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Optimal search efficiency of Barker's algorithm with an exponential fitness function

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Abstract Markov Chain Monte Carlo (MCMC) methods may be employed to search for a probability distribution over a bounded space of function arguments to estimate which argument(s) optimize(s) an objective function. This search-based optimization requires sampling the suitability, or fitness, of arguments in the search space. When the objective function or the fitness of arguments vary with time, significant exploration of the search space is required. Search efficiency then becomes a more relevant measure of the usefulness of an MCMC method than traditional measures such as convergence speed to the stationary distribution and asymptotic variance of stationary distribution estimates. Search efficiency refers to how quickly prior information about the search space is traded-off for search effort savings. Optimal search efficiency occurs when the entropy of the probability distribution over the space during search is maximized. Whereas the Metropolis case of the Hastings MCMC algorithm with fixed candidate generation is optimal with respect to asymptotic variance of stationary distribution estimates, this paper proves that Barker's case is optimal with respect to search efficiency if the fitness of the arguments in the search space is characterized by an exponential function. The latter instance of optimality is beneficial for time-varying optimization that is also model-independent.

Keywords Markov chain Monte Carlo · Maximum entropy · Search efficiency · Selective generation · Stochastic optimization in dynamic environments

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1 Introduction

Markov Chain Monte Carlo (MCMC) algorithms [6,4,3,2] are useful for simulating large random fields through sampling, and are frequently employed in statistical mechanics applications [2]. MCMC algorithms utilize an irreducible, aperiodic, time-homogeneous Markov chain such that the stationary distribution, π, is the target distribution. Since convergence to the target distribution is easier to check for reversible Markov chains, these Markov chains are the most frequent case of MCMC algorithms [2].

To optimize an objective function, MCMC algorithms can be used to convert a prior uniform probability distribution over a bounded search space of arguments that are candidates for function optimization to a target probability distribution that is concentrated in a neighborhood at the location of one or more arguments that achieve function optimization. This conversion process can be accomplished through sampling the suitability, or fitness, of the candidate arguments. The extent to which the target probability distribution is concentrated in a neighborhood may be tuned, with a limiting case of tunability being a distribution consisting of a delta function at the location of an argument that exactly optimizes the function. This paper proves that, under certain conditions, a well-known MCMC algorithm utilizing a reversible, irreducible, aperiodic, time-homogeneous Markov chain accomplishes optimization by searching for π efficiently, where this optimal search efficiency is defined as the quickest trade-off of prior information about the search space for search effort savings [8]. Such savings are important when significant exploration of the search space is required, for instance, in model-independent optimization with time-varying objective function or argument fitnesses (e.g., [12]). Optimal search efficiency is characterized by a method that maximizes the entropy of the probability distribution over the search space during the search [7,8]. Hence, this paper clarifies the conditions under which the well-known MCMC algorithm, Barker's algorithm [1], maximizes entropy.

The approach in this paper is different from the covariance matrix adaptation evolution strategy [5], which employs a maximum entropy probability distribution but is concerned with the propagation of a covariance matrix in a manner similar to gradient-based search that is unsuited to time-varying fitness landscapes. The approach is also not related to the cross-entropy method for optimization [15], which deploys a cross-entropy heuristic unlike this paper's adaptation of the theory of rational behavior [11] for Markov chains that yields and explains cross-entropy. Instead, the approach is a novel optimization method based on the new theory that is equivalent to Barker's algorithm.

Additionally, this paper's goal of search efficiency is different from asymptotic variance, which is the variance of estimates of the stationary distribution when an MCMC algorithm is started close to stationarity. Optimal asymptotic variance is characterized by low values that indicate a lack of volatility in the algorithm's converged solution. Examining the search efficiency of an MCMC optimization algorithm is more useful than determining its asymptotic variance when the objective function or the fitness values of the arguments in the search space vary with time because the target distribution correspondingly varies, despite the algorithm being close to stationarity prior to an objective function or fitness change.

Search efficiency is also different from convergence speed to the stationary distribution, which, for a time-homogeneous, irreducible, ergodic Markov chain, is given by the second-largest eigenvalue modulus of the matrix of transition probabilities. Again, examining the search efficiency of an MCMC optimization algorithm is more useful than determining its stationary distribution convergence speed when the objective function or the fitness values of the arguments in the search space vary with time because it is desirable for the algorithm to utilize information previously gained about the search space to improve its convergence speed after an objective function or fitness change.

The remainder of this paper is as follows. Section 2 sets up the optimization problem to be solved by an MCMC search algorithm, and briefly highlights two well-known MCMC methods. Section 3 provides sufficient conditions for optimal search efficiency through an extension of the theory of rational behavior to Markov chains. Section 4 develops a technique that satisfies the sufficient conditions for optimal search efficiency and explains the method's equivalence to Barker's algorithm. Section 5 presents conclusions.

The primary original contributions of this paper are the claims in Theorems 2 and 3 and their proofs. A preliminary version of the technique in Section 4 appears in [13], and a few biological parallels of this technique are noted in [14].

2 Background

2.1 Problem Definition

Let X be a search space with elements x_i, $1 \leq i \leq n$. The problem seeks a probability density function $\phi_X : X \rightarrow \mathbb{R}^+$ that accomplishes the specified objective below. Let $z : X \rightarrow Z$ be an unknown, computable, and possibly changing function that we are interested in. The set Z is a metric space. Suppose that we are given a desired element z_{des} in the image of z, and we wish to find $x \in X$ such that $||z(x) - z_{des}||$ is small (i.e., $z(x) \approx z_{des}$). Formally, we want a ϕ_X that helps achieve a known expected value $Y \geq 0$, i.e.,

$$\mathrm{E}_{\phi_X}[||z(x) - z_{des}||] = Y. \tag{1}$$

In the above, Y is effectively a tolerance, i.e., it is the acceptable mean distance between candidates in the image of z compared to the desired image value. Let $y(x) = ||z(x) - z_{des}||$. The scheme to find ϕ_X should be efficient in that it trades off prior information about X for search effort savings as quickly as possible. Let $f : Z \rightarrow \mathbb{R}^+$. We allow the method to employ a function $F : X \rightarrow \mathbb{R}^+ : x \mapsto F(x) = (f \circ z)(x) = f(z(x))$, a real-valued, positive fitness function.

2.2 MCMC Design

The design of an MCMC algorithm involves finding an ergodic matrix of transition probabilities $\mathbf{P}$ with elements P_{ij} that satisfy

$$\pi_i P_{ij} = \pi_j P_{ji}, \; \forall i, j. \tag{2}$$

Here, π_i denotes the i-th element of the stationary distribution vector π over X, and P_{ij} represents the probability of transitioning from element x_i to element x_j. The distribution π is the sought ϕ_X in Section 2.1. A typical choice [2] of P_{ij} has the form

$$P_{ij} = Q_{ij}\alpha_{ij},\ \forall j \neq i. \tag{3}$$

Here, $\mathbf{Q}$ is a probability transition matrix (called the *candidate-generating matrix*) with elements Q_{ij} representing the probability of "tentatively" choosing a transition from x_i to x_j, and α is a probability transition matrix with elements α_{ij} representing the probability of accepting that transition. A generic formulation for the acceptance probabilities is specified by the Hastings algorithm, which sets

$$\alpha_{ij} = \frac{S_{ij}}{1+\frac{\pi_i Q_{ij}}{\pi_j Q_{ji}}}, \tag{4}$$

where S_{ij} are the elements of a symmetric matrix $\mathbf{S}$. Special cases of the Hastings algorithm include the Metropolis algorithm, which is used in simulated annealing [10], and Barker's algorithm.

2.3 Metropolis Algorithm

The acceptance probability for the Metropolis algorithm sets $S_{ij} = 1+\min\left(\frac{\pi_i Q_{ij}}{\pi_j Q_{ji}}, \frac{\pi_j Q_{ji}}{\pi_i Q_{ij}}\right)$ in (4) [2], so that

$$\alpha_{ij} = \min\left(1, \frac{\pi_j Q_{ji}}{\pi_i Q_{ij}}\right). \tag{5}$$

In the case of purely random $\mathbf{Q}$ (Q_{ij} is constant), this becomes

$$\alpha_{ij} = \min\left(1, \frac{\pi_j}{\pi_i}\right). \tag{6}$$

The Metropolis algorithm is optimal with respect to asymptotic variance in the class of Hastings algorithms with fixed $\mathbf{Q}$ [2].

2.4 Barker's Algorithm

The acceptance probability for Barker's algorithm sets $S_{ij} = 1$ in (4) [2], so that

$$\alpha_{ij} = \frac{1}{1+\left(\frac{\pi_i}{\pi_j}\right)\left(\frac{Q_{ij}}{Q_{ji}}\right)}. \tag{7}$$

In the case of purely random $\mathbf{Q}$, this becomes

$$\alpha_{ij} = \frac{1}{1+\left(\frac{\pi_i}{\pi_j}\right)}. \tag{8}$$

3 Sufficient Conditions for Efficient Search

Extending the theory of rational behavior [11] to Markov chains yields sufficient conditions for optimal search efficiency. Let $(X,\mathbf{P})$ be a time-homogeneous, irreducible, ergodic Markov chain, where $X=\{x_1,x_2,\ldots,x_n\}$ is the set of states of a Markov process, $\mathbf{P}\in\mathbb{R}^{n\times n}$ is the matrix of transition probabilities for these states, and $n<\infty$ is the number of states. Assume that the initial probability distribution over the states is known, i.e., we are given an n-vector $\mathbf{p}(0)$ having elements $p_i(0)=\Pr[\mathscr{X}(0)=x_i]$ for all $x_i\in X$, where $\mathscr{X}(0)$ denotes the state realization at time 0, and we have $\sum\limits_{i=1}^{n} p_i(0)=1$. Since we have assumed that the states in X are ergodic and irreducible, they admit a unique stationary probability distribution [2]. Let $\pi=\begin{bmatrix}\pi_1 & \pi_2 & \ldots & \pi_n\end{bmatrix}$ be the row vector of these stationary probabilities, satisfying the constraints $\pi_i>0\ \forall i$, and $\sum\limits_{i=1}^{n}\pi_i=1$. Let $F:X\rightarrow\mathbb{R}^+$ be a positive fitness function. Let $N\in\mathbb{N}$ be a natural number.

Definition 1 The time-homogeneous, irreducible, ergodic Markov chain $(X,\mathbf{P})$ is said to *behave rationally* with respect to fitness F with level N if

$$\frac{\pi_i}{\pi_j}=\left(\frac{F(x_i)}{F(x_j)}\right)^N,\ 1\leq i\leq n,\ 1\leq j\leq n. \tag{9}$$

This is a definition of *global rationality*, which refers to the ratio of the probabilities.

Each stationary probability can also be explicitly characterized to ensure Markov chain rational behavior.

Theorem 1 *The time-homogeneous, irreducible, ergodic Markov chain $(X,\mathbf{P})$ behaves rationally with respect to fitness F with level N if and only if*

$$\pi_i=\frac{F(x_i)^N}{\sum\limits_{k=1}^{n}F(x_k)^N},\ 1\leq i\leq n. \tag{10}$$

Proof See [12].

Here, we have a more general, probabilistic version of the optimization of an objective function. A Markov chain that behaves rationally selects the state of maximum fitness with the highest stationary probability, and, in the limit as N approaches ∞, this probability is 1. That is, N tunes the concentration of the stationary probability distribution around the state of maximum fitness, and in the limit as N approaches ∞, the problem and solution then revert to one of standard optimization. Remarkably, rational behavior in Markov chains is the result of a subsidiary optimization.

Theorem 2 *The stationary distribution π of the time-homogeneous, irreducible, ergodic Markov chain $(X,\mathbf{P})$ that behaves rationally with respect to fitness F with level N solves the optimization problem*

$$\min_{\pi_1,\ldots,\pi_n} U(\pi)=-\sum_{i=1}^{n}\varphi_i\ln(\pi_i), \tag{11}$$

subject to the constraints $\sum_{i=1}^{n} \pi_i = 1$, *and* $\pi_i > 0,\ \forall i$, *utilizing the fitness distribution*

$$\varphi_i = \frac{F\left(x_i\right)^N}{\sum_{k=1}^{n} F\left(x_k\right)^N},\ 1 \le i \le n. \tag{12}$$

Proof We use the method of Karush-Kuhn-Tucker (KKT) multipliers to solve the optimization problem

$$\min_{\pi_1,\ldots,\pi_n} \Phi(\pi) = -\sum_{i=1}^{n} F(x_i)^N \ln(\pi_i),$$

subject to $\sum_{i=1}^{n} \pi_i - 1 = 0$, and $-\pi_i < 0,\ 1 \le i \le n$. Let

$$L(\pi_1,\ldots,\pi_n,\lambda,\mu_1,\ldots,\mu_n) = -\sum_{i=1}^{n} F(x_i)^N \ln(\pi_i) + \lambda\left(\sum_{i=1}^{n} \pi_i - 1\right) - \sum_{i=1}^{n} \mu_i \pi_i.$$

The KKT necessary conditions for optimality are

$$\frac{-F(x_i)^N}{\pi_i} + \lambda - \mu_i = 0,\ 1 \le i \le n;\ \sum_{i=1}^{n} \pi_i - 1 = 0;\ -\pi_i < 0,\ 1 \le i \le n;\ \lambda \ge 0;$$

$$\mu_i \ge 0,\ 1 \le i \le n;\ \lambda\left(\sum_{i=1}^{n} \pi_i - 1\right) = 0;\ \mu_i \pi_i = 0,\ 1 \le i \le n.$$

The first necessary condition becomes

$$-F(x_i)^N + \lambda \pi_i - \mu_i \pi_i = 0,\ 1 \le i \le n.$$

Since $\mu_i \pi_i = 0$ for all i, we obtain

$$-F(x_i)^N + \lambda \pi_i = 0,\ 1 \le i \le n.$$

Next, the constraint $\pi_i > 0$ for all i and the positive nature of $F(x_i)^N$ imply that $\lambda \neq 0$. Therefore,

$$\pi_i = \frac{F(x_i)^N}{\lambda},\ 1 \le i \le n,$$
$$\sum_{i=1}^{n} \pi_i = \sum_{i=1}^{n} \frac{F(x_i)^N}{\lambda},\ 1 \le i \le n.$$

Since $\sum_{i=1}^{n} \pi_i = 1$, we find that

$$\lambda = \sum_{i=1}^{n} F(x_i)^N,$$

and hence,

$$\pi_i = \frac{F(x_i)^N}{\sum_{k=1}^{n} F(x_k)^N}, \ 1 \le i \le n.$$

Thus, the stationary distribution in (10) satisfies the first order necessary conditions for optimality.

Moreover, we have

$$\frac{\partial^2 \Phi(\pi)}{\partial \pi_j \partial \pi_i} = 0 \text{ for } j \neq i,$$
$$\frac{\partial^2 \Phi(\pi)}{\partial \pi_i^2} = \frac{F(x_i)^N}{\pi_i^2} > 0.$$

Hence, the optimization problem has a strictly convex cost function and linear constraints. Thus, the solution of the first order necessary conditions is the global optimizer.

Note that in (9), rational behavior is invariant under positive scaling of fitness. Hence, there is no loss of generality in assuming that the fitness function is normalized. Accordingly, let $\varphi = [\varphi_1 \ \varphi_2 \ \dots \ \varphi_n]$ be the distribution of the N^{th} power of fitness, where

$$\varphi_i = \frac{F(x_i)^N}{\sum_{k=1}^{n} F(x_k)^N}, \ 1 \le i \le n.$$

Let

$$U(\pi) = \frac{\Phi(\pi)}{\sum_{k=1}^{n} F(x_k)^N}.$$

Then, the optimization problem can be normalized as $\min_{\pi_1,\dots,\pi_n} U(\pi) = -\sum_{i=1}^{n} \varphi_i \ln(\pi_i)$, subject to the constraints $\sum_{i=1}^{n} \pi_i - 1 = 0$, and $-\pi_i < 0, \ 1 \le i \le n$, which completes the proof.

Theorem 2 states that at the optimum, the stationary distribution agrees with the fitness distribution, i.e., $\pi = \varphi$. Using the notion of entropy, we can interpret (11) as follows. First, we recognize the term $-\ln(\pi_i)$ as the information content of state x_i [16]. Hence, the right hand side of (11) represents the "fitness-expectation of information." Moreover, we have the following.

Corollary 1 *The time-homogeneous, irreducible, ergodic Markov chain $(X, \mathbf{P})$ behaves rationally with respect to fitness F with level N if and only if its stationary probability distribution minimizes the fitness-expectation of information. At the optimum, this fitness-expectation of information is the entropy of the fitness distribution, i.e.,*

$$U^* = H(\varphi) = -\sum_{i=1}^{n} \varphi_i \ln(\varphi_i). \tag{13}$$

For Markov chains that behave rationally, and therefore possess fitness fractions that are distributed over the set of states as in (12), the entropy quantifies how egalitarian or elitist the states are. That is, the entropy is highest when all states have equal fitness; conversely, the entropy is lowest when there is only one state with a fitness fraction of unity and all other fitness fractions are zero. Equation (11) is also derived and discussed in [9] within the context of Information Theory [16].

Entropy maximization is important for search: 'In making inferences on the basis of partial information, the maximum entropy probability distribution subject to whatever is known is the only unbiased assignment we can make; to use any other would amount to arbitrary assumption of information which by hypothesis we do not have' [7]. The relationship between entropy maximization and optimal search is clarified in [8]. The optimal search policy for cells with exponential "sizes" 'appears very much like an irreversible process in thermodynamics, in which an initially non-equilibrium state relaxes in the the equilibrium state of maximum entropy. But now it is only our state of knowledge that relaxes to the "equilibrium" condition of maximum uncertainty' [8].

Applying these results from [7] and [8] to eliminate search biases during model-independent optimization with time-varying objective function or state fitnesses, an exponential normalized fitness function relates rational behavior, entropy and optimal search through the following.

Theorem 3 *Let $y : X \to \mathbb{R}$ be an unknown function for which an expected value, $\mathrm{E}[y(x)]$, is a known number Y. The normalized fitness*

$$\varphi_i = \alpha e^{-\beta y(x_i)},\ 1 \le i \le n, \tag{14}$$

and the stationary distribution π of the time-homogeneous, irreducible, ergodic Markov chain $(X, \mathbf{P})$ that behaves rationally with respect to fitness F with level N solves the optimization problem

$$\max_{\varphi_1,\ldots,\varphi_n} \min_{\pi_1,\ldots,\pi_n} U(\varphi,\pi) = -\sum_{i=1}^{n} \varphi_i \ln(\pi_i), \tag{15}$$

subject to the constraint

$$\mathrm{E}[y(x)] = Y. \tag{16}$$

Proof We use the method of Karush-Kuhn-Tucker (KKT) multipliers to solve the optimization problem

$$\max_{\varphi_1,\ldots,\varphi_n} H(\varphi) = -\sum_{i=1}^{n} \varphi_i \ln(\varphi_i),$$

subject to $\sum_{i=1}^{n} \varphi_i - 1 = 0,\ -\varphi_i < 0,\ 1 \le i \le n$, and $\mathrm{E}[y(x)] - \sum_{i=1}^{n} \varphi_i y(x_i) = 0$. Let $L(\varphi_1,\ldots,\varphi_n,\lambda_1,\lambda_2,\mu_1,\ldots,\mu_n) =$

$$-\sum_{i=1}^{n} \varphi_i \ln(\varphi_i) + \lambda_1 \left(\sum_{i=1}^{n} \varphi_i - 1\right) + \lambda_2 \left(\mathrm{E}[y(x)] - \sum_{i=1}^{n} \varphi_i y(x_i)\right) - \sum_{i=1}^{n} \mu_i \varphi_i.$$

The KKT necessary conditions for optimality are

$$-\ln \varphi_i - 1 + \lambda_1 - \lambda_2 y(x_i) - \mu_i = 0,\ 1 \le i \le n;\ \sum_{i=1}^{n} \varphi_i - 1 = 0;\ -\varphi_i < 0,\ 1 \le i \le n;$$

$$\lambda_1 \ge 0;\ \lambda_2 \ge 0;\ \mu_i \ge 0,\ 1 \le i \le n;\ \lambda_1 \left(\sum_{i=1}^{n} \varphi_i - 1 \right) = 0;$$

$$\lambda_2 \left(\mathrm{E}\left[y(x)\right] - \sum_{i=1}^{n} \varphi_i y(x_i) \right) = 0;\ \mu_i \varphi_i = 0,\ 1 \le i \le n.$$

The first necessary condition becomes

$$-\ln \varphi_i = \lambda_1 - \lambda_2 y(x_i) - \mu_i - 1,\ 1 \le i \le n,$$
$$\varphi_i = e^{(\lambda_1 - \lambda_2 y(x_i) - \mu_i - 1)},\ 1 \le i \le n.$$

Since $\varphi_i \neq 0$ for all i, $\mu_i = 0$ for all i. We obtain

$$\varphi_i = e^{\lambda_1 - 1} \cdot e^{-\lambda_2 y(x_i)},\ 1 \le i \le n,$$

or equivalently,

$$\varphi_i = \alpha e^{-\beta y(x_i)},\ 1 \le i \le n.$$

Hence, a scheme with underlying Markov chain dynamics that behave rationally also maximizes the entropy of the fitness distribution when the fitness function is exponential. The implication is that a fitness function like

$$F(x_i) = e^{-\left((z(x_i) - z_{des})^2\right)} \tag{17}$$

together with a scheme that makes use of rational behavior (see Section 4) guarantees efficient search-based optimization.

4 Barker's Algorithm Satisfies the Sufficient Conditions for Efficient Search

We first develop an MCMC method that optimizes through efficient search and then demonstrate that algorithm's equivalence to Barker's algorithm. The technique developed here is that of Selective Evolutionary Generation Systems [12], which arose in the context of tunable, responsive, model-independent optimization.

4.1 Selective Evolutionary Generation Systems

Definition 2 A *Selective Evolutionary Generation System* (SEGS) is a quintuple $\Gamma = (X,R,P,G,F)$, where

- X is a set of arguments that are candidates for objective function optimization, $X = \{x_1, x_2, \ldots, x_n\}$;
- R is a set whose elements can be utilized to transition between arguments, $R = \{r_1, r_2, \ldots, r_m\}$;
- $P : R \to (0,1]$ is a probability mass function on R, given by $P(r_i) = \Pr[\mathscr{R} = r_i] = p_i$, $\sum_{k=1}^{m} p_k = 1$;
- $G : X \times R \to X$ is a mapping from one argument to another using an element from R;
- $F : X \to \mathbb{R}^+$ is a function that evaluates argument fitness;
- X is reachable through G and R; and
- the dynamics of the system are given by

$$\mathscr{X}(t+1) = Select(\mathscr{X}(t), G(\mathscr{X}(t), \mathscr{R}(t)), N), \tag{18}$$

where $Select : X \times X \times \mathbb{N} \to X$ is a random function such that if $x_1 \in X$ and $x_2 \in X$ are any two arguments, and $N \in \mathbb{N}$ is the *level of selectivity*, then

$$Select(x_1, x_2, N) = \begin{cases} x_1 & \text{with probability } \frac{F(x_1)^N}{F(x_1)^N + F(x_2)^N}, \\ x_2 & \text{with probability } \frac{F(x_2)^N}{F(x_1)^N + F(x_2)^N}. \end{cases} \tag{19}$$

In (18), $\mathscr{X}(t)$ denotes the realization of a random argument at time t, $\mathscr{R}(t)$ denotes the realization of a random element from R at time t, $G(\mathscr{X}(t), \mathscr{R}(t))$ denotes the outcome argument mapped from the realized argument at time t utilizing the element from R at time t, and $\mathscr{X}(0)$ has a known probability mass function.

The *Select* function has a number of interesting properties [12], including, for all N,

$$\frac{\Pr[Select(x_1, x_2, N) = x_1]}{\Pr[Select(x_1, x_2, N) = x_2]} = \left(\frac{F(x_1)}{F(x_2)}\right)^N. \tag{20}$$

That is, the ratio of the probabilities of selecting any two cells is equal to the ratio of their respective fitnesses raised to the power N. This property is called *local rationality*.

Definition 3 Let $\Gamma = (X,R,P,G,F)$ be a SEGS. Let $x_i, x_j \in X$ and $r_k \in R$. The *descendancy tensor, δ,* has elements

$$\delta_{ijk} = \begin{cases} 1 & \text{if } x_j = G(x_i, r_k),\ 1 \le i \le n,\ 1 \le j \le n,\ 1 \le k \le m, \\ 0 & \text{otherwise.} \end{cases} \tag{21}$$

Hence, the descendancy tensor indicates whether it is possible to produce x_j in one step from x_i, using r_k. We can use this tensor to create a matrix that represents the conditional probability of transitioning to x_j from x_i, by utilizing the probability of selecting each available element in R and summing over all m elements as follows.

Definition 4 For the SEGS $\Gamma = (X,R,P,G,F)$, the matrix γ, called the unselective matrix of transition probabilities, has elements

$$\gamma_{ij} = \Pr[\text{offspring is } x_j \mid \text{progenitor is } x_i] = \sum_{k=1}^{m} \delta_{ijk} p_k, \; 1 \le i \le n, \; 1 \le j \le n. \quad (22)$$

This matrix is a stochastic matrix (see [12]).

For the SEGS $\Gamma = (X,R,P,G,F)$, the matrix of transition probabilities, $\mathbf{P}$, has elements

$$P_{ij} = \Pr[\mathscr{X}(t+1) = x_j \mid \mathscr{X}(t) = x_i], \quad (23)$$

$$= \begin{cases} \Pr[Select(x_i,x_j,N) = x_j \mid \mathscr{X}(t) = x_i] \\ \times \Pr[\text{offspring is } x_j \mid \text{progenitor is } x_i], & \forall j \ne i, \\ \\ \Pr[Select(x_i,x_i,N) = x_i \mid \mathscr{X}(t) = x_i] \\ \times \Pr[\text{offspring is } x_i \mid \text{progenitor is } x_i] \\ + \sum_{\substack{k=1 \\ k \ne i}}^{n} \Pr[Select(x_i,x_k,N) = x_i \mid \mathscr{X}(t) = x_i] \\ \times \Pr[\text{offspring is } x_k \mid \text{progenitor is } x_i], & \text{if } j = i. \end{cases} \quad (24)$$

$$= \begin{cases} \frac{1}{1+\left(\frac{F(x_i)}{F(x_j)}\right)^N} \gamma_{ij}, & \forall j \ne i, \\ \gamma_{ii} + \sum_{\substack{j=1 \\ j \ne i}}^{n} \frac{1}{1+\left(\frac{F(x_j)}{F(x_i)}\right)^N} \gamma_{ij}, & \text{if } j = i. \end{cases} \quad (25)$$

The matrix of transition probabilities in (25) is also a stochastic matrix (see [12]).

Theorem 4 *For the ergodic SEGS $\Gamma = (X,R,P,G,F)$, assume that γ is symmetric. Then the Markov chain representing the stochastic dynamics of the ergodic SEGS behaves rationally with fitness F and level N. That is, the row vector $\pi = [\pi_1 \; \pi_2 \; \dots \; \pi_n]$, where π_i satisfies* (10)*, is a left eigenvector of $\mathbf{P}$, the matrix of transition probabilities for Γ, with corresponding eigenvalue 1 (i.e., $\pi\mathbf{P} = \pi$). Hence, π is the vector of stationary probabilities for the SEGS.*

Proof See [12].

The symmetry condition on γ implies that there exists equiprobable forward and reverse transitions between any pair of arguments prior to the selection process.

Theorem 5 *For the ergodic SEGS $\Gamma = (X,R,P,G,F)$, assume that γ is symmetric. Then the Markov chain representing the stochastic dynamics of the ergodic SEGS is time-reversible, i.e.,*

$$\pi_i P_{ij} = \pi_j P_{ji}, \; \forall i, j. \quad (26)$$

Proof See [12].

As a consequence, the Markov chain representing the stochastic dynamics of the SEGS and its time reversed form are statistically the same.

4.2 Barker's Algorithm and SEGS

Comparing a SEGS to the treatment in Section 2, a SEGS has $\mathbf{Q} = \gamma$. For rational behavior, we impose a symmetry condition resulting in $Q_{ij} = Q_{ji}$. Setting $S_{ij} = 1$ in (4), the definition of rational behavior implies that the acceptance probability utilized by the SEGS algorithm is

$$\alpha_{ij} = \frac{1}{1 + \left(\frac{\pi_i}{\pi_j}\right)}. \tag{27}$$

From (8) and (27), Barker's algorithm and the SEGS algorithm are the same.

5 Conclusions

Since Barker's algorithm and the SEGS technique are equivalent, and a SEGS has the capacity for optimal search efficiency by Theorem 3 (which has its hypothesis satisfied by Theorem 4), it follows that Barker's algorithm with an exponential fitness function is optimally search efficient.

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