Proceedings of the 2004 Winter Simulation Conference
R .G. Ingalls, M. D. Rossetti, J. S. Smith, and B. A. Peters, eds.

SIMULATION-BASED OPTIMIZATION USING SIMULATED ANNEALING WITH CONFIDENCE INTERVAL

Talal M. Alkhamis
Mohamed A. Ahmed

Department of Statistics and Operations Research
Kuwait University
P. O. Box 5969, Safat, KUWAIT

ABSTRACT

This paper develops a variant of Simulated Annealing (SA) algorithm for solving discrete stochastic optimization problems where the objective function is stochastic and can be evaluated only through Monte Carlo simulations. In the proposed variant of SA, the Metropolis criterion depends on whether the objective function values indicate statistically significant difference at each iteration. The differences between objective function values are considered to be statistically significant based on confidence intervals associated with these values. Unlike the original SA, our method uses a constant temperature. We show that the configuration that has been visited most often in the first m iterations converges almost surely to a global optimizer.

1 INTRODUCTION

In this paper, we consider a class of optimization problems where the objective function is a stochastic discrete function and can be evaluated only through Monte Carlo simulation. A general problem of discrete stochastic optimization can be defined as

$$\min_{i \in S} f(i) = E[Y(i, \omega)], \tag{1}$$

where S , the search space, is a large, finite, and discrete set; i is the design parameters; $f(i)$ is the performance measure of interest; and $Y(i, \omega)$ represents the sample performance function based on a sample realization ω (ω can be thought of as representing the randomness in the system, e.g., all the random numbers in a simulation run). If the expected value $E[Y(i, \omega)]$ can be found analytically for all i then, (1) represents a deterministic optimization problem which can be solved either analytically or numerically by methods of numerical programming. We are interested in those systems whose $f(i)$ cannot be easily obtained through analytical means and therefore must be estimated from sample paths, e.g., via discrete event simulation. Many real-life systems such as communication networks, computer systems, production systems, transportation networks, reliability systems, flow networks and flexible manufacturing systems can be modeled as discrete-event systems. These systems are driven by the occurrence of discrete events. Due to the complex interactions of such discrete events overtime, the performance analysis and optimization of these systems can be difficult tasks. At the same time, since such systems are becoming more widespread as a result of modern technological advances, it is important to develop efficient methods for optimizing the parameters of these systems.

Simulated annealing (SA) was proposed originally by Kirkpatrick et al. (1983) for solving complex deterministic optimization problems with discrete space. SA has shown successful applications in a wide range of combinatorial optimization problems, and this fact has motivated researchers to use SA in simulation optimization. However SA still needs to evaluate the objective function values accurately, and there have been few theoretical studies for the SA algorithm when the objective function is estimated through simulation.

Gelfand and Mitter (1989) presented a theoretical analysis for the SA algorithm when the objective function includes noise. They showed that under suitable conditions on the noise, the modified annealing algorithm exhibits the same convergence in probability to the globally minimum energy states as the original annealing algorithm. Gutjahr and Pflug (1996) generalized the classical convergence result for the SA algorithm to the case where cost function observations are disturbed by random noise. They showed that for a certain class of noise distributions, the convergence assertion remains valid, provided that the standard deviation of the noise is reduced in the successive steps of cost function evaluation with a speed O($k^{-\gamma}$), where γ is an arbitrary constant larger than one.

Roenko (1990) applied SA algorithm to a stochastic optimization problem. His approach, however, makes it necessary to store all feasible solutions encountered during the execution of the algorithm and to compare them with each newly generated solution. It seems that this approach is not realistic for practical applications due to the computational burden involved.

Alrefaei and Andradottir (1999) presented a modification of the SA algorithm for discrete stochastic optimization problems. Their modification differs from the original SA algorithm in that it uses a constant (rather than decreasing) temperature. Also for estimating the optimal solution they considered two approaches. The first approach uses the number of visits the algorithm makes to the different states (divided by a normalizer) to estimate the optimal solution. The second approach uses the state that has the best average estimated objective function value as an estimate of the optimal solution. They showed that both approaches are guaranteed to converge almost surely to the set of global optimal solutions.

Alkhamis et al. (1999) presented a variant of the SA algorithm for discrete stochastic optimization problems. The basic idea of their modification is to make the comparison between state (solution) *i* and state *j* based on whether the objective function value indicates statistically significant difference at each iteration. The differences between objective function values are considered to be statistically significant based on confidence intervals associated with these values. They showed that under suitable conditions on the random noise, the modified annealing algorithm converges in probability to the set of optimal solutions.

In this paper we present different variant of SA that is based on the approach of Alkhamis et al., but instead of using decreasing temperature we use constant temperature, also for estimating the optimal solution we use the state that is visited most often by the algorithm as the estimated optimal solution (this is similar to the approach proposed by Andradottir (1995, 1996), Alrefaei and Andradottir (1999)). We show that our new variant of SA algorithm converges almost surely to the set of optimal solutions.

The paper is organized as follows. In section 2, we review the original SA algorithm and present our modification of SA to handle objective functions disturbed with noise. Next, in Section 3, we present our convergence proof to the modified annealing algorithm. Finally, section 4 contains some concluding remarks.

2 THE MODIFIED SIMULATED ANNEALING ALGORITHM

2.1 SA with Deterministic Cost Function

In this section, we give a brief description to the original SA algorithm so as to further motivate our modification. To describe SA algorithm we need the following definitions and assumption.

Definition 1 For each $i \in S$ there exists a subset N(i) of S - $\{i\}$ which is called the set of neighbors of i, such that each point in N(i) can be reached from i in a single transition.

Definition 2 A function G : S× S $\rightarrow$ [0,1] is said to be a generating probability function for S and N if

1. $G_{ij} > 0 \Leftrightarrow j \in N(i)$ *and*
2. $\sum_{j \in S} G_{ij} = 1$ *for all* $i, j \in S$.

Here G_{ij} is the probability of generating solution point j as a candidate for the next solution point, when the system is in solution point i. We will consider G_{ij} such that the probability is distributed uniformly over $N(i)$.

Assumption 1 *For any pair* $(i, j) \in S \times S$, j *is reachable from* i, *i.e. there exists a finite sequence,* $\{n_m\}_{m=0}^{\ell}$ *for some* ℓ, *such that* $i_{n_0} = i, i_{n_\ell} = j$ *and* $i_{n_{m+1}} \in N(i_{n_m})$, $m = 0, 1, 2, ..., \ell - 1$.

In SA, one needs a sequence of positive real numbers $\{T_k, k = 0,1,...\}$ satisfying $T_k \geq 0$, $T_{k+1} < T_k \ \forall k$, and $lim_{k \to \infty} T_k = \infty$. T_k is called the temperature at the kth iteration and the sequence $\{T_k, k = 0,1,...\}$ is called the Cooling schedule. The SA algorithm can be described as a sequence of Markov chains with the state space being the domain of the objective function to be minimized. Let X_k denotes the state of the system visited by the SA algorithm at the kth step. Now we state the original simulated annealing algorithm:

Algorithm 1

1. Obtain an initial solution $X_0 \in S$. Set $k = 0$. Obtain an initial temperature $T_k > 0$.
2. Given $X_k = i$, choose a candidate $Z_k \in N(i)$ with probability distribution $P[Z_k = j \mid X_k = i] = G_{ij}$, $j \in N(i)$.
3. Given $Z_k = j$, generate $U_k \sim U[0,1]$, and set

$$X_{k+1} = \begin{cases} Z_k & \text{if } U_k \leq exp\left[\dfrac{-[f(j) - f(i)]^+}{T_k}\right] \\ X_k & \text{otherwise,} \end{cases}$$

(w

here for all $a \in R$, $a^+ = a$ if $a > 0$, and $a^+ = 0$ otherwise)

4. Set $k = k + 1$. Update T_k and go to step 2.

The stochastic random process $\{X_k\}$ produced by the SA algorithm above is a discrete-time inhomogeneous Markov

chain defined over states *S*, and its state transition probability is given by

$$P_{ij}(k) = P[X_{k+1} = j \mid X_k = i]$$
$$= \begin{cases} G_{ij} \min[1, exp\text{-}(f(j) - f(i))/T_k] & if \quad j \in N(i), \\ 1 - \sum_{\ell \in N(i)} P_{i\ell}(T_k) & if \quad i = j, \end{cases} \quad (2)$$

where G_{ij} denotes the generating probability, and $\min[1, exp\text{-}(f(j) - f(i))/T_k]$ denotes the acceptance probability, i.e. the probability of accepting state j, once it is generated from state i, and T_k denotes the temperature control parameter. If we fix the temperature T_k at T, i.e., $T_k = T$, for all k, then the Markov chain constructed by algorithm 1 is a time-homogeneous Markov chain with transition probability matrix P defined as follows:

$$P_{ij} = P[X_{k+1} = j \mid X_k = i]$$
$$= \begin{cases} G_{ij} \min[1, exp\text{-}(f(j) - f(i))/T] & if \quad j \in N(i), \\ 1 - \sum_{\ell \in N(i)} P_{i\ell}(T) & if \quad i = j, \end{cases} \quad (3)$$

The Markov chain, defined in (3), has stationary distribution $\pi(T)$, whose components are given by

$$\pi_i(T) = \frac{|N(i)| \exp(-f(i)/T)}{\sum_{j \in S} |N(j)| \exp(-f(j)/T)}, \quad for\ all\ i \in S. \quad (4)$$

Aarts and Korts (1989), discuss conditions under which the above SA algorithm converges asymptotically to the global minimum.

As it can be seen in algorithm 1, the SA algorithm needs to evaluate the objective function value $f(i)$ accurately. Here we are considering situation where $f(i)$ can only be evaluated via Monte Carlo simulation. Since the input processes driving the simulation are random, the output from the simulation is also random. The runs of the simulation do not directly yield the desired measures of system performance but they only give estimates of the performance measures. Since the estimators are themselves random variables, they are subject to sampling error. Accordingly, SA algorithm must be modified to handle the stochastic nature of the simulation output.

2.2 The Modified SA Algorithm

Now we describe our modified simulated annealing algorithm. On the kth iteration with current configuration (state) i and a candidate configuration j, we generate N_k independent observations of the difference $D_{ji} = Y_j - Y_i$ between the cost of Y_j of state j and the cost Y_i of state i. Let

$$\overline{D}_{ji} = \overline{Y}_j - \overline{Y}_i = \frac{1}{N_k} \sum_{\ell=1}^{N_k} D_{ji}^{\ell}$$

and

$$\hat{\sigma}_k = \frac{1}{\sqrt{N_k}} \sqrt{\frac{1}{N_k - 1} \sum_{\ell=1}^{N_k} (D_{ji}^{\ell} - \overline{D}_{ji})^2}$$

respectively denote the sample mean and sample standard error of the mean based on the observed sample of D_{ji}. Let t_k denote a selected upper critical value of student's t-distribution with $N_k - 1$ degrees of freedom. In the proposed variant of SA, the Metropolis criterion has the form

$$min\left\{1, exp\left[\frac{-[\overline{Y}_j - \overline{Y}_i - t_k \hat{\sigma}_k]}{T}\right]\right\}.$$

The transition matrix for the kth step is given by

$$\widetilde{P}_{ij}(k) = P\{X_{k+1} = j \mid X_k = i\}$$
$$= \begin{cases} G_{ij}\ P\left\{U_k \le \exp\left[\frac{-[\overline{Y}_j - \overline{Y}_i - t_k \hat{\sigma}_k]^+}{T}\right]\right\} & j \in N(i), \\ 1 - \sum_{\ell \in N(i)} P_{i\ell}(k) & j = i, \end{cases} \quad (5)$$

where U_k is a uniform random variable defined on the interval [0,1]. Note that if $j \in N(i)$, then

$$P\left\{U_k \le \exp\left[\frac{-[\overline{Y}_j - \overline{Y}_i - t_k \hat{\sigma}_k]^+}{T}\right]\right\}$$
$$= \mathrm{E}\left\{\exp\left[\frac{-[\overline{Y}_j - \overline{Y}_i - t_k \hat{\sigma}_k]^+}{T}\right]\right\}.$$

Before presenting the modified SA algorithm, we need the following assumption.

Assumption 2 *Let* $\{N_k\}$ *be a sequence of positive integers such that* $N_k \to \infty$ *as* $k \to \infty$.

The steps for the modified SA algorithm are as follows.

Algorithm 2

1. Select a starting point $i_0 \in S$. Let $V_0(i_0) = 1$ and $V_0(j) = 0$ for all $j \in S$, $j \neq i_0$. Let $k = 0$ and $X_k^* = i_0$. Go to step 2.
2. Given $X_k = i$, choose a candidate $Z_k \in N(i)$ with probability distribution $P[Z_k = j \mid X_k = i] = G_{ij}$, $j \in N(i)$.
3. Given $Z_k = j$, generate two N_k independent observations $Y_i^1, Y_i^2, \ldots, Y_i^{N_k}$ and $Y_j^1, Y_j^2, \ldots, Y_j^{N_k}$. Evaluate $\overline{Y}_i, \overline{Y}_j$ *and* $\hat{\sigma}_k$.
4. Given $Z_k = j$, generate $U_k \sim U[0,1]$, and set

$$X_{k+1} = \begin{cases} Z_k & \text{if } U_k \le exp\left[\dfrac{-[\overline{Y}_j - \overline{Y}_i - t_k\hat{\sigma}_k]^+}{T}\right], \\ X_k & \text{otherwise.} \end{cases}$$

5. Set $k = k+1$, $V_k(X_k) = V_{k-1}(X_k) + 1$ and $V_k(j) = V_{k-1}(j)$, for all $j \in S$ and $j \neq X_k$. If $\dfrac{V_k(X_k)}{|N(X_k)|} > \dfrac{V_k(X_{k-1}^*)}{|N(X_{k-1}^*)|}$ then let $X_k^* = X_k$; otherwise let $X_k^* = X_{k-1}^*$. Update N_k,, go to step 2.

The stochastic process $\{X_k, k = 0, 1, 2, \ldots\}$ generated by algorithm 2 is a time inhomogeneous Markov chain with transition matrix given in (5).

3 CONVERGENCE OF THE MODIFIED SA ALGORITHM

In this section we discuss the convergence of our modified SA algorithm and show that our approach is guaranteed to converge almost surly to the set of global optimal solutions.

Proposition 1 $\widetilde{P}_{ij}(k) \to P_{ij}$ *as* $k \to \infty$, *for all* $i, j \in S$ *where* $\widetilde{P}_{ij}(k)$ *and* P_{ij} *are the transition probabilities matrices given in equations* (5) *and* (3) *respectively.*

Proof If $i \neq j$, then $\lim_{k\to\infty} \widetilde{P}_{ij}(k) =$

$$G_{ij} \lim_{k\to\infty} E\left[exp\left[\frac{-[\overline{Y}_j - \overline{Y}_i - t_k\hat{\sigma}_k]^+}{T}\right]\right].$$

Since

$$\left|exp\left[\frac{-[\overline{Y}_j - \overline{Y}_i - t_k\hat{\sigma}_k]^+}{T}\right]\right| \le 1,$$

the bounded convergence theorem gives

$$\begin{aligned} \lim_{k\to\infty} \widetilde{P}_{ij}(k) &= G_{ij} \lim_{k\to\infty} E\left[exp\left[\frac{-[\overline{Y}_j - \overline{Y}_i - t_k\hat{\sigma}_k]^+}{T}\right]\right] \\ &= G_{ij}\ E\left[exp\left[\frac{-[f(j) - f(i)]^+}{T}\right]\right] \\ &= P_{ij} \end{aligned}$$

where the third equality follows from the strong law of large number and the assumption that $N_k \to \infty$ as $k \to \infty$. Note that

$$\frac{1}{N_k - 1}\sum_{\ell=1}^{N_k}(D_{ji}^{\ell} - \overline{D}_{ji})^2 \xrightarrow{p} \sigma_j^2 + \sigma_i^2 \text{ as } N_k \to \infty,$$

therefore

$$\hat{\sigma}_k \xrightarrow{p} 0 \text{ as } N_k \to \infty.$$

Proposition 2 *The Markov chain with the transition matrix P given in equation* (3) *is irreducible, aperiodic and has stationary distribution* $\{\pi_j, j \in S\}$ *given in equation* (4).

Proof Assumptions 1-3 imply that all states can be reached from each other, then the transition probability matrix P is irreducible. To proof that the Markov chain is aperiodic, we need to show that $p_{ii} > 0$. Since periodicity is class properties. Let $i^* \in S^*$ and $i \in N(i^*)$ with $f(i^*) < f(i)$. Then, from the definition of P, $p_{i^*i^*} > 0$ and therefore, P is aperiodic. The proof that $\{\pi_j, j \in S\}$ is the stationary distribution of P can be found in proposition 3.1 in Mitra et al. (1986). Note that, the Markov chain with the transition matrix P is irreducible aperiodic with positive recurrent states, that is, $\pi_j = \underset{n\to\infty}{Lim} P_{ij}^n > 0$. In this case, $\{\pi_j, j \in S\}$ is a stationary distribution and there exists no other stationary distribution.

Lemma 1 (Andradottir (1995), Lemma 3.1)
Suppose that $\{X_k\}$ *is a non-homogeneous Markov chain with a finite state space* S *and transition matrix* $\widetilde{P}_{ij}(k) \to P_{ij}$ *as* $k \to \infty$ *for all* $i, j \in S$ *and* P *is an irreducible and aperiodic Markov chain, let* $g : S \to R$ *be a real valued function on the state space S. Then* $Lim \dfrac{1}{m}\sum_{k=1}^{m} g(X_k) = \sum_{i\in S}\pi_i g(i)$ almost surely *as* $m \to \infty$, where $\{\pi_j, j \in S\}$ is the equilibrium distribution of P.

Corollary 1 *Let*

$$g(X_k) = 1_{\{X_k = j\}} = \begin{cases} 1 & \text{if } X_k = j, \\ 0 & \text{other wise,} \end{cases}$$

then

$$P(\lim_{M\to\infty} \frac{1}{M} \sum_{k=1}^{M} 1_{\{X_{k=j}\}} = \pi_j) = 1.$$

In other words, if we observe the process $\{X_k\}$, the average number of visits to state j during the first M iterations converges to π_j for large M. Note that $V_M(j) = \sum_{k=1}^{M} 1_{\{X_k = j\}}$ which implies that $\frac{V_M(j)}{M}$ asymptotically equals π_j. Now we state and prove the convergence theorem of algorithm 1.

THEOREM 1 *The sequence $\{X_k^*\}$ generated by algorithm 2 converges almost surely to S^*; i.e., $P\{\lim_{k\to\infty} 1_{\{X_k^* = S^*\}} = 1\} = 1$, where S^* is the set that contains the optimal configurations.*

Proof The Markov chain with transition matrix P is irreducible and aperiodic (Aarts and Korst (1989)). By Proposition 1, we have $\widetilde{P}_{ij}(k) \to P_{ij}$ as $k \to \infty$. Suppose that $i \in S^*$ and $j \notin S^*$, then $f(i) \le f(j)$. Then by the definition of π_j, we have $\frac{\pi_j}{|N(j)|} \le \frac{\pi_i}{|N(i)|}$. Since $i \in S^*$ and $j \notin S^*$ are arbitrary, this shows that if $\frac{\pi_i}{|N(i)|} = \max_{\ell \in S} \frac{\pi_\ell}{|N(\ell)|}$, then $i \in S^*$ for all $i \in S$. Let η denotes the difference between the best and the 2nd best of the equilibrium distributions weighted by the size of the neighborhood, i.e., $\eta = \min_{i \in S^*} (\frac{\pi_i}{|N((i)|}) - \max_{j \in \bar{S}^*} (\frac{\pi_j}{|N(j)|})$ where $S^* \subset S$ denote the set of global maximizers and $\bar{S}^* = S - S^*$. Now define $A = \{\omega: P(\lim_{k\to\infty} \frac{V_k(i,\omega)}{k|N(i)|} = \frac{\pi_i}{|N(i)|}) = 1$ for all $i \in S\}$ be such that $P(A) = 1$. Since $P(\lim_{k\to\infty} \frac{V_k(i)}{k|N(i)|} = \frac{\pi_i}{|N(i)|}) = 1$, (by corollary 1), then for almost all ω there exist $k_i(\omega)$ such that $P(\frac{V_k(i)}{k|N(i)|} - \frac{\pi_i}{|N(i)|} < \frac{\eta}{2}, k > k_i(\omega) \forall i \in S) = 1$. Therefore, since $|S| < \infty$, $P(X_k^*(\omega) \in S^*, k > k_\omega^* = \max_i k_i(\omega)) = 1$. Then, $P\{\lim_{k\to\infty} 1_{\{X_k^* = S^*\}} = 1\} = 1$, and this completes the proof.

Corollary 2 *If there is only one point in S^*, i^*, then $X_k^* \to i^*$ as $k \to \infty$ almost surely.*

4 CONCLUSION

In this paper, we have proposed a new variant of Simulated Annealing algorithm for solving discrete stochastic optimization problems where the objective function is stochastic and can be evaluated only through Monte Carlo simulations. This variant is important when either the objective function cannot be computed exactly or such an evaluation is computationally expensive. In the proposed variant, the Metropolis criterion depends on whether the objective function values indicate statistically significant difference at each iteration. The differences between objective function values are considered to be statistically significant based on confidence intervals associated with these values. This new variant uses a convergence criterion where we use the number of visits by the Markov chain generated by the proposed algorithm to the different states to estimate the optimal solution. Unlike the original SA, our method uses a constant temperature and is guaranteed to converge almost surely to a global optimal solution.

REFERENCES

Aarts, E. H. L., and J. Korst. 1989. *Simulated Annealing and Boltzmann Machines.* New York: John Wiley & Sons.

Alkhamis, T. M., M. A. Ahmed, and V. K. Tuan. 1999. Simulated Annealing for Discrete Optimization with Estimation. *European Journal of Operational Research* 116: 530 544.

Alrefaei, M. H., and S. Andradottir. 1999. A simulated Annealing Algorithm with Constant Temperature for Discrete Stochastic Optimization. *Management Science* 45 (5): 748 764.

Andradottir, S. 1995. A Method for Discrete Stochastic Optimization. *Management Science* 41 (12): 1946 1961.

Andradottir, S. 1996. Global Search for Discrete Stochastic Optimization. *SIAM J. Optimization* 6 (2): 513 530.

Gelfand, S. B. and S. K. Mitter. 1989. Simulated Annealing with Noisy or Imprecise Energy Measurements. *Journal of Optimization Theory and Applications* 62: 49 62.

Gutjahr, W. J. and G. C. Pflug. 1996. Simulated Annealing for Noisy Cost Functions. *Journal of Global Optimization* 8: 1 13.

Kirkpatrick, S.,C. D. Gelatt, and M. P. Vecchi. 1983. Optimization by Simulated Annealing. *Science* 221: 671 680.

Mitra, D., F. Romeo, and A. Sangiovanni-Vincentelli. 1986. Convergence and finite-time of simulated annealing. *Adv. Appl. Prob* 18: 747 771.

Roenko N. 1990. Simulated Annealing under Uncertainty. Technical Report, Inst. F. Operations Research, Univ. Zurich.

AUTHOR BIOGRAPHIES

TALAL M. ALKHAMIS is an associate professor in the Department of Statistics and Operations Research at Kuwait University. He received a B.S. in Computer Science & Statistics from Kuwait University, a M.S. in Computer Science, and a Ph.D. in Operations Research from the Florida Institute of Technology. His research interests include discrete Optimization, meta-heuristics, and stochastic optimization. His e-mail address is <alkhamis@kuc01.kuniv.edu.kw>.

MOHAMED A. AHMED is an associate professor in the Department of Statistics and Operations Research at Kuwait University. He received a B.S. in Production Engineering from Helwan University-Egypt, a M.S. and a Ph.D. in Operations Research from George Washington University. His research interests lie in the area of inventory control, simulation, stochastic optimization, and applied probability. His e-mail address is <wakeel@kuc01.kuniv.edu.kw>.