L\}$ and the expectation over W is of I , the indicator function satisfying $I(i, j, k, w) \in \{0, 1\}$ where for $w = 1, \dots, L - 1$ it is 1 if $k = (i_1, \dots, i_w, j_{w+1}, \dots, j_L)$, for $w = 0$, if $k = j$, and for $w = L$, if $k = i$.

Also define for $\beta \in [0, 1]$ the operator $\mu_\beta : \Xi \rightarrow \Xi$ defined by

$$\mu_\beta\xi(i) = \sum_{j=0}^{N-1} \beta^{H(i, j)} (1 - \beta)^{L-H(i, j)} \xi(j), \quad (2)$$

where $H(i, j) = \sum_{k=1}^L |i_k - j_k|$ is the Hamming distance between $i = (i_1, i_2, \dots, i_L)$ and $j = (j_1, j_2, \dots, j_L)$ in S . This is the *mutation operator* on $S' \times S'$.

The selection operator $\psi : \Xi \rightarrow \Xi$ is defined by

$$\psi\xi(i) = \frac{\xi(i)R(i)}{\sum_{j=0}^{N-1} \xi(j)R(j)}. \quad (3)$$

The operator $\Psi_\beta : \Xi \times \Xi \rightarrow [0, 1]$ defined by

$$\Psi_\beta(\xi_2, \xi_1) = \binom{M}{M\xi_2(0), M\xi_2(1), \dots, M\xi_2(N-1)} \prod_{j=0}^{N-1} (\mu_{\beta\tau}\psi\xi_1(j))^{M\xi_2(j)}, \quad (4)$$

where $\binom{a}{b_1, \dots, b_j} = \frac{a!}{b_1! \dots b_j!}$ is the multinomial coefficient, defines a transition probability from $\xi_1 \in \Xi$ to $\xi_2 \in \Xi_0$, hence also from Ξ_0 into itself. Since for scalars $t > 0$ $\psi(t\xi) = \psi\xi$, there is an equivalent representation in terms of a transition matrix $Q_\beta^{(\tau)}$ on $S' \times S'$ whose entries are

$$q_\beta^{(\tau)}(\bar{m}_2 | \bar{m}_1) = \binom{M}{m_2(0), m_2(1), \dots, m_2(N-1)} \prod_{j=0}^{N-1} (\mu_{\beta\tau}\psi m_1(j))^{m_2(j)}, \quad (5)$$

where $\bar{m}_j = (m_j(0), m_j(1), \dots, m_j(N-1)) \in S'$ and

$$\Psi_\beta(\xi_2, \xi_1) = q_\beta^{(\tau)}((M\xi_2(0), \dots, M\xi_2(N-1)) | (M\xi_1(0), M\xi_1(1), \dots, M\xi_1(N-1))).$$

The matrix Q_β is square and stochastic with $\binom{M+N-1}{M}$ rows.

3. Fixed probability of crossover

In this section the consequences of sending the mutation rate to zero geometrically fast are investigated. It is shown that by employing a crossover scheme, called wrong-side-of-the-tracks (wst-crossover), which allows “tempered restarting” of the GA, a cross between a member of the current population with a randomly chosen member of S , the probability the goal has not been encountered by the n th generation decreases to zero geometrically quickly while this need not occur for the usual crossover scheme.

Suppose it is desired to maximize the function R on the set S . It is shown that employing the fixed crossover $\tau_{\alpha, \nu}$, where $\nu = v$, the uniform distribution on S , and $\alpha \in (0, 1)$ is arbitrary, the sequence of states (distributions $\bar{m}_n \in S'$) of the Markov chain whose transition matrix at the n th epoch is Q_{β_n} , where $\beta_n = (1 + \lambda^2)^{-n}$, $\lambda \neq 0$, has the property that the probability the populations up to epoch n have excluded a point at which R achieves its global maximum on S decreases to 0 as η^n for some

$\eta < 1$. Thus “rapid” identification of the global optimum is assured even though the mutation probability is decreasing to 0 rapidly. It is shown, furthermore, that for any $\alpha \in (0, 1)$ this fails for the traditional crossover $\tau_{\alpha, \xi}$. Thus without the crossover which includes the possibility of crosses with general elements of the state space S , mutation rates tending to 0 this rapidly, and even more slowly, result in a positive probability of never seeing the global maximum of the function.

3.1. Deleted transition matrix

In this section it is assumed without loss of generality that the function R assumes its maximum value at $j = 0$ so that $R(0) > R(j)$ for $j = 1, \dots, N - 1$. Consider the set X consisting of points

$$\{x = (m(1), m(2), \dots, m(N - 1)) : m(0) = 0, (m(0), m(1), \dots, m(N - 1)) \in S'\}$$

and, fixing τ , define the *deleted transition matrix* P_β on $X \times X$ as the submatrix of Q_β restricted to the states in X by

$$p_\beta(x_2|x_1) = q_\beta^{(\tau)}((0, x_2)|(0, x_1)).$$

Note that q_β are all polynomials in β of degree ML and write

$$q_\beta(\bar{n}|\bar{m}) = \sum_{j=0}^{ML} a_j(\bar{n}, \bar{m})\beta^j.$$

The limiting matrix is $P = \lim_{\beta \rightarrow 0} P_\beta = P_0$ and plainly

$$p(x_2|x_1) = a_0((0, x_2), (0, x_1)).$$

and

$$p_\beta(x_2|x_1) - p(x_2|x_1) = \beta a_1((0, x_2), (0, x_1)) + O(\beta^2).$$

3.2. Geometric convergence and wst-crossover

We shall employ Lemma A2 of [4] to prove that shrinking the mutation probability quickly does not hinder the rapid identification of the goal state as long as wrong side of the tracks crossover (wst-cross) is used, but that if one employs ordinary crossover as described in [1] (for example) there is even a positive probability that the goal state will never be identified. The result quoted from [4] runs as follows.

Lemma 1. (A2 of [4]) *If for some $\gamma > 1$, $\sum_{n \geq 1} \gamma^n \|P_n - P\| < \infty$ and for some $k \geq 1$, P^k has norm $\delta < 1$, then there is a constant $K < \infty$ and an $\eta \in (0, 1)$ such that for all n and m*

$$\|P_m P_{m+1} \cdots P_{m+n-1}\| < K\eta^n. \quad (6)$$

We can now prove that by “restarting” the GA, that is by allowing a crossover of any of the current members of the elite population with any member of the space S , a mutation rate tending to zero geometrically fast does not hinder rapid identification of the extremal value of the objective function.

Theorem 1. *Under the crossover measure $\tau_{\alpha, v}$, $\alpha \in (0, 1)$ and the geometrically decreasing mutation rate $\beta_n = (1 + \lambda^2)^{-n}$ there is an $\eta < 1$ and constant $K < \infty$ such that*

$$P[\cap_{j=1}^n \{m_j(0) = 0\}] \leq K\eta^n.$$

Proof. Since

$$\pi' P_1 P_2 \dots P_n e = P[\cap_{j=1}^n \{m_j(0) = 0\}],$$

where e is the deleted vector of ones and π is the deleted vector of initial probabilities, it suffices to prove the truth of (6). The norm of P is $\max_{x \in X} \sum_{y \in X} p(y|x)$; the norm of $P_\beta - P$ is $\max_{x \in X} \sum_{y \in X} |p_\beta(y|x) - p(y|x)|$ and is clearly no greater than $\beta(A + O(\beta))$ for some $A < \infty$. For each $x \in X$, $\sum_{y \in X} p(y|x)$ is $1 - \pi_x$, where π_x is the probability $P[m(0) > 0 | (0, x)]$.

Clearly the conditions of the lemma will be satisfied if $\pi_x > 0$ for each $x \in X$ since this is a finite set. Since

$$\tau\psi(\bar{m})(k) = \alpha \sum_{i \in S} \sum_{j \in S} \frac{E[I(i, j, k, W)]}{N} \psi(\bar{m})(i) + (1 - \alpha)\psi(\bar{m})(k),$$

$P[W = 0] = 1/(L + 1) > 0$, and $v(0) = 1/N > 0$ one has for $k = 0$ and any \bar{m} that

$$\tau\psi(\bar{m})(0) \geq \alpha N^{-1}(L + 1)^{-1}.$$

Thus for any $x \in X$, $\mu_0 \tau\psi((0, x))(0) = \pi_x \geq \alpha N^{-1}(L + 1)^{-1} > 0$.

3.3. Non-convergence for ordinary crossover

If one sends the mutation rate to 0 geometrically fast (or even more slowly - see below) and uses crossover $\tau_{\alpha, \xi}$ as in Davis and Principe [1], then the geometric

convergence of the tail probabilities, indeed the convergence to zero at all, need not hold. In [1] the mutation probability $p_m(k)$, called here κ_k , is sent to 0 with the generation count k . They liken this to cooling in a simulated anneal and show their algorithm converges asymptotically to one of the absorbing states of the chain, a population all of whose members are the same, provided cooling is slow enough. A rate guaranteeing that type of convergence is $\kappa_k = k^{-ML}$ where M is population size and L is the string size. Let $L = 3$ and $M = 4$ and let the algorithm start in the state $\bar{m} = (M, 0, \dots, 0) \in R^8$. Thus the entire population consists of the element $(0, 0, 0)$. Then under their selection rule (also called roulette wheel selection and the same as our ψ) including crossover, the same population will result on every generation unless there is a mutation event. But in fact there is a positive probability this will not occur. The probability that the algorithm remains in this starting population indefinitely is given by

$$\prod_{k \geq 1} (1 - \kappa_k)$$

and this infinite product is zero if and only if the infinite sum $\sum_{k \geq 1} \kappa_k$ is unbounded. However, if κ_k converges to zero even as slowly as their rate and certainly as fast as geometrically, this infinite sum is finite.

4. Process initiated crossover

In the last section it was shown that rapid convergence of the mutation rate to zero, and hence increasing protection from taking wrong paths deep into the search, need not hinder a rapid encounter with the goal. On the other hand, the crossover scheme by which this is accomplished is applied with constant probability over time, rather than when needed; namely, when progress in the algorithm has slowed or ceased. In this section a scheme is proposed, called *r-cross*, which executes a crossover only when necessary, not with constant probability over time, but depending on the progress of the algorithm. It is shown that even with geometrically decreasing mutation rates, this new method of initiating a crossover results in rapid encounter of the goal.

4.1. Motivation for r-cross

A Bayesian argument is offered in favor of the rule we shall adopt. Consider a situation in which one observes iid $\mathcal{B}(1, p)$ random variables (Bernoulli random variables) and in which there is a prior distribution $\pi_{\alpha, \beta} = Be(\alpha, \beta)$ on the success probability p , a Beta distribution. After the observations x_1, x_2, \dots, x_n the conditional probability distribution

$$\xi(p|x_1, \dots, x_n) \propto p^{\alpha-1}(1-p)^{\beta-1} \prod_{j=1}^n p^{x_j}(1-p)^{1-x_j}$$

so $p|x_1, \dots, x_n \sim Be(\alpha + s_n, \beta + n - s_n)$, where $s_n = \sum_{j=1}^n x_j$. In particular, if $x = 1$ corresponds to “a higher value is observed than any seen to date” and $x = 0$ corresponds to the complement, and if no improvement over a span of n trials has been seen (so $s_n = 0$) then the posterior distribution of p , the probability of a better value on the next trial is $\xi_n(p) = Be(\alpha, \beta + n)$. Taking $\alpha = \beta = 1$ the prior density reflects no knowledge of the underlying probability p ; it is uniform and the posterior density is simply

$$f_n(p) = (n+1)(1-p)^n I_{(0,1)}(p).$$

Thus, for example, the posterior probability assigned to the event that the probability of seeing anything better is less than 0.01 after not having seen an improvement in 10 trials is $\int_0^{0.01} f_{10}(p) dp = -(1-p)^{11} \Big|_0^{0.01} = 1 - (0.99)^{11} \approx 1 - 0.895 = 0.100466$. After 50 trials it would be approximately 0.4 and after 100 it would be roughly 0.63. In fact, the posterior assessment that the probability of seeing anything better is no more than c/n after not having seen anything better in $n-1$ trials is, for large n ,

$$1 - \left(1 - \frac{c}{n}\right)^n \approx 1 - e^{-c}.$$

This suggests the following rule for executing a crossover, although of course, the situation is more complicated in the case of GA.

Crossover Heuristic: Assuming a large posterior probability, say 0.85, is desired that the probability of seeing anything better is small, say less than 0.01, take $1 - e^{-c} = 0.85$. Solve for c obtaining in this case $c = 1.897$ and initiate a crossover if $c/n < 0.01$; that is, if no improvement has been seen in $1.897/0.01 = 189.7$ trials.

Less stringent requirements lead to more frequent crossovers: if a posterior probability of, say 0.5, is desired that the probability of there being a better value forthcoming

is less than, say 0.3, then initiate a crossover if $1 - (1 - 0.3)^{n+1} < 0.5$, or whenever an improvement has not been seen in 1 trial.

4.2. State space and transition matrix for r-cross

As above, denote distributions on the set $S = \{0, 1\}^L$ by

$$\bar{m} = (m(0), m(1), \dots, m(2^L - 1)),$$

where $m(j)$ are all non-negative integers, $\sum_{j=0}^N m(j) = M$, and $N = 2^L - 1$. The space of distributions on S is denoted S' . Our state space in this section is the set $C = (S')^r$ consisting of r -vectors $c = (\bar{m}_1, \bar{m}_2, \dots, \bar{m}_r)$. We think of the subscripts as increasing with time so the only transitions between states c_1 and c_2 with non-zero probabilities are those when the c 's are of the form

$$c_1 = (\bar{m}_1, \bar{m}_2, \dots, \bar{m}_{r-1}, \bar{m}_r) \rightarrow (\bar{m}_2, \bar{m}_3, \dots, \bar{m}_r, \bar{m}_{r+1}) = c_2$$

so that the last $r - 1$ distributions of c_1 are shifted to the left and a new one is added in the last position to form c_2 . To describe the transition probability, introduce the functions $\Delta(c)$, on C and σ defined on S' . For $\bar{m} \in S'$, retaining the notation R for the objective function, let

$$\sigma(\bar{m}) = \max\{R(j) : m(j) > 0, 0 \leq j \leq N\}.$$

The function Δ takes values in $\{0, 1\}$ and is 1 at $c = (\bar{m}_1, \dots, \bar{m}_r)$ iff

$$\max_{2 \leq j \leq r} \sigma(\bar{m}_j) > \sigma(\bar{m}_1).$$

Thus Δ simply indicates whether or not the supports of the measures on that stretch of r distributions have seen any improvement in the objective function R (assuming the maximum of R is sought).

Denoting the crossover to be applied in this section, determined simply by the failure to improve the objective over the course of r generations, as $\tau = \tau_{\alpha=1, \nu=v}$, for c_1 such that $\Delta(c_1) = 1$, where $c_1 = (\bar{m}_{n+1}, \dots, \bar{m}_{n+r})$, the transition probability from c_1 to $c_2 = (\bar{m}_{n+2}, \dots, \bar{m}_{n+r}, \bar{m}_{n+r+1})$ is given by

$$a(\bar{m}_{n+1+r} | \bar{m}_{n+r}) = q_0^{(e)}(\bar{m}_{n+1+r} | \bar{m}_{n+r}) = \binom{M}{\bar{m}_{n+r+1}} \prod_{j=0}^{N-1} (\psi(\bar{m}_{n+r})(j))^{m_{n+r+1}(j)},$$

above since no crossover ($\tau = e$, the identity) is applied in this case and $\mu_0 = e$. The transition in case $\Delta(c_1) = 0$ is

$$b(\bar{m}_{n+1+r}|\bar{m}_{n+r}) = q_0^{(\tau)}(\bar{m}_{n+1+r}|\bar{m}_{n+r}) = \binom{M}{\bar{m}_{n+r+1}} \prod_{j=0}^{N-1} (\tau\psi(\bar{m}_{n+r})(j))^{m_{n+r+1}(j)}.$$

Thus for the case of r-cross, one can write the transition probability on $C \times C$ as

$$T(c_2|c_1) = (a(c_{2,r}|c_{1,r}))^{\Delta(c_1)} (b(c_{2,r}|c_{1,r}))^{1-\Delta(c_1)},$$

where $c_j = (c_{j,1}, c_{j,2}, \dots, c_{j,r})$, if $c_{2,i} = c_{1,i+1}$ for $i = 1, 2, \dots, r-1$ and 0 otherwise.

4.3. Deleted transition and geometric convergence for r-cross

Introduce the deleted transition matrix Σ defined on $D \times D$, where $D = X^r$, by

$$\Sigma(d_2|d_1) = T(((0, d_{2,1}), \dots, (0, d_{2,r}))|((0, d_{1,1}), \dots, (0, d_{1,r}))).$$

The chain on $C \times C$ with positive mutation rate has $a_\beta(\bar{m}|\bar{n}) = q_\beta^{(e)}(\bar{m}|\bar{n})$ and $b_\beta(\bar{m}|\bar{n}) = q_\beta^{(\tau)}(\bar{m}|\bar{n})$ and we denote by T_β its transition matrix and by Σ_β the corresponding deleted transition matrix. For any sequence $c = (\bar{m}_1, \dots, \bar{m}_r)$ of states in S' let $Z(c) = 0$ if $m_j(0) = 0$ for every $j = 1, \dots, r$ and otherwise $Z(c) = 1$. Letting the chain's state at generation j be C_j , the main theorem can now be proven.

Theorem 2. *Under r-cross and shrinking the mutation rate according to $\beta_n = (1 + \lambda^2)^{-n}$, one has for some $K < \infty$ and $\eta < 1$*

$$P[\cap_{j=1}^n \{Z(C_j) = 0\}] \leq K\eta^n. \quad (7)$$

Proof. With an initial probability vector π , a deleted vector $\hat{\pi}$, and the deleted vector of ones, $\hat{1}$, since

$$\hat{\pi}' \prod_{i=1}^r P_{\beta_i}^{(e)} \prod_{j=r+1}^n \Sigma_{\beta_j} \hat{1} = P[\cap_{k=1}^n \{Z(C_k) = 0\}]$$

it suffices to prove for some $\gamma > 1$, positive integer k and $\delta < 1$ that $\sum_{j \geq 1} \gamma^j \|\Sigma_{\beta_j} - \Sigma\| < \infty$ and $\|\Sigma^k\| < \delta$.

Consider first

$$\|\Sigma_\beta - \Sigma\| = \max_{d \in D} \sum_{d' \in D} |\Sigma_\beta(d'|d) - \Sigma(d'|d)|.$$

Since for $d_1, d_2 \in D$ one has $a_\beta((0, d_{2,r})|(0, d_{1,r}))$ a polynomial in β of degree ML whose value at $\beta = 0$ is $a((0, d_{2,r})|(0, d_{1,r}))$ and similarly for b_β , it follows that for some $A < \infty$, $\|\Sigma_\beta - \Sigma\| = \beta(A + O(\beta))$.

Next, taking $k = (N - 1)(r - 1) + 1$, it is shown that $\|\Sigma^k\| < 1$. Since D is a finite set and $\|\Sigma^k\| = \max_{d \in D} \sum_{d' \in D} \Sigma^k(d'|d)$, it suffices to prove that for each $d \in D$ one has $\sum_{d'} \Sigma^k(d'|d) < 1$. The latter is simply the probability under no mutation that starting with an element $d \in D, d = ((0, x_1), (0, x_2), \dots, (0, x_r)), x_i \in X$ one passes through successive generations of the form $(0, x_{r+1}), \dots, (0, x_{N_r})$ to arrive at $d' = ((0, x_{(N-1)r+1}), \dots, (0, x_{N_r}))$. It will be shown that this probability is less than 1.

If $\Delta(d) = 0$ then there will be a wst-crossover to get to the $r + 1$ st generation and since $\cup_{x \in X} \{C_{2,r} = (0, x)\} = \{C_{2,r}(0) = 0\}$ if one has $P[C_{2,r}(0) > 0|d] > 0$ then the claim will be shown for d such that $\Delta(d) = 0$, for then it will have been shown that the probability one exits D immediately and thereby includes the goal state in the elite set at that stage is positive so the probability of remaining in D is less than 1. Now the marginal distribution of $C_{2,r}(0)|d$ is binomial, $\mathcal{B}(M, \pi_d)$ where $\pi_d = \mu_0 \tau \psi((0, x_r))(0)$. As before, a lower bound on this quantity, because of wst-crossover, is $N^{-1}(L + 1)^{-1}$ uniformly in $x_r \in X$ and hence in $d \in D$. This concludes the case $\Delta(d) = 0$.

For $\Delta(d) = 1$ there are $r - 1$ cases: the improvement occurs last at index 2, 3, \dots , r and it will be shown that in this instance, a stretch of length $(N - 1)(r - 1) + 1$ beginning at our first index 1 must encompass either a transition out of the states in D or at least one stretch of length r over which no improvement in the objective occurs. Indeed, the most favorable circumstance in generating long stretches of no improvement may be described in terms of the ordered values $R_1 < R_2 < \dots, R_N$ of the objective function. We could have R_1 as our first maximum and repeated $r - 1$ times, then R_2 repeated $r - 1$ times, so that in any sequence of $(N - 1)(r - 1) + 1$ states, one must have exited the suboptimal states or must have encountered a stretch of length at least r over which no improvement was observed. As the former is precluded in this case of examining the probabilities of transitions among the states D , such a stretch must occur. As has been seen immediately above, once such a stretch occurs, there is a positive probability of leaving D . One concludes, therefore, that $\|\Sigma^{(N-1)(r-1)+1}\| < 1$

5. General r-cross

Geometric convergence of tail probabilities also holds for more general schemes for both mutation and crossover initiated after a fixed number of non-improvements.

5.1. General crossover

Suppose there is a family of m mappings $F^{(v)}, v = 1, \dots, m$ from $S \times S$ into S . Denoting, for $j \in S$ fixed, by $F_j^{(v)}$ the transformation from S into S defined by $F_j^{(v)}(i) = F^{(v)}(i, j)$ the family $\{F^{(v)}\}_{v=1}^m$ of transformations will be said to be *adequate* if for every $k \in S$ and $j \in S$ one has

$$\bigcup_{v=1}^m \left(F_j^{(v)}\right)^{-1}(k) \neq \emptyset. \quad (8)$$

Define the associated crossover operator on Ξ by

$$\tau\xi(k) = \sum_{v=1}^m \sum_{i \in S} \sum_{j \in S} \delta(v)\nu(i)\xi(j)I_{A_v(k)}(i, j), \quad (9)$$

where $A_v(k) = \{(i, j) \in S^2 : F^{(v)}(i, j) = k\}$. Geometric convergence will still hold under r-cross using this crossover under conditions which also amount to tempered restarting. Specifics are in Theorem 3, whose proof can be carried out just as in the case of Theorem 2.

Theorem 3. *If the family $F^{(v)}, v = 1, \dots, m$ satisfies (8) then under r-cross with τ as defined in (9) and shrinking the mutation rate according to $\beta_n = (1 + \lambda^2)^{-n}$, one has for some $K < \infty$ and $\eta < 1$ that (7) holds if $\delta(v) > 0$ for $v = 1, \dots, m$ and $\nu(i) > 0$ for every $i \in S$.*

Proof. Observe that because of (8), for each $k, j \in S \times S$ one must have $\sum_{v=1}^m I_{A_v(k)}(i, j) > 0$ for some $i \in S$. Under the conditions of the theorem, no choice of $\xi \in \Xi$ yields $\tau\xi(k) = 0$; in fact, these quantities are uniformly bounded below over $\xi \in \Xi$ and $k \in S$ by a positive quantity. This bound now plays the same role in the proof as did $N^{-1}(L+1)^{-1}$ in the proof of Theorem 2; otherwise, the proof is the same.

In the case of wst-cross, for example, $\nu(i) = N^{-1} > 0$ and $\delta(v) = 1/m$, where $m = L+1$ and wst-cross satisfies (8) trivially since for one of the v 's we had $F^{(v)}(i, j) = i$ for all i, j . Obviously, many other crossing schemes are covered by Theorem 3.

5.2. General mutation

The essential feature of the mutation operator μ_β is that it satisfy

$$\|\mu_\beta - e\| = \beta(A + O(\beta)), \quad (10)$$

where e is the identity. As long as this feature holds then under r-cross with an *adequate* crossover scheme, the convergence of tail probabilities for geometrically decreasing mutation rates will itself be geometric.

6. Examples

In this section some examples are provided to illustrate the ideas of the previous sections.

Example 1. In this example the success of GA's in maximizing the function f defined in (11) is investigated. The number of bits is $L = 10$ so that, interpreting $i \in S$ as a binary representation, $i = 0, 1, \dots, 1023$. The objective function (called R above) is f given by

$$f(i) = \frac{100}{1 + i^{7/10}} [1 + \cos(\frac{\pi(i - 60)}{50})] \quad (11)$$

and has a global maximum at $i = 0$ and local maxima at $i = 60, 160, 260, \dots$. Population size was $M = 4$ for each of three GA implementations. The traditional (T) had a fixed mutation rate $\lambda_t = \lambda$ and crossover only between members of the current population. Traditional with decreasing mutation rate (TD) retained the same crossover and mutation but the mutation rate $\lambda_t = \lambda^t$ decreased geometrically with t . Finally the r-cross (RX) version had $\lambda_t = \lambda^t$ and executed crossover only after a prescribed number r of failures to improve, and then implemented wst-cross between randomly selected members of the current and S rather than just ordinary crossover. In each case implementation involved : (1) roulette wheel selection; (2) crossover selection; (3) with probability $p_m(t)$ mutate every bit of a randomly selected offspring.

Consulting Table 1 one finds that in both cases the algorithm often failed to find the optimum within the allotted 7K iterations. In Table 2 can be found averages for r-cross for various r where its superior performance is clear.

More detail is provided by selected histograms. In Figure 1 one sees data for which a 68% success rate was observed for ordinary GA, namely (T), with λ_t identically 0.95.

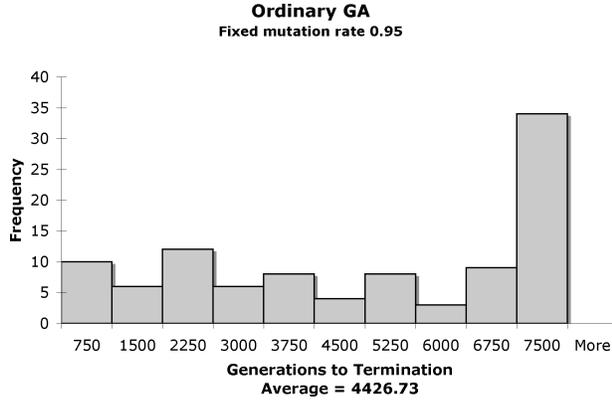


FIGURE 1: Histogram for ordinary GA, $\lambda = 0.95$. Success rate 68%.

(T) Average	(T) success rate	λ	(TD) Average	(TD) success rate
3867.09	0.75	0.99	4057.63	0.43
4426.73	0.68	0.95	6304.24	0.10
4305.24	0.61	0.90	6721.1	0.04
4459.07	0.57	0.80	7000	0.00
3193.65	0.88	0.7	6860.15	0.02

TABLE 1: Generations till termination of (T) and (TD).

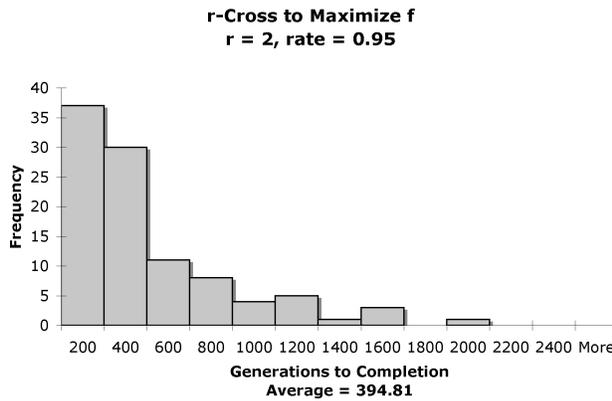
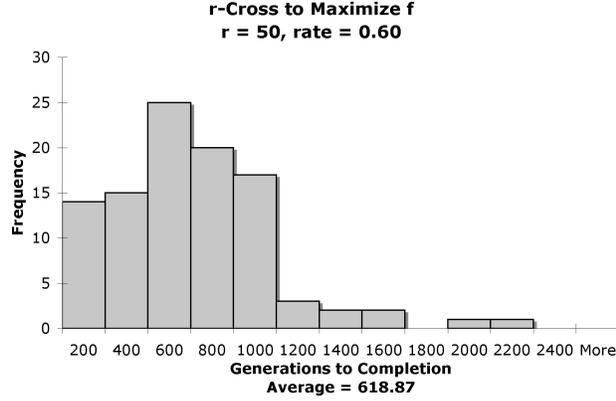


FIGURE 2: Histogram for r-cross, $r = 2$, $\lambda = 0.95$.

In Figures 2,3, and 4 can be found plots histograms detailing the performance of (RX) in selected cases. In table 2 one sees the much smaller average iterations till the goal

FIGURE 3: Histogram for r-cross, $r = 50$, $\lambda = 0.60$.

	r			
	2	5	10	20
0.99	468.12	416.45	494.53	424.52
0.95	394.81	421.32	432.03	437.03
λ 0.90	362.85	426.71	434.60	483.53
0.80	426.82	377.08	435.99	449.86
0.70	341.32	427.58	394.11	446.76

TABLE 2: Average generations till termination of (RX). Success rate 1 in all cases.

was found. The histograms show in addition that typically the number of iterations was far smaller than the average, a typical situation of smaller median than mean for these more or less exponentially shaped distributions.

Example 2 below, in which GA is applied to finding the maximum permanent of a matrix, provides an instance requiring the more general mutation and crossover schemes discussed in section 5. In coding the 14×14 0-1 matrix as a length 196 vector of 0's and 1's, one cannot simply flip bits indiscriminately since one must obtain a 196-vector with exactly 40 ones and 156 zeros. The crossover operation described above has similar problems. Thus, alterations must be made.

Example 2. Effectiveness of GA with tempered restart is compared with that of ordinary GA in maximizing a permanent. The permanent of a square matrix is obtained

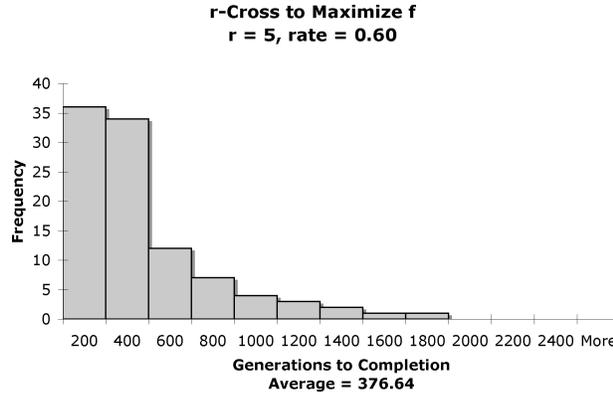


FIGURE 4: Histogram for r-cross, $r = 5$, $\lambda = 0.60$.

by taking all signs to be positive in the expansion of its determinant. The optimization problem consists of attempting to find the 14×14 0-1 matrix with the maximum permanent, subject to the constraint that there are exactly 40 ones (and thus 156 zeros) in the matrix. The authors have previously investigated in [4] the effectiveness of restarted simulated annealing in finding the maximum for this problem. Reported herein are the results of experiments comparing the performance of an ordinary GA with r-cross GA.

Ordinary GA, with crossover executed only between randomly selected members of the current population and with a fixed mutation rate, was compared with r-cross for varying values of the parameters r and the mutation rate λ_t . For ordinary GA the rate was fixed at $\lambda_t = \text{Rate}$ while for r-cross the rate was geometrically decreasing satisfying $\lambda_t = \text{Rate}^t$. The r-cross had wst-crossovers only when the objective had not shown improvement over r generations; so mating was allowed between members of the current population and a general element of the state space S . In Tables 3 and 4 can be found the numerical results of running the algorithms on the permanent problem with a 14×14 matrix of zeros and ones and containing exactly 40 ones.

Many alternatives are possible to the mutation operation. The operator of (2) describes the situation of flipping all bits independently with probability λ_t , but the one employed in this example simply selects at random a location in the matrix at which a 1 is located and selects at random (probability $1/4$ each since the matrix is 2-dimensional) from the locations adjacent to it in the matrix one which contains a zero

and interchanges the zero and one. If there are none it selects again, and again until the switch is accomplished. At generation t the mutation is performed on a randomly selected member of the current population with probability λ_t . Letting $i \in \{0, 1\}^{196}$ be an arbitrary matrix with 40 ones and 156 zeros, the probability $\rho_{i,j}$ that i is the result of a mutation from the matrix represented by j clearly does not depend upon any of the other problem parameters so

$$\mu_\beta \xi(i) = \beta \sum_j \rho_{i,j} \xi(j) + (1 - \beta) \xi(i)$$

and it is seen that (10) is satisfied.

Crossover requires a new scheme since by the usual one the offspring of two parents i and j could have an incorrect number of ones. The crossover used for this example compared locations and swapped 0's and 1's in such a way as to preserve the number of ones, 40 in this case, in the offspring. The important feature is that one of the crossover operations was the identity so that the requirements of Theorem 3 were met. Thus the geometric convergence to 0 was assured in the tempered restarted GA in this example.

<i>Average Best Objective Value</i>						
	Ordinary GA	r-cross				
Rate		$r = 5$	10	50	100	200
0.99	863.20	1254.40	928.00	1108.80	1000.00	1272.00
0.90	972.80	1161.60	1257.60	1048.00	1281.60	1043.20
0.80	643.60	1062.40	1121.60	932.80	1003.20	1040.00
0.70	685.60	1042.80	1259.20	1098.00	1160.00	1430.40

TABLE 3: Average over 5 runs for 40K generations, population size 30.

7. Discussion

It has been shown that implementations of genetic algorithms which send the mutation rate to 0 geometrically fast and execute crossover only after a fixed number of non-improvements have the property that the probability the goal has not been encountered yet tends to zero geometrically if, in a sort of anti-eugenics way, crossover

<i>Maximum Best Objective Value</i>						
	Ordinary GA	r-cross				
Rate		$r = 5$	10	50	100	200
0.99	1200	1728	1620	1344	1152	1584
0.90	1152	1440	1728	1296	1944	1152
0.80	792	1344	1200	1056	1120	1512
0.70	768	1296	2016	1452	1728	2016

TABLE 4: Maximum over the 5 runs.

allows matings between members of the elite and the original population rather than just between members of the elite population. By itself geometric convergence to zero of this tail probability of not having seen the goal is not a strong recommendation for the method; after all, simply guessing each time by selecting a random population has the same property. However, if the crossover mechanism is selected carefully and appropriately to fit the problem, great gains in the speed of identifying the goal can be achieved. The idea of the algorithm is simply that in the initial stages of a search for the maximum one should allow large probability of moving around freely; since the selection mechanism will quickly weed out unfit members the algorithm will proceed to the more promising directions rapidly. However, keeping a fixed mutation rate will introduce chaff at a constant rate and unduly burden the selection mechanism. Instead, by sending the mutation rate to zero, promising directions can be examined more thoroughly without jumping far away by a mutation, as long as the crossover mechanism is *tame*; it stays close in terms of function values in the sense that for all $(i, j) \in S \times S$ and for most $v \in \{1, \dots, m\}$ one has that $|R(F^{(v)}(i, j)) - R(j)|$ is small. This should not hold for all v since, having sent the mutation rate to something small, if the region of examination ceases to offer improvement after a sufficient time, at least one of the randomly selected crossover $F^{(v)}$ should allow escape from the region. Thus for an *adequate* (see (8)) collection this can happen with probability determined by the distribution δ .

For example, in the case of maximizing a continuous function R on an interval $[0, 1]$ with the members of $i \in S$ being the binary expansion coefficients $(i_1, \dots, i_L), i_t \in$

$\{0, 1\}$ the collection

$$F^{(v)}(i, j) = (j_1, j_2, \dots, j_v, i_{v+1}, \dots, i_L) \quad (12)$$

will, depending on the smoothness of R satisfy the criterion quite well for $v \geq 2$ for the crossover operator in (9) while the crossover $G^{(v)}(i, j) = (i_1, \dots, i_v, j_{v+1}, \dots, j_L)$ would not satisfy this criterion and the resulting algorithm would be expected to perform poorly. The choice of r in waiting for improvement should allow an examination of the directions from a given point in the population assuming the crossover is *tame*. For the case of the continuous function R on the line, r should be small, around 2, while for the permanent problem 200 looks more reasonable since the members of S constitute 196-vectors.

8. Acknowledgments

F. Mendivil gratefully acknowledges support for this work from the Natural Sciences and Engineering Research Council of Canada (NSERC).

References

- [1] DAVIS, T. AND PRINCIPE, J. (1993). A markov framework of the simple genetic algorithm. *J. Evolut. Comp.* **1**, 269–288.
- [2] HU, A., SHONKWILER, R. AND SPRUILL, M. C. (2002). Estimating the convergence rate of a restarted search process. *Int. J. Comput. Numer. Anal. Appl.* **1**, 353–367.
- [3] LÖWE, M. (1996). On the convergence of genetic algorithms. *Exposition. Math.* **14**, 289–312.
- [4] MENDIVIL, F., SHONKWILER, R. AND SPRUILL, M. C. (2001). Restarting search algorithms with applications to simulated annealing. *Adv. in Appl. Probab.* **33**, 242–259.
- [5] SHONKWILER, R. AND VAN VLECK, E. (1994). Parallel speed-up of Monte Carlo methods for global optimization. *J. Complexity* **10**, 64–95.