

An Analytically Derived Cooling Schedule
for Simulated Annealing *

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Abstract

We present an analytically derived cooling schedule for a simulated annealing algorithm applicable to both continuous and discrete global optimization problems. An adaptive search algorithm is used to model an idealized version of simulated annealing which is viewed as consisting of a series of Boltzmann distributed sample points. Our choice of cooling schedule ensures linearity in the expected number of sample points needed to become arbitrarily close to a global optimum.

Keywords: simulated annealing, cooling schedule, adaptive search

1 Introduction

Simulated annealing is a stochastic method for searching for global optima of discrete and continuous optimization problems [1, 7, 8, 11]. The origination of simulated annealing is from an analogy with the physical annealing process of finding low energy states of a solid in a heat bath [14]. The algorithm avoids getting trapped in local optima by allowing moves that may lead to a deterioration in objective function value. The probability of accepting a worse candidate point is controlled by a time-dependent temperature parameter, which descends asymptotically to zero in the course of the optimization process. From both practical and theoretical points of view, the cooling schedule for the temperature plays an important role in simulated annealing. Various choices for cooling schedule have been proposed and computationally tested in the literature [3, 6, 9]. Moreover, sufficient conditions for many of these cooling schedules have been established that guarantee convergence to the global optimum [4, 12, 13, 18]. Most conditions simply require the cooling not be too rapid but are otherwise not specific in specifying what rates might lead to the fastest convergence to optimal. Indeed, for globally reaching Markov chain samplers like Hit-and-Run [18, 19], any cooling schedule converging to zero at any rate guarantees convergence to optimal in the limit. In this paper, we

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propose an analytic cooling schedule which leads to a linear in dimension number of sample points.

2 Adaptive Search for Continuous and Discrete Problems

In this paper we derive an adaptive cooling schedule for simulated annealing applicable to both continuous and discrete optimization problems. The cooling schedule strategies are developed based on the adaptive search algorithm introduced by Romeijn and Smith [19]. Adaptive search (AS) is an ideal algorithm that models simulated annealing by assuming points can be sampled according to a sequence of Boltzmann distributions. An attractive property of AS is that the expected number of record values generated by the algorithm increase at most linearly in dimension of the problem for a large class of continuous/discrete optimization problems [19, 23]. In addition, a natural choice of cooling schedule for AS was derived in [19], which maintained the linearity result on the expected number of sample points required for AS for solving a class of convex problems with a quadratic type of objective function. In this paper, we develop a cooling schedule for AS applied to the more general class of Lipschitz objective functions over both continuous and discrete domains. In light of the difficulty of generating Boltzmann distributed points with low temperature values, the cooling schedule attempts to keep the temperature of each AS iteration as high as possible while maintaining a linear complexity in expected number of sample points.

We consider two global optimization programs, one with a continuous domain and one with a discrete domain. The continuous problem is

$$\begin{aligned}
 \text{(P1)} \quad & \max \quad f(x) \\
 & \text{s.t.} \quad x \in S
 \end{aligned}$$

where S is a convex, compact, and full dimensional subset of \mathfrak{R}^n , and the objective function f is a real-valued continuous function defined over S . Let ρ denote the diameter of S . Let x^* be an optimal solution of (P1) and f^* be the global optimum, $f^* = \max_{x \in S} f(x)$. We assume that f satisfies the *Lipschitz condition* with Lipschitz constant K , i.e.,

$$|f(x) - f(y)| \leq K\|x - y\|, \quad \forall x, y \in S, \tag{1}$$

where $\|\cdot\|$ is the Euclidean norm on \mathfrak{R}^n .

The discrete problem is

$$\begin{aligned}
 \text{(P2)} \quad & \max \quad \tilde{f}(\tilde{x}) \\
 & \text{s.t.} \quad \tilde{x} \in \tilde{S}
 \end{aligned}$$

where \tilde{S} is the collection of integer points contained in an n -dimensional hyperrectangle $[a_1, b_1] \times [a_2, b_2] \times \dots \times [a_n, b_n]$, where $a_i \leq b_i$ and $a_i, b_i \in Z$ for $i = 1, \dots, n$. Let $\tilde{\rho}$ denote the largest width of the hyperrectangle, i.e., $\tilde{\rho} = \max_{i=1, \dots, n} (b_i - a_i)$. Let \tilde{x}^* be an optimal solution of (P2) and \tilde{f}^* be the global optimum, $\tilde{f}^* = \max_{\tilde{x} \in \tilde{S}} \tilde{f}(\tilde{x})$. Notice that a condition analogous to the Lipschitz condition is satisfied for (P2), that is

$$|\tilde{f}(\tilde{x}) - \tilde{f}(\tilde{y})| \leq \tilde{K} \max_{i=1, \dots, n} (|\tilde{x}_i - \tilde{y}_i|), \quad \forall \tilde{x}, \tilde{y} \in \tilde{S}, \quad (2)$$

where \tilde{K} is a positive constant and $\tilde{x} = (\tilde{x}_1, \dots, \tilde{x}_n)$, $\tilde{y} = (\tilde{y}_1, \dots, \tilde{y}_n)$. Note that because \tilde{S} is a finite set, a positive constant \tilde{K} exists, with $\tilde{K} \leq \tilde{f}^* - \tilde{f}_*$, where $\tilde{f}_* = \min_{\tilde{x} \in \tilde{S}} \tilde{f}(\tilde{x})$.

We center our attention on adaptive search, introduced in Romeijn and Smith [19], to solve (P1) and (P2). In [19], adaptive search models simulated annealing by assuming points can be exactly sampled according to a sequence of Boltzmann distributions. Adaptive search has an attractive complexity property for solving continuous/discrete global optimization problems. Romeijn and Smith showed in 1994 that the expected number of record values required for adaptive search to solve (P1) over the continuous space S grows linearly in the dimension of the problem [19, Theorem 1]. In 2003, Shen, Zabinsky and Smith [20] (see also [21, 23]) extended the linearity result to a finite domain within an n -dimensional lattice.

Neither Romeijn and Smith [19] nor Shen et al. [20] offer algorithms for computing the cooling schedule whose existence guarantees the linearity result. In this paper, we derive formulas for an analytic cooling schedule guaranteed to result in at most a linear number of temperature changes. If a procedure were to be discovered to sample efficiently from the corresponding Boltzmann distributions, adaptive search would thereby be efficiently implementable through use of this cooling schedule.

2.1 The Adaptive Search Algorithm

Adaptive search [19] is motivated by the idea of approximating the global optimum by generating points according to a sequence of Boltzmann distributions parameterized by decreasing temperatures (see e.g.

Pincus [15], Rubinstein [17]). As the temperature parameter decreases to zero, the Boltzmann distribution concentrates more around the global optimum. To be precise, let $\pi_{f,T}$ be the Boltzmann distribution corresponding to (P1),

$$\pi_{f,T}(S_i) = \frac{\int_{S_i} e^{f(x)/T} dx}{\int_S e^{f(w)/T} dw},$$

and let $\tilde{\pi}_{\tilde{f},\tilde{T}}$ be the Boltzmann distribution corresponding to (P2),

$$\tilde{\pi}_{\tilde{f},\tilde{T}}(\tilde{S}_i) = \frac{\sum_{\tilde{x} \in \tilde{S}_i} e^{\tilde{f}(\tilde{x})/\tilde{T}}}{\sum_{\tilde{w} \in \tilde{S}} e^{\tilde{f}(\tilde{w})/\tilde{T}}},$$

where $S_i \subseteq S$, $\tilde{S}_i \subseteq \tilde{S}$, and T and \tilde{T} are referred to as the *temperature parameters*.

The adaptive search algorithm [19] is stated below.

Adaptive Search (AS)

Step 0: Set $k = 0$. Generate X_0 uniformly over the feasible region. Set $Y_0 = f(X_0)$ and $T_0 = \tau(Y_0)$, where τ is a nonnegative real valued nonincreasing function.

Step 1: Generate Z from the Boltzmann distribution with parameter T_k over the feasible region. If $f(Z) > Y_k$, set $X_{k+1} = Z$. Otherwise, repeat Step 1.

Step 2: Set $Y_{k+1} = f(X_{k+1})$ and set the temperature parameter $T_{k+1} = \tau(Y_{k+1})$. If stopping criteria has not been met, increment k and return to Step 1.

Intermediate points Z generated in step 1 are called trial points or sample points. The sequence $(X_k; k \geq 0)$ is a sequence of record points. Defined in this way, the last sampled point generated by step 1 in each iteration is then a record point (i.e., an improving point). Lastly, the function τ generating the sequence of temperature parameters $(T_k; k \geq 0)$ is called the *cooling schedule*.

The expected number of record points of adaptive search has been shown to increase linearly in the dimension of the problem for both continuous (P1) and discrete (P2) problems [19, 23]. However, the number of sample points needed to obtain a record value needs to be considered to reflect the overall performance of the algorithm. To maintain linear performance, we would like to manipulate the cooling schedule to maintain a constant $(1 - \alpha)$ probability of achieving an improving point. This leads to our choice of cooling schedule.

2.2 Characterization of the Adaptive Search Cooling Schedule

The following principle for a cooling schedule characterizes Adaptive Search (AS).

Choose the temperature for the next iteration of adaptive search so that the probability of generating an improving point under the Boltzmann distribution is at least $1 - \alpha$.

Defining the cooling schedule in this way, the expected number of sample points in each iteration will be $1/(1 - \alpha)$ where $0 \leq \alpha < 1$, independent of the dimension n of the problem. As a result, not only the expected number of record points, but also the expected number of sample points of the adaptive search algorithm will grow linearly in the dimension of the problem. (The task of generating Boltzmann distributed sample points remains of course a challenging task that we will not address here.)

To construct the cooling schedule, we first define the improving region corresponding to the continuous problem (P1) as follows

$$S_{f(X_k)} = \{x \in S : f(x) > f(X_k)\},$$

where X_k is the record point sampled at the k^{th} iteration of AS. And similarly, let \tilde{X}_k be the record point on the k^{th} iteration of AS for solving the discrete problem (P2), and define the corresponding improving region as

$$\tilde{S}_{\tilde{f}(\tilde{X}_k)} = \{\tilde{x} \in \tilde{S} : \tilde{f}(\tilde{x}) > \tilde{f}(\tilde{X}_k)\}.$$

For (P1) with $0 \leq \alpha < 1$, we want to derive the temperature T_k such that the probability of generating an improving point according to the Boltzmann distribution satisfies the following cooling schedule condition

$$\pi_{f, T_k}(S_{f(X_k)}) = \frac{\int_{S_{f(X_k)}} e^{f(x)/T_k} dx}{\int_S e^{f(x)/T_k} dx} \geq 1 - \alpha, \quad (3)$$

and similarly for (P2), find the temperature \tilde{T}_k such that

$$\tilde{\pi}_{\tilde{f}, \tilde{T}_k}(\tilde{S}_{\tilde{f}(\tilde{X}_k)}) = \frac{\sum_{\tilde{x} \in \tilde{S}_{\tilde{f}(\tilde{X}_k)}} e^{\tilde{f}(\tilde{x})/\tilde{T}_k}}{\sum_{\tilde{x} \in \tilde{S}} e^{\tilde{f}(\tilde{x})/\tilde{T}_k}} \geq 1 - \alpha. \quad (4)$$

Note that a temperature close to zero will satisfy the required probability, as in equations (3) and (4). However, for a practical algorithm, in general the lower the temperature, the higher the difficulty to achieve the Boltzmann distribution. In order to be tractable computationally, we want to find the

highest temperature possible that satisfies the required probability. We also want the cooling schedule to be applicable to a broad family of optimization problems since in general little is known about the problem before us. This leads to our worst case approach discussed in the next section.

3 An Analytical Cooling Schedule

In this section, we develop cooling schedules for (P1) and (P2) that satisfy inequalities (3) and (4) respectively, based on a worst case analysis.

3.1 Worst Case Functions

Given the current record value, the temperature consistent with the principle of an adaptive search cooling schedule will be calculated based upon the worst case function among those consistent with the Lipschitz constants K and \tilde{K} respectively.

The worst case functions for the continuous and discrete problems are constructed as follows.

Definition 1 *Given the record point X_k generated at the k^{th} iteration of AS for solving (P1), define a function $h(x)$ over \mathfrak{R}^n as follows*

$$h(x) = \max\{f(X_k), (f^* - K||x - x^*||)\}$$

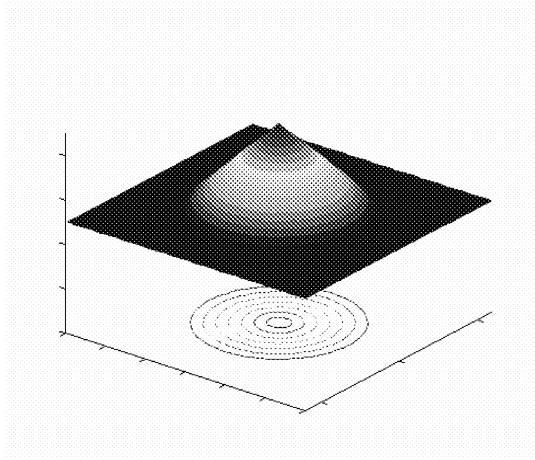
for all $x \in \mathfrak{R}^n$.

Definition 2 *Given the record point \tilde{X}_k generated at the k^{th} iteration of AS for solving (P2), define a function \tilde{h} over Z^n as follows*

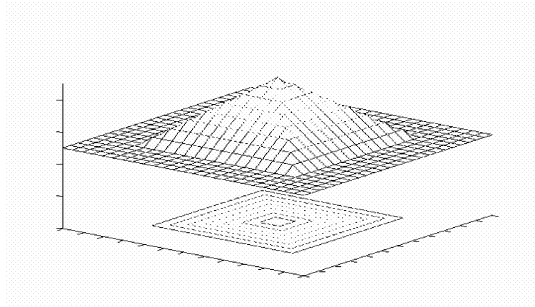
$$\tilde{h}(\tilde{x}) = \max\left\{\tilde{f}(\tilde{X}_k), \left(f^* - \tilde{K} \max_{i=1, \dots, n} (|\tilde{x}_i - \tilde{x}_i^*|)\right)\right\}$$

for all $\tilde{x} \in Z^n$.

An illustration of $h(x)$ and $\tilde{h}(\tilde{x})$ in two dimensions is given in Figure 1.



(1a): Worst case function for continuous problem in two dimensions.



(1b): Worst case function for discrete problem in two dimensions

Figure 1: Worst case functions in two dimensions.

Let $S_{h(X_k)}$ and $\tilde{S}_{\tilde{h}(\tilde{X}_k)}$ denote the improving regions of the h function and \tilde{h} function respectively, i.e.,

$$S_{h(X_k)} = \{x \in S : h(x) > h(X_k)\},$$

$$\tilde{S}_{\tilde{h}(\tilde{X}_k)} = \{\tilde{x} \in \tilde{S} : \tilde{h}(\tilde{x}) > \tilde{h}(\tilde{X}_k)\}.$$

The following theorem states the functions h and \tilde{h} are worse than the original functions f and \tilde{f} , respectively, in the sense that the probability of sampling an improving point with the worst case function is smaller than the probability of sampling an improving point with the original function.

Theorem 1 *Let X_k and \tilde{X}_k be the record points at the k^{th} iteration of AS for solving (P1) and (P2) respectively. Under the same temperature and feasible region, the probability of sampling a point on the improving region according to the Boltzmann distribution corresponding to the worst function is less than*

that of sampling a point on the improving region according to the Boltzmann distribution with respect to the original functions $f(x)$ and $\tilde{f}(\tilde{x})$, i.e.,

$$\pi_{f,T_k}(S_{f(X_k)}) \geq \pi_{h,T_k}(S_{h(X_k)}), \text{ and} \quad (5)$$

$$\tilde{\pi}_{\tilde{f},\tilde{T}_k}(\tilde{S}_{\tilde{f}(\tilde{X}_k)}) \geq \tilde{\pi}_{\tilde{h},\tilde{T}_k}(\tilde{S}_{\tilde{h}(\tilde{X}_k)}). \quad (6)$$

Proof. We only show the proof for the continuous case. The proof for the discrete case is similar. The proof of the theorem relies on Lemma 4, which appears in Appendix A, and states that, for $a, b \in \mathfrak{R}$, $b > a$, $b > 0$, if $c \geq 0$ then $\frac{a+c}{b+c} \geq \frac{a}{b}$.

Let x be any point in the region $S_{h(X_k)}$, where $S_{h(X_k)} = \{x \in S : h(x) > h(X_k)\}$. Then $f(x) \geq h(x)$, where $h(x) = f^* - K\|x - x^*\|$. Because the original objective function $f(x)$ is a Lipschitz function with Lipschitz constant K , we have

$$f^* - f(x) \leq K\|x - x^*\|,$$

which is equivalent to

$$f(x) \geq f^* - K\|x - x^*\|.$$

By the definition of $h(x)$ and the Lipschitz condition, for any $x \in S_{h(X_k)}$, one has $f(x) \geq h(x)$, which implies that

$$S_{h(X_k)} \subseteq S_{f(X_k)}.$$

Next, by applying Lemma 4 and using the facts that $S_{h(X_k)} \subseteq S_{f(X_k)}$ and $f(x) \geq h(x)$ for any $x \in S_{h(X_k)}$, we show that $\pi_{f,T_k}(S_{f(X_k)}) \geq \pi_{h,T_k}(S_{h(X_k)})$.

According to the definition of the Boltzmann distribution, we have,

$$\begin{aligned} \pi_{f,T_k}(S_{f(X_k)}) &= \frac{\int_{S_{f(X_k)}} e^{f(x)/T_k} dx}{\int_S e^{f(x)/T_k} dx} \\ &= \frac{\int_{S_{f(X_k)}} e^{f(x)/T_k} dx}{\int_{S \setminus S_{f(X_k)}} e^{f(x)/T_k} dx + \int_{S_{f(X_k)}} e^{f(x)/T_k} dx} \end{aligned}$$

and applying the fact that $S_{h(X_k)} \subseteq S_{f(X_k)}$, we have,

$$= \frac{\int_{S_{h(X_k)}} e^{f(x)/T_k} dx + \int_{S_{f(X_k)} \setminus S_{h(X_k)}} e^{f(x)/T_k} dx}{\int_{S \setminus S_{f(X_k)}} e^{f(x)/T_k} dx + \int_{S_{h(X_k)}} e^{f(x)/T_k} dx + \int_{S_{f(X_k)} \setminus S_{h(X_k)}} e^{f(x)/T_k} dx}.$$

We apply Lemma 4, $(a + c)/(b + c) \geq a/b$ for $b > a > 0$ and $c > 0$, and use

$$\begin{aligned}
a &= \int_{S_{h(X_k)}} e^{f(x)/T_k} dx + \int_{S_{f(X_k)} \setminus S_{h(X_k)}} e^{f(X_k)/T_k} dx \\
b &= \int_{S \setminus S_{f(X_k)}} e^{f(x)/T_k} dx + \int_{S_{h(X_k)}} e^{f(x)/T_k} dx + \int_{S_{f(X_k)} \setminus S_{h(X_k)}} e^{f(X_k)/T_k} dx \\
c &= \int_{S_{f(X_k)} \setminus S_{h(X_k)}} e^{f(x)/T_k} dx - \int_{S_{f(X_k)} \setminus S_{h(X_k)}} e^{f(X_k)/T_k} dx.
\end{aligned}$$

Note that $c > 0$ because for all $x \in S_{f(X_k)}$, $f(x) \geq f(X_k)$. This yields,

$$\begin{aligned}
\pi_{f, T_k}(S_{f(X_k)}) &\geq \frac{\int_{S_{h(X_k)}} e^{f(x)/T_k} dx + \int_{S_{f(X_k)} \setminus S_{h(X_k)}} e^{f(X_k)/T_k} dx}{\int_{S \setminus S_{f(X_k)}} e^{f(x)/T_k} dx + \int_{S_{h(X_k)}} e^{f(x)/T_k} dx + \int_{S_{f(X_k)} \setminus S_{h(X_k)}} e^{f(X_k)/T_k} dx} \\
&\geq \frac{\int_{S_{h(X_k)}} e^{f(x)/T_k} dx}{\int_{S \setminus S_{f(X_k)}} e^{f(x)/T_k} dx + \int_{S_{h(X_k)}} e^{f(x)/T_k} dx + \int_{S_{f(X_k)} \setminus S_{h(X_k)}} e^{f(X_k)/T_k} dx}.
\end{aligned}$$

We again apply Lemma 4 by setting

$$\begin{aligned}
a &= \int_{S_{h(X_k)}} e^{h(x)/T_k} dx \\
b &= \int_{S \setminus S_{f(X_k)}} e^{f(x)/T_k} dx + \int_{S_{h(X_k)}} e^{h(x)/T_k} dx + \int_{S_{f(X_k)} \setminus S_{h(X_k)}} e^{f(X_k)/T_k} dx \\
c &= \int_{S_{h(X_k)}} e^{f(x)/T_k} dx - \int_{S_{h(X_k)}} e^{h(x)/T_k} dx,
\end{aligned}$$

where $c > 0$ since $f(x) \geq h(x)$ for all $x \in S_{h(X_k)}$. This yields,

$$\pi_{f, T_k}(S_{f(X_k)}) \geq \frac{\int_{S_{h(X_k)}} e^{h(x)/T_k} dx}{\int_{S \setminus S_{f(X_k)}} e^{f(x)/T_k} dx + \int_{S_{h(X_k)}} e^{h(x)/T_k} dx + \int_{S_{f(X_k)} \setminus S_{h(X_k)}} e^{f(X_k)/T_k} dx}$$

and because for all $x \in S \setminus S_{f(X_k)}$, $f(x) \leq f(X_k)$, we have,

$$\begin{aligned}
&\geq \frac{\int_{S_{h(X_k)}} e^{h(x)/T_k} dx}{\int_{S \setminus S_{f(X_k)}} e^{f(X_k)/T_k} dx + \int_{S_{h(X_k)}} e^{h(x)/T_k} dx + \int_{S_{f(X_k)} \setminus S_{h(X_k)}} e^{f(X_k)/T_k} dx} \\
&= \frac{\int_{S_{h(X_k)}} e^{h(x)/T_k} dx}{\int_{S \setminus S_{h(X_k)}} e^{f(X_k)/T_k} dx + \int_{S_{h(X_k)}} e^{h(x)/T_k} dx} \\
&= \pi_{h, T_k}(S_{h(X_k)}).
\end{aligned}$$

Therefore, $\pi_{f, T_k}(S_{f(X_k)}) \geq \pi_{h, T_k}(S_{h(X_k)})$, i.e., $h(x)$ is a function ‘‘worse’’ than the original function $f(x)$. \blacksquare

3.2 Calculation of the Adaptive Search Cooling Schedule

Given the k^{th} record values for (P1) and (P2), we next develop a method to calculate T_k and \tilde{T}_k respectively such that

$$\pi_{h,T_k}(S_{h(X_k)}) \geq 1 - \alpha, \text{ and} \quad (7)$$

$$\tilde{\pi}_{\tilde{h},\tilde{T}_k}(\tilde{S}_{\tilde{h}(\tilde{X}_k)}) \geq 1 - \alpha, \quad (8)$$

for $0 \leq \alpha < 1$. Note that if inequalities (7) and (8) are satisfied with respect to T_k and \tilde{T}_k , then according to Theorem 1, the desired results

$$\pi_{f,T_k}(S_{f(X_k)}) \geq 1 - \alpha \text{ and } \tilde{\pi}_{\tilde{f},\tilde{T}_k}(\tilde{S}_{\tilde{f}(\tilde{X}_k)}) \geq 1 - \alpha$$

are also satisfied.

For both continuous and discrete cases, the probability of sampling the improving region of the worst case function not only depends on the current record value but also depends on the location of the global optimal point. For example, in the continuous case, if x^* is an interior point and $(f^* - f(X_k))/K$ is less than the shortest distance from x^* to the boundary of the feasible set S , then the improving region $S_{h(X_k)}$ is a full n -dimensional ball with center at x^* . But if x^* is located on the boundary of the set S , then no matter how small the value of $(f^* - f(X_k))/K$, $S_{h(X_k)}$ is always a part of the n -dimensional ball. In general, the location of the global point is unknown. The following theory allows a general location of the optimal point, however a tighter bound is possible if some information on the location of the optimal point is known.

Theorem 2 *Consider the program (P1) with the convex feasible region S and the program (P2) with the feasible region \tilde{S} being the collection of integer points contained in an n -dimensional hyperrectangle. Suppose X_k , $f(X_k)$ and T_k are given for current iteration k for (P1) and \tilde{X}_k , $\tilde{f}(\tilde{X}_k)$ and \tilde{T}_k are given for current iteration k for (P2). Define the continuous sets B_θ , B_ρ , $\tilde{B}_{\tilde{\theta}}$ and $\tilde{B}_{\tilde{\rho}}$ as follows*

$$B_\theta = \{x \in \mathfrak{R}^n : \|x - x^*\| \leq (f^* - f(X_k))/K = \theta\}$$

$$B_\rho = \{x \in \mathfrak{R}^n : \|x - x^*\| \leq \rho\}$$

$$\tilde{B}_{\tilde{\theta}} = \{\tilde{x} \in \mathfrak{R}^n : \max_{i=1,\dots,n} |\tilde{x}_i - \tilde{x}_i^*| \leq \lfloor (f^* - \tilde{f}(\tilde{X}_k))/\tilde{K} \rfloor + 0.5 = \tilde{\theta}\}$$

$$\tilde{B}_{\tilde{\rho}} = \{\tilde{x} \in \mathfrak{R}^n : \max_{i=1,\dots,n} |\tilde{x}_i - \tilde{x}_i^*| \leq \tilde{\rho} + 1\}.$$

Then

$$\pi_{h,T_k}(S_{h(X_k)}) \geq \frac{\int_{B_\theta} e^{h(x)/T_k} dx}{\int_{B_\rho} e^{h(x)/T_k} dx} \quad \text{and} \quad \tilde{\pi}_{\tilde{h},\tilde{T}_k}(\tilde{S}_{\tilde{h}(\tilde{X}_k)}) \geq \frac{\sum_{\tilde{x} \in (\tilde{B}_\theta \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k}}{\sum_{\tilde{x} \in (\tilde{B}_\rho \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k}}.$$

Proof. See Appendix B. ■

According to Theorem 2, the probability of sampling the improving region of the worst case function corresponding for the continuous program (P1) is bounded by the probability of sampling the n -dimensional ball B_θ with center x^* over the larger ball B_ρ . And for the discrete program (P2), the probability of sampling the improving region of \tilde{h} is bounded by the probability of sampling the discrete points contained in the n -dimensional hypercube \tilde{B}_θ with center \tilde{x}^* over the discrete domain contained in the hypercube \tilde{B}_ρ . The locations of the optimal points of both continuous and discrete programs do not influence the shapes of B_θ and \tilde{B}_θ , which suggests a way of calculating a lower bound on the probability of sampling the improving region without the knowledge of the optimal point.

We next discuss a method to calculate T_k and \tilde{T}_k respectively such that

$$\frac{\int_{B_\theta} e^{h(x)/T_k} dx}{\int_{B_\rho} e^{h(x)/T_k} dx} \geq 1 - \alpha, \quad \text{and} \quad (9)$$

$$\frac{\sum_{\tilde{x} \in (\tilde{B}_\theta \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k}}{\sum_{\tilde{x} \in (\tilde{B}_\rho \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k}} \geq 1 - \alpha, \quad (10)$$

for $0 \leq \alpha < 1$. Note that if (9) and (10) are satisfied with respect to T_k and \tilde{T}_k , then (7) and (8) are also satisfied by Theorem 2.

We first consider solving for T_k for the continuous problem. The following theorem states that solving for the temperature T_k for the continuous problem to satisfy (9) is equivalent to solving (11) in Theorem 3 for z and using z to determine T_k .

Theorem 3 Consider the continuous problem defined by (P1) with optimal objective function value f^* . Let

$M = \left(\frac{K}{f^* - f(X_k)} \right)^n \cdot \left(\frac{1-\alpha}{\alpha} \right) \cdot \frac{v_n(B_\rho \setminus B_\theta)}{2\pi^{n/2}/\Gamma(\frac{n}{2})}$. Then solving for z that satisfies

$$p_M(z) = (n-1)! - \sum_{i=0}^{n-1} \frac{(n-1)!}{i!} z^i e^{-z} - M z^n e^{-z} \geq 0 \quad (11)$$

and setting $T_k = (f^* - f(X_k))/z$, provides T_k that satisfies the inequality $\frac{\int_{B_\theta} e^{h(x)/T_k} dx}{\int_{B_\rho} e^{h(x)/T_k} dx} \geq 1 - \alpha$.

Proof.

$$\frac{\int_{B_\theta} e^{h(x)/T_k} dx}{\int_{B_\rho} e^{h(x)/T_k} dx} = \frac{\int_{B_\theta} e^{h(x)/T_k} dx}{\int_{B_\rho \setminus B_\theta} e^{h(x)/T_k} dx + \int_{B_\theta} e^{h(x)/T_k} dx}$$

and by definition, $h(x) = f^* - K\|x - x^*\|$ for all $x \in B_\theta$, and $h(x) = f(X_k)$ for all $x \in B_\rho \setminus B_\theta$, thus,

$$\begin{aligned} &= \frac{\int_{B_\theta} e^{(f^* - K\|x - x^*\|)/T_k} dx}{\int_{B_\rho \setminus B_\theta} e^{f(X_k)/T_k} dx + \int_{B_\theta} e^{(f^* - K\|x - x^*\|)/T_k} dx} \\ &= \frac{e^{f^*/T_k} \cdot \int_{B_\theta} e^{-K\|x - x^*\|/T_k} dx}{e^{f(X_k)/T_k} \cdot v_n(B_\rho \setminus B_\theta) + e^{f^*/T_k} \cdot \int_{B_\theta} e^{-K\|x - x^*\|/T_k} dx}. \end{aligned}$$

By substituting $u = x - x^*$ and changing the integration from rectangular coordinates to polar coordinates,

with $G = \{u \in \mathfrak{R}^n : \|u\| \leq (f^* - f(X_k))/K = \theta\}$, we obtain

$$\begin{aligned} \frac{\int_{B_\theta} e^{h(x)/T_k} dx}{\int_{B_\rho} e^{h(x)/T_k} dx} &= \frac{e^{f^*/T_k} \cdot \int_G e^{-K\|u\|/T_k} du}{e^{f(X_k)/T_k} \cdot v_n(B_\rho \setminus B_\theta) + e^{f^*/T_k} \cdot \int_G e^{-K\|u\|/T_k} du} \\ &= \frac{(2\pi^{n/2}/\Gamma(n/2)) \cdot e^{f^*/T_k} \cdot \int_0^\theta r^{n-1} e^{-Kr/T_k} dr}{v_n(B_\rho \setminus B_\theta) \cdot e^{f(X_k)/T_k} + \frac{2\pi^{n/2}}{\Gamma(n/2)} \cdot e^{f^*/T_k} \cdot \int_0^\theta r^{n-1} e^{-Kr/T_k} dr} \end{aligned}$$

Therefore, the inequality $\frac{\int_{B_\theta} e^{h(x)/T_k} dx}{\int_{B_\rho} e^{h(x)/T_k} dx} \geq 1 - \alpha$ is equivalent to

$$\frac{(2\pi^{n/2}/\Gamma(n/2)) \cdot e^{f^*/T_k} \cdot \int_0^\theta r^{n-1} e^{-Kr/T_k} dr}{v_n(B_\rho \setminus B_\theta) \cdot e^{f(X_k)/T_k} + \frac{2\pi^{n/2}}{\Gamma(n/2)} \cdot e^{f^*/T_k} \cdot \int_0^\theta r^{n-1} e^{-Kr/T_k} dr} \geq 1 - \alpha. \quad (12)$$

Carrying out the integration, inequality (12) is,

$$(n-1)! - \sum_{i=0}^{n-1} \frac{(n-1)!}{i!} \left(\frac{f^* - f(X_k)}{T_k} \right)^i e^{(f(X_k) - f^*)/T_k} - \left(\frac{K}{T_k} \right)^n \left(\frac{1-\alpha}{\alpha} \right) \frac{v_n(B_\rho \setminus B_\theta)}{2\pi^{n/2}/\Gamma(\frac{n}{2})} e^{(f(X_k) - f^*)/T_k} \geq 0.$$

Substituting $z = (f^* - f(X_k))/T_k$ and $M = \left(\frac{K}{f^* - f(X_k)} \right)^n \cdot \left(\frac{1-\alpha}{\alpha} \right) \cdot \frac{v_n(B_\rho \setminus B_\theta)}{2\pi^{n/2}/\Gamma(\frac{n}{2})}$ into the above equation, we

have

$$(n-1)! - \sum_{i=0}^{n-1} \frac{(n-1)!}{i!} z^i e^{-z} - M z^n e^{-z} \geq 0.$$

Therefore solving for T_k in inequality $\frac{\int_{B_\theta} e^{h(x)/T_k} dx}{\int_{B_\rho} e^{h(x)/T_k} dx} \geq 1 - \alpha$ is equivalent to solving for z in (11) and setting

$T_k = (f^* - f(X_k))/z$. ■

Theorem 3 transfers the problem of solving for T_k in inequality $\frac{\int_{B_\theta} e^{h(x)/T_k} dx}{\int_{B_\rho} e^{h(x)/T_k} dx} \geq 1 - \alpha$ to the problem of solving for z in Eq. 11. Later in this section, we discuss characteristics of $p_M(z)$. Next, in Theorem 4,

we derive an analogous expression to solve for the temperature \tilde{T}_k in the discrete problem. For the discrete problem, we consider two cases; when there is a single discrete point contained in the region $\tilde{B}_{\tilde{\delta}}$, and when there are several discrete points contained in the region. In the first case, \tilde{T}_k is calculated directly. In the latter case, \tilde{T}_k is calculated using $p_{\tilde{M}}(\tilde{z})$. The proof of Theorem 4 relies on two lemmas, Lemma 4 and Lemma 5, which appear in the appendices.

Theorem 4 Consider the discrete problem defined by (P2) with optimal objective function value \tilde{f}^* . If $\frac{\tilde{f}^* - \tilde{f}(\tilde{X}_k)}{\tilde{K}} < 1$, then $\tilde{T}_k \leq \frac{\tilde{f}^* - \tilde{f}(\tilde{X}_k)}{\ln[\frac{1-\alpha}{|\tilde{B}_{\tilde{\delta}} \cap Z^n| - 1}]}$ solves the inequality $\frac{\sum_{\tilde{x} \in (\tilde{B}_{\tilde{\delta}} \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k}}{\sum_{\tilde{x} \in (\tilde{B}_{\tilde{\delta}} \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k}} \geq 1 - \alpha$. Moreover, if $\frac{\tilde{f}^* - \tilde{f}(\tilde{X}_k)}{\tilde{K}} \geq 1$, setting $\tilde{M} = \left(\frac{\tilde{K}}{\tilde{f}^* - \tilde{f}(\tilde{X}_k)}\right)^n \cdot \left(\frac{1-\alpha}{\alpha}\right) \cdot \frac{|\tilde{B}_{\tilde{\delta}} \cap Z^n| - (2\tilde{\delta})^n}{2^{n \cdot n}}$, with $\hat{f}^* = \tilde{f}^* - 0.5\tilde{K}$ and $|\tilde{B}_{\tilde{\delta}} \cap Z^n|$ representing the number of discrete points contained in the hypercube $\tilde{B}_{\tilde{\delta}}$ and $\tilde{\delta} = \frac{\tilde{f}^* - \tilde{f}(\tilde{X}_k)}{\tilde{K}}$, we have that solving for \tilde{z} satisfying

$$p_{\tilde{M}}(\tilde{z}) = (n-1)! - \sum_{i=0}^{n-1} \frac{(n-1)!}{i!} \tilde{z}^i e^{-\tilde{z}} - \tilde{M} \tilde{z}^n e^{-\tilde{z}} \geq 0 \quad (13)$$

and setting $\tilde{T}_k = (\hat{f}^* - \tilde{f}(\tilde{X}_k))/\tilde{z}$ provides a \tilde{T}_k that satisfies the inequality $\frac{\sum_{\tilde{x} \in (\tilde{B}_{\tilde{\delta}} \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k}}{\sum_{\tilde{x} \in (\tilde{B}_{\tilde{\delta}} \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k}} \geq 1 - \alpha$.

Proof. If $\frac{\tilde{f}^* - \tilde{f}(\tilde{X}_k)}{\tilde{K}} < 1$, then there is only one lattice point, \tilde{x}^* , contained in the hypercube $\tilde{B}_{\tilde{\delta}}$. Hence

$$\frac{\sum_{\tilde{x} \in (\tilde{B}_{\tilde{\delta}} \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k}}{\sum_{\tilde{x} \in (\tilde{B}_{\tilde{\delta}} \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k}} = \frac{e^{\tilde{f}^*/\tilde{T}_k}}{e^{\tilde{f}^*/\tilde{T}_k} + (|\tilde{B}_{\tilde{\delta}} \cap Z^n| - 1)e^{\tilde{f}(\tilde{X}_k)/\tilde{T}_k}} \geq 1 - \alpha,$$

which is equivalent to

$$\tilde{T}_k \leq \frac{\tilde{f}^* - \tilde{f}(\tilde{X}_k)}{\ln[\frac{1-\alpha}{|\tilde{B}_{\tilde{\delta}} \cap Z^n| - 1}]}.$$

Therefore, if $\frac{\tilde{f}^* - \tilde{f}(\tilde{X}_k)}{\tilde{K}} < 1$, $\tilde{T}_k \leq \frac{\tilde{f}^* - \tilde{f}(\tilde{X}_k)}{\ln[\frac{1-\alpha}{|\tilde{B}_{\tilde{\delta}} \cap Z^n| - 1}]}$ solves $\frac{\sum_{\tilde{x} \in (\tilde{B}_{\tilde{\delta}} \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k}}{\sum_{\tilde{x} \in (\tilde{B}_{\tilde{\delta}} \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k}} \geq 1 - \alpha$.

Now consider the case $\frac{\tilde{f}^* - \tilde{f}(\tilde{X}_k)}{\tilde{K}} \geq 1$, which implies

$$\frac{\sum_{\tilde{x} \in (\tilde{B}_{\tilde{\delta}} \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k}}{\sum_{\tilde{x} \in (\tilde{B}_{\tilde{\delta}} \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k}} = \frac{\sum_{\tilde{x} \in (\tilde{B}_{\tilde{\delta}} \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k}}{\sum_{\tilde{x} \in (\tilde{B}_{\tilde{\delta}} \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k} + \sum_{\tilde{x} \in (\tilde{B}_{\tilde{\delta}} \cap Z^n) \setminus (\tilde{B}_{\tilde{\delta}} \cap Z^n)} e^{\tilde{f}(\tilde{X}_k)/\tilde{T}_k}}.$$

We let $m = \lfloor \frac{\tilde{f}^* - \tilde{f}(\tilde{X}_k)}{\tilde{K}} \rfloor$, and since $(\tilde{B}_{\tilde{\delta}} \cap Z^n) = \{\tilde{x} \in Z^n : \max_{i=1, \dots, n} (|\tilde{x}_i - \tilde{x}_i^*|) \leq m\}$, this implies that the number of lattice points contained in the set $\tilde{B}_{\tilde{\delta}}$ is $(2m+1)^n$. Consequently, we have

$$\frac{\sum_{\tilde{x} \in (\tilde{B}_{\tilde{\delta}} \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k}}{\sum_{\tilde{x} \in (\tilde{B}_{\tilde{\delta}} \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k}} = \frac{\sum_{\tilde{x} \in (\tilde{B}_{\tilde{\delta}} \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k}}{\sum_{\tilde{x} \in (\tilde{B}_{\tilde{\delta}} \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k} + \left(|\tilde{B}_{\tilde{\delta}} \cap Z^n| - (2m+1)^n\right) e^{\tilde{f}(\tilde{X}_k)/\tilde{T}_k}}$$

and applying Lemma 4 and Lemma 5 yields

$$\geq \frac{\int_0^{\tilde{\delta}} e^{(\hat{f}^* - u\tilde{K})/\tilde{T}_k} \cdot 2n \cdot (2u)^{n-1} du}{\int_0^{\tilde{\delta}} e^{(\hat{f}^* - u\tilde{K})/\tilde{T}_k} \cdot 2n \cdot (2u)^{n-1} du + \left(|\tilde{B}_{\tilde{\rho}} \cap Z^n| - (2m+1)^n \right) e^{\tilde{f}(\tilde{X}_k)/\tilde{T}_k}}$$

and using the fact that $\tilde{\delta} \leq m + 0.5$, one has

$$\geq \frac{\int_0^{\tilde{\delta}} e^{(\hat{f}^* - u\tilde{K})/\tilde{T}_k} \cdot 2n \cdot (2u)^{n-1} du}{\int_0^{\tilde{\delta}} e^{(\hat{f}^* - u\tilde{K})/\tilde{T}_k} \cdot 2n \cdot (2u)^{n-1} du + \left(|\tilde{B}_{\tilde{\rho}} \cap Z^n| - (2\tilde{\delta})^n \right) e^{\tilde{f}(\tilde{X}_k)/\tilde{T}_k}}.$$

Therefore, if $\frac{\tilde{f}^* - \tilde{f}(\tilde{X}_k)}{\tilde{K}} \geq 1$, \tilde{T}_k can be determined by solving the inequality

$$\frac{\sum_{\tilde{x} \in (\tilde{B}_{\tilde{\rho}} \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k}}{\sum_{\tilde{x} \in (\tilde{B}_{\tilde{\rho}} \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k}} \geq \frac{\int_0^{\tilde{\delta}} e^{(\hat{f}^* - u\tilde{K})/\tilde{T}_k} \cdot 2n \cdot (2u)^{n-1} du}{\int_0^{\tilde{\delta}} e^{(\hat{f}^* - u\tilde{K})/\tilde{T}_k} \cdot 2n \cdot (2u)^{n-1} du + \left(|\tilde{B}_{\tilde{\rho}} \cap Z^n| - (2\tilde{\delta})^n \right) e^{\tilde{f}(\tilde{X}_k)/\tilde{T}_k}} \geq 1 - \alpha.$$

Following the similar method used for proving Theorem 3 and the fact that

$$\int_0^{\tilde{\delta}} e^{(\hat{f}^* - u\tilde{K})/\tilde{T}_k} \cdot 2n \cdot (2u)^{n-1} du = 2^n n \cdot \left(\frac{\tilde{T}_k}{\tilde{K}} \right)^n \cdot \left[(n-1)! - e^{-\tilde{K}\tilde{\delta}/\tilde{T}_k} \sum_{i=0}^{n-1} \frac{(n-1)!}{i!} \left(\tilde{K}\tilde{\delta}/\tilde{T}_k \right)^i \right] \cdot e^{\hat{f}^*/\tilde{T}_k},$$

it is easy to prove that solving for \tilde{T}_k satisfying the second inequality above is equivalent to solving for \tilde{z} in the inequality (13) and setting $\tilde{T}_k = (\hat{f}^* - \tilde{f}(\tilde{X}_k))/\tilde{z}$. ■

Theorem 3 and Theorem 4 provide a way to solve for T_k and \tilde{T}_k for the continuous problem and the discrete problem, respectively. Both theorems are related to the function

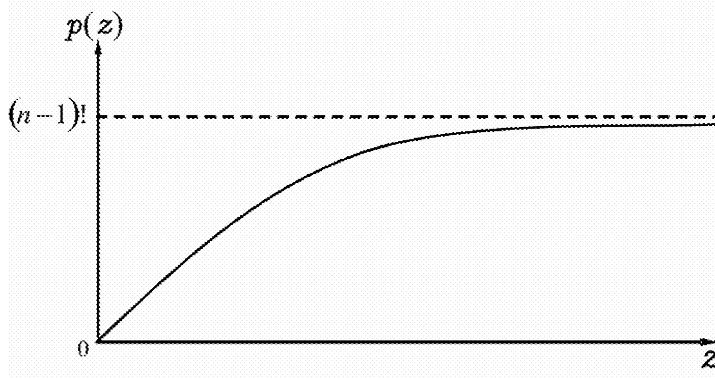
$$p_{\mathcal{M}}(z) = (n-1)! - \sum_{i=0}^{n-1} \frac{(n-1)!}{i!} z^i e^{-z} - \mathcal{M} z^n e^{-z}$$

with $\mathcal{M} = M$ for the continuous problem and $\mathcal{M} = \tilde{M}$ for the discrete problem. Next we discuss the characteristics of the $p_{\mathcal{M}}(z)$ function.

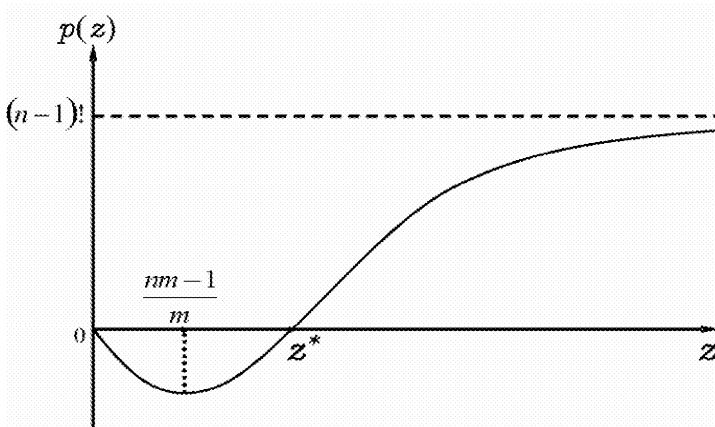
Lemma 1 Consider the function $p_{\mathcal{M}}(z) = (n-1)! - \sum_{i=0}^{n-1} \frac{(n-1)!}{i!} z^i e^{-z} - \mathcal{M} z^n e^{-z}$ with $z \in \mathfrak{R}^+$. Then

- (1) if $n\mathcal{M} \leq 1$, $p_{\mathcal{M}}(z) > 0$ for all $z > 0$;
- (2) if $n\mathcal{M} > 1$, the equation $p_{\mathcal{M}}(z) = 0$ has an unique solution z^* such that $z^* > \frac{n\mathcal{M}-1}{\mathcal{M}}$, and for all $z \geq z^*$ one has $p_{\mathcal{M}}(z) \geq 0$

Proof. The lemma is proved by analyzing the shape of the function $p_{\mathcal{M}}(z)$ corresponding to the parameters n and \mathcal{M} . The detailed proof is given in Appendix D. ■



(2a): the graph of the function $p(z)$ for $n\mathcal{M} \leq 1$.



(2b): the graph of the function $p(z)$ for $n\mathcal{M} > 1$

Figure 2: Two cases of the graph of the function $p(z)$.

According to Lemma 1, finding z such that $p_{\mathcal{M}}(z) \geq 0$ can be separated into two cases based on the parameters n and \mathcal{M} . These two cases are illustrated in figure 2. If $n\mathcal{M} \leq 1$, any positive value of z satisfies $p_{\mathcal{M}}(z) \geq 0$; if $n\mathcal{M} > 1$, any $z \geq z^*$ will satisfy $p_{\mathcal{M}}(z) \geq 0$, where z^* solves equation $p_{\mathcal{M}}(z) = 0$. Lemma 1 guarantees the uniqueness and existence of z^* , which implies that z^* can be calculated numerically by any simple line search algorithm, e.g. bisection. An important issue for those line search algorithms are the choice of initial points, i.e. the upper and lower bounds of z^* . Lemma 1 provides a lower bound, $\frac{n\mathcal{M}-1}{\mathcal{M}} < z^*$. Next, in Lemmas 2 and 3, we present upper bounds on z^* corresponding to the continuous and

discrete problems respectively.

Lemma 2 Consider the continuous problem (P1) and the function

$$p_M(z) = (n-1)! - \sum_{i=0}^{n-1} \frac{(n-1)!}{i!} z^i e^{-z} - M z^n e^{-z}$$

where z and M are defined as in Theorem 3. If $nM > 1$, let z^* be the solution to $p_M(z) = 0$, then

$$z^* \leq \frac{L}{(1-\varepsilon)} \quad (14)$$

where $0 < \varepsilon < 1$, $L = \ln\left(\frac{1-\alpha}{\alpha} \cdot \frac{v_n(B_\rho) - v_n(B_{\hat{\varepsilon}})}{v_n(B_{\hat{\varepsilon}})}\right)$, $0 \leq \alpha < 1$, $B_{\hat{\varepsilon}}$ is an n -dimensional ball with radius $\hat{\varepsilon} = \varepsilon(f^* - f(X_k))/K$ and B_ρ is an n -dimensional ball with radius ρ as defined in Theorem 2.

Proof. See Appendix E. ■

Now we turn to an upper bound on \tilde{z}^* for the discrete problem.

Lemma 3 Consider the discrete problem (P2) and the function

$$p_{\tilde{M}}(\tilde{z}) = (n-1)! - \sum_{i=0}^{n-1} \frac{(n-1)!}{i!} \tilde{z}^i e^{-\tilde{z}} - \tilde{M} \tilde{z}^n e^{-\tilde{z}}$$

where \tilde{z} and \tilde{M} are defined as in Theorem 4. If $\frac{\hat{f}^* - \hat{f}(\tilde{X}_k)}{K} \geq 1$ and $n\tilde{M} > 1$, letting \tilde{z}^* be the solution to $p_{\tilde{M}}(\tilde{z}) = 0$, we have that

$$\tilde{z}^* \leq \frac{\tilde{L}}{(1-\varepsilon)} \quad (15)$$

where $0 < \varepsilon < 1$, $\tilde{L} = \ln\left(\frac{1-\alpha}{\alpha} \cdot \frac{|\tilde{B}_{\tilde{\rho}} \cap Z^n| - (2\varepsilon\tilde{\delta})^n}{(2\varepsilon\tilde{\delta})^n}\right)$, $0 \leq \alpha < 1$, $\tilde{\delta}$ and \hat{f}^* are defined as in Theorem 4, $\tilde{B}_{\tilde{\rho}}$ is defined as in Theorem 2, and $|\tilde{B}_{\tilde{\rho}} \cap Z^n|$ denotes the number of integer points contained in $\tilde{B}_{\tilde{\rho}}$.

Proof. See Appendix E. ■

3.3 Cooling Schedule Strategy

We are now ready to summarize the cooling schedule strategy for the adaptive search algorithm. This cooling schedule strategy ensures that the probability of sampling an improving point is not less than $1 - \alpha$.

Consequently the expected number of record points and sample points is linear in the dimension of the problem. This linearity result assumes that points are sampled according to a Boltzmann distribution. Since generating points according to a Boltzmann distribution is in general more difficult when the temperature is small, we endeavor to keep T_k as high as possible in our cooling schedule strategy.

Cooling Schedule Strategy for (P1):

- Keep $T_k = \infty$ until $nM > 1$, where M is defined in Theorem 3.
- When $nM > 1$, either
 - i*) use a numerical method to calculate z^* by solving $p_M(z) = 0$ as in Theorem 3 Eq. (11) and set $T_k = (f^* - f(X_k))/z^*$, or
 - ii*) use the upper bound on z^* in Lemma 2 Eq. (14) to calculate $T_k = \frac{(1-\epsilon)(f^* - f(X_k))}{L}$, where L is defined in Lemma 2.

Cooling Schedule Strategy for (P2):

- Keep $\tilde{T}_k = \infty$ until $n\tilde{M} > 1$, where \tilde{M} is defined in Theorem 4.
- When $n\tilde{M} > 1$ and $\tilde{f}^* - \tilde{f}(\tilde{X}_k)/\tilde{K} < 1$, set $\tilde{T}_k = \frac{\tilde{f}^* - \tilde{f}(\tilde{X}_k)}{\ln((|\tilde{B}_{\tilde{\sigma}} \cap Z^n| - 1)(1-\alpha)/\alpha)}$.
- When $n\tilde{M} > 1$ and $\tilde{f}^* - \tilde{f}(\tilde{X}_k)/\tilde{K} \geq 1$, either
 - i*) use a numerical method to calculate \tilde{z}^* by solving $p_{\tilde{M}}(\tilde{z}) = 0$ as in Theorem 4 Eq. (13) and set $\tilde{T}_k = (\hat{f}^* - \tilde{f}(\tilde{X}_k))/\tilde{z}^*$, where $\hat{f}^* = \tilde{f}^* - 0.5\tilde{K}$ as defined in Theorem 4, or
 - ii*) use the upper bound on \tilde{z}^* in Lemma 3 Eq. (15) to calculate $\tilde{T}_k = \frac{(1-\epsilon)(\hat{f}^* - \tilde{f}(\tilde{X}_k))}{\tilde{L}}$, where \tilde{L} is defined in Lemma 3.

To implement the cooling schedule strategies, we need to know several pieces of information: dimension n , the current record value $f(X_k)$ or $\tilde{f}(\tilde{X}_k)$, the Lipschitz constant K for (P1) or \tilde{K} for (P2), the optimal value f^* , and the n -dimensional volume of the feasible set. For a specific problem, we certainly know the dimension. At the k^{th} iteration, we also know the record value. The constant K or \tilde{K} is assumed to be

known, but an estimate that is an upper bound may also be used [16]. In general, the maximum function value f^* is unknown. However any lower bound to f^* that exceeds $f(X_k)$ may be used at the sacrifice of a cooler temperature than needed. In the following computational study, we estimate f^* using order statistics as in [18]. Similarly, any upper bound on the volume of the feasible region may be used while maintaining the linearity properties of the resulting cooling schedule.

4 Numerical Results

We have performed a computational study comparing an adaptive cooling schedule with several other cooling schedules on continuous and discrete test problems from the literature. The other cooling schedules include: a cooling schedule proposed by Bohachevsky et al. [5], an exponential cooling schedule [11], and a logarithmic cooling schedule [10]. Several parameters and implementations are considered and are summarized below.

Adaptive Cooling Schedule (summarized in Section 3.3)

$$f^* \text{ known, } \alpha = 0.01, 0.05, 0.9, T_k = \frac{f^* - f(X_k)}{z}$$

$$\hat{f} \text{ estimate, } \alpha = 0.01, 0.05, 0.9, T_k = \frac{\hat{f} - f(X_k)}{z}$$

Fixed Beta Cooling Schedule [5]

$$f^* \text{ known, } \beta = 0.01, 1, 100, T_k = \beta(f^* - f(X_k))$$

$$\hat{f} \text{ estimate, } \beta = 0.01, 1, 100, T_k = \beta(\hat{f} - f(X_k))$$

Exponential Cooling Schedule [11] $T_k = T_0 \gamma^k$

$$T_0 = 0.01, 1, 100 \text{ and } \gamma = 0.01, 0.99$$

Logarithmic Cooling Schedule [10] $T_k = \frac{T_0}{\ln(k+1)}$

$$T_0 = 0.01, 1, 100$$

The adaptive cooling schedule developed in this paper uses the information of f^* . In the computational study, we tested two cases, one is to give a known global optimum, and the other is to estimate and update

\hat{f} during the process of running the algorithm. The estimate \hat{f} for f^* is based on order statistics and was used in [18],

$$\hat{f} = f(X_k) + \frac{f(X_k) - f(X_{k-1})}{(1-q)^{-n/2} - 1}, \quad (16)$$

where $f(X_k)$ and $f(X_{k-1})$ are the first and second best points found so far, n is the dimension of the test problem and we chose $q = 0.1$.

The adaptive cooling schedule is summarized in Section 3.3, where z is calculated every time an improving point is found. The problem specific parameters (including an upper bound on the Lipschitz constant) used in this calculation are summarized with the test problems given in Appendix F. The other parameter specific to this cooling schedule is α , where $1 - \alpha$ is the desired probability of sampling an improving point. Three values of α , 0.01, 0.05 and 0.9, were used in the computational study to represent a spread of values.

The cooling schedule suggested by Bohachevsky et al. [5] has a form $T_k = \beta(f^* - f(X_k))$ where the parameter value of β is chosen at the one set and held constant throughout the algorithm. The temperature is updated every time an improving point is found. This fixed beta cooling schedule was also run when the global optimum f^* is known and when it is estimated with \hat{f} as in Eq. (16). Typically the parameter value β is determined by trial and error, and we used three values of β , 0.01, 1 and 100, where the smallest value was determined by trial and error to provide good performance. The two other values were chosen to represent a spread.

The exponential cooling schedule [11] of the form $T_k = T_0\gamma^k$ was used and the temperature was updated every iteration (in contrast to the previous cooling schedules that updated temperature when an improving point was found). Values of T_0 , 0.01, 1 and 100, and γ , 0.01, 0.99, were chosen by trial and error, and to represent a spread of values.

The logarithmic cooling schedule [10] of the form $T_k = \frac{T_0}{\ln(k+1)}$ was also implemented where temperature was updated every iteration, and three values of T_0 , 0.01, 1 and 100, were used.

The candidate point generator used in the simulated annealing algorithm is from the family of Hit-and-Run methods with continuous and discrete versions [22, 21]. Four test problems, described in Appendix F, were used, two in a continuous form and two in a discrete form. The sinusoidal function was introduced in [24], used in [2], and was motivated by an engineering design problem of composite laminate structures.

For each cooling schedule, 100 runs with random starting points were performed on each test problem. The computational results are shown in the following tables and graphs. Tables 1 to 4 show the performance of the 21 different cooling schedules with parameters for solving test problems 1 to 4, where in each cell the upper integer indicates the number of successful runs out of 100 that achieved a value no worse than the associated y value, and the lower number indicates the average number of function evaluations of the successful runs to achieve the y value. The bold line indicates the parameter value with the best performance. The four graphs show the performance of each cooling schedule with its best parameter value for solving each test problem.

The numerical results indicate that in most of the cases, the adaptive cooling schedule with its best choice of parameter was first or second best compared to the others, and its performance is not very sensitive to the choice of α . The performance of the fixed beta cooling schedule and the logarithmic cooling schedule highly depends on the choice of parameter (among three parameter values, only one of them performs well and the other two have among the four worst performance). And in most of the cases the performance of the fixed beta cooling schedule and the logarithmic cooling schedule with their best choice of parameters (among the three tested values) is worse than that of our adaptive cooling schedule with the best choice of α . The performance of the exponential cooling schedule is very close to the performance of the adaptive cooling schedule. In most of the cases, the performance of adaptive cooling schedule with known f^* is better than the performance using \hat{f} estimated by Eq. (16). For fixed beta cooling schedule, the performance with known f^* for solving two test problems out of four is better than the performance using \hat{f} . A big advantage of our robust adaptive cooling schedule is eliminating the need for trial and error to determine parameter values.

y	2.0	2.2	2.4	2.6	2.8	3.0	3.2
Adap (given f^*) $\alpha=0.01$	100 77.5	100 84.2	100 93.8	100 103.5	100 121.9	98 186.9	65 236.0
Adap (given f^*) $\alpha=0.05$	100 75.5	100 82.2	100 92.0	100 101.3	100 119.4	98 184.8	65 232.8
Adap (given f^*) $\alpha=0.9$	100 74.7	100 82.0	100 91.7	100 100.5	100 118.6	96 172.1	65 230.3
Adap (estimate f^*) $\alpha=0.01$	99 77.2	99 86.6	99 95.5	99 104.5	99 123.9	95 164.8	67 238.1
Adap (estimate f^*) $\alpha=0.05$	99 77.3	99 86.5	99 95.9	99 104.8	99 125.0	95 164.6	67 240.9
Adap (estimate f^*) $\alpha=0.9$	99 69.5	99 78.7	99 90.9	99 100.9	99 121.9	95 170.6	68 240.8
Fixed Beta (given f^*) $\beta=0.01$	100 69.0	100 75.8	100 85.1	100 97.8	100 115.9	98 199.0	60 259.7
Fixed Beta (given f^*) $\beta=1$	100 179.4	100 241.9	98 329.0	98 399.0	95 488.7	85 635.2	31 884.2
Fixed Beta (given f^*) $\beta=100$	99 285.0	95 388.6	89 508.3	71 590.5	38 667.2	14 593.8	0 -
Fixed Beta (estimate f^*) $\beta=0.01$	99 82.0	99 91.2	99 100.3	99 109.2	99 130.3	96 189.3	66 253.3
Fixed Beta (estimate f^*) $\beta=1$	100 118.2	100 149.3	100 188.5	98 272.6	96 375.3	86 520.1	27 536.4
Fixed Beta (estimate f^*) $\beta=100$	100 287.2	96 371.4	92 479.5	72 573.3	40 647.9	16 754.2	0 -
Exp ($\gamma=0.99$) $T0=0.01$	100 68.2	100 75.0	100 83.8	100 96.8	100 113.5	96 189.0	62 229.2
Exp ($\gamma=0.99$) $T0=1$	100 101.7	100 113.4	100 130.8	100 145.2	100 176.7	96 254.0	59 406.0
Exp ($\gamma=0.99$) $T0=100$	100 243.5	100 324.0	100 378.6	100 468.0	100 556.4	96 675.2	68 813.6
Exp ($\gamma=0.01$) $T0=0.01$	100 86.3	100 93.4	100 101.9	100 113.5	100 134.4	95 207.9	61 274.8
Exp ($\gamma=0.01$) $T0=1$	100 88.6	100 95.7	100 103.8	100 115.6	100 135.0	95 204.2	62 269.3
Exp ($\gamma=0.01$) $T0=100$	100 85.4	100 93.2	100 101.8	100 113.3	100 130.8	96 195.3	63 249.0
Log $T0=0.01$	100 79.4	100 86.64	100 95.31	100 107.94	100 129.46	98 215.85	60 251.03
Log $T0=1$	100 72.1	100 82.8	100 90.0	100 99.0	100 128.8	100 212.8	60 597.0
Log $T0=100$	99 272.8	96 360.7	95 501.5	73 603.0	45 735.6	8 976.9	0 -

Table 1: Number of successful runs out of 100 and average number of function evaluations for successful runs for the continuous 6-dimensional Hartmann test problem.

y	0.02	0.04	0.06	0.08	0.10	0.12	0.14	0.16
Adap (given f*) $\alpha=0.01$	100 563.2	100 613.1	100 613.1	100 1080.7	100 1080.7	100 1080.7	100 1081.0	100 1081.0
Adap (given f*) $\alpha=0.05$	100 579.9	100 645.9	100 645.9	100 1095.1	100 1095.1	100 1095.1	100 1095.5	100 1095.5
Adap (given f*) $\alpha=0.9$	100 576.7	100 634.3	100 634.3	100 977.2	100 977.2	100 977.2	100 977.5	100 977.5
Adap (estimate f*) $\alpha=0.01$	100 422.7	100 1861.9	100 1861.9	100 2194.7	100 2194.7	100 2196.1	100 2196.4	100 2196.4
Adap (estimate f*) $\alpha=0.05$	100 430.6	100 1995.1	100 1995.1	100 2347.9	100 2347.9	100 2349.3	100 2349.6	100 2349.6
Adap (estimate f*) $\alpha=0.9$	100 427.6	100 1505.6	100 1505.6	100 1824.9	100 1824.9	100 1826.6	100 1827.5	100 1827.5
Fixed Beta (given f*) $\beta=0.01$	100 557.3	100 953.7	100 953.7	100 1340.9	100 1340.9	100 1341.3	100 1341.4	100 1341.4
Fixed Beta (given f*) $\beta=1$	100 511.7	100 553.9	100 553.9	90 8710.4	90 8710.4	90 8710.4	90 8890.9	90 8890.9
Fixed Beta (given f*) $\beta=100$	100 532.0	100 586.2	100 586.2	88 10131.4	88 10131.4	88 10131.4	86 10512.9	86 10512.9
Fixed Beta (estimate f*) $\beta=0.01$	100 479.1	100 2229.3	100 2229.3	100 2532.8	100 2532.8	100 2533.5	100 2533.9	100 2533.9
Fixed Beta (estimate f*) $\beta=1$	100 584.0	100 623.4	100 623.4	97 7571.8	97 7571.8	97 7571.8	97 7909.4	97 7909.4
Fixed Beta (estimate f*) $\beta=100$	100 517.5	100 574.0	100 574.0	91 10284.4	91 10284.4	91 10395.3	89 10745.5	89 10745.5
Exp ($\gamma=0.99$) T0=0.01	100 405.3	100 1214.7	100 1214.7	100 1468.2	100 1468.2	100 1469.1	100 1469.1	100 1469.1
Exp ($\gamma=0.99$) T0=1	100 422.6	100 792.3	100 792.3	100 1675.1	100 1675.1	100 1676.2	100 1676.5	100 1676.5
Exp ($\gamma=0.99$) T0=100	100 507.2	100 633.0	100 633.0	100 1975.3	100 1975.3	100 1975.6	100 1976.1	100 1976.1
Exp ($\gamma=0.01$) T0=0.01	100 409.9	100 1708.7	100 1708.7	100 1862.2	100 1862.2	100 1863.9	100 1864.6	100 1864.6
Exp ($\gamma=0.01$) T0=1	100 397.2	100 1754.0	100 1754.0	100 1932.7	100 1932.7	100 1935.8	100 1935.9	100 1935.9
Exp ($\gamma=0.01$) T0=100	100 376.0	100 1633.7	100 1633.7	100 1767.3	100 1767.3	100 1769.5	100 1770.0	100 1770.0
Log T0=0.01	100 474.46	100 828.04	100 828.04	100 1172	100 1172	100 1172	100 1172	100 1172
Log T0=1	100 526.5	100 570.4	100 570.4	97 8879.5	97 8879.5	97 8963.0	95 9276.8	95 9276.8
Log T0=100	100 532.0	100 586.2	100 586.2	87 10357.6	87 10357.6	87 10357.6	85 10723.4	85 10723.4

Table 2: Number of successful runs out of 100 and average number of function evaluations for successful runs for the discrete 6-dimensional Hartmann test problem.

γ	1.0	1.5	2.0	2.5	3.0	3.465
Adap (given f*) $\alpha=0.01$	98 921.7	98 953.6	98 1027.3	98 1249.1	91 1733.0	91 3921.8
Adap (given f*) $\alpha=0.05$	100 1206.3	100 1237.9	100 1312.7	100 1532.4	92 1874.9	92 4100.5
Adap (given f*) $\alpha=0.9$	99 1089.9	99 1123.6	99 1208.0	99 1614.6	93 2245.2	93 4438.5
Adap (estimate f*) $\alpha=0.01$	100 775.1	91 1228.5	91 1297.2	91 1496.1	87 1569.7	87 3858.6
Adap (estimate f*) $\alpha=0.05$	100 775.2	91 1228.9	91 1297.3	91 1498.6	87 1575.2	87 3858.3
Adap (estimate f*) $\alpha=0.9$	100 775.4	91 1229.1	91 1297.4	91 1496.6	87 1576.3	87 3810.4
Fixed Beta (given f*) $\beta=0.01$	100 1281.8	100 1315.0	100 1413.5	100 1865.1	96 2171.1	95 3875.1
Fixed Beta (given f*) $\beta=1$	100 2951.3	71 18540.4	2 18918.0	0 -	0 -	0 -
Fixed Beta (given f*) $\beta=100$	100 3345.3	61 20012.7	3 14022.3	0 -	0 -	0 -
Fixed Beta (estimate f*) $\beta=0.01$	100 695.7	91 893.4	91 960.5	91 1166.2	86 1396.6	86 3691.6
Fixed Beta (estimate f*) $\beta=1$	100 1016.0	99 2314.1	82 10498.8	43 15589.3	14 16582.1	1 10178.0
Fixed Beta (estimate f*) $\beta=100$	100 3339.4	69 19613.0	2 14795.0	0 -	0 -	0 -
Exp ($\gamma =0.99$) T0=0.01	100 1061.4	89 1847.1	89 1911.0	89 2130.4	83 2664.6	83 4866.9
Exp ($\gamma =0.99$) T0=1	100 440.1	97 670.8	97 754.1	97 985.2	93 1231.5	93 3260.9
Exp ($\gamma =0.99$) T0=100	100 864.6	99 995.8	99 1078.3	99 1298.9	96 1549.8	96 3544.3
Exp ($\gamma =0.01$) T0=0.01	100 828.6	87 1078.8	87 1139.9	87 1339.8	82 1676.5	82 3968.4
Exp ($\gamma =0.01$) T0=1	100 932.7	88 1334.1	88 1400.8	88 1610.4	83 1750.9	83 4021.9
Exp ($\gamma =0.01$) T0=100	100 1504.8	90 2975.2	90 3039.1	90 3231.2	84 3488.3	84 5671.4
Log T0=0.01	95 934.65	89 2126.3	89 2190	89 2392.8	85 2907.4	85 5157.8
Log T0=1	100 380.8	100 579.0	100 958.7	100 4593.9	100 11367.0	0 -
Log T0=100	100 3148.0	64 19023.1	2 23262.0	0 -	0 -	0 -

Table 3: Number of successful runs out of 100 and average number of function evaluations for successful runs for the continuous 10-dimensional sinusoidal test problem.

y	1.0	1.5	2.0	2.5	3.0	3.5
Adap (given f^*) $\alpha=0.01$	100 115.7	100 183.6	100 318.7	100 774.4	100 2742.3	99 19620.0
Adap (given f^*) $\alpha=0.05$	100 113.3	100 173.3	100 319.2	100 748.8	100 2143.8	100 19224.9
Adap (given f^*) $\alpha=0.9$	100 116.5	100 179.4	100 330.7	100 758.8	100 1874.6	100 19168.4
Adap (estimate f^*) $\alpha=0.01$	100 126.6	100 211.1	100 441.6	100 942.5	100 3570.8	98 20583.9
Adap (estimate f^*) $\alpha=0.05$	100 126.6	100 211.1	100 441.6	100 942.5	100 3568.7	98 20506.9
Adap (estimate f^*) $\alpha=0.9$	100 127.2	100 210.8	100 440.1	100 931.4	100 3651.2	98 20614.6
Fixed Beta (given f^*) $\beta=0.01$	100 97.0	100 157.3	100 324.3	100 769.8	100 3653.7	97 18951.3
Fixed Beta (given f^*) $\beta=1$	100 2373.1	95 17530.7	2 9485.0	0 -	0 -	0 -
Fixed Beta (given f^*) $\beta=100$	100 2315.3	71 17855.8	2 38299.5	0 -	0 -	0 -
Fixed Beta (estimate f^*) $\beta=0.01$	100 126.7	100 220.3	100 529.9	100 1058.2	100 4495.2	99 21273.5
Fixed Beta (estimate f^*) $\beta=1$	100 409.9	100 2337.5	91 9870.0	51 15599.2	17 23929.1	0 -
Fixed Beta (estimate f^*) $\beta=100$	100 2591.9	82 16956.9	3 14490.0	0 -	0 -	0 -
Exp ($\gamma=0.99$) $T0=0.01$	100 89.4	100 141.1	100 252.9	100 649.3	100 1873.8	100 18070.1
Exp ($\gamma=0.99$) $T0=1$	100 282.6	100 362.1	100 503.9	100 1018.6	100 2684.4	99 18907.2
Exp ($\gamma=0.99$) $T0=100$	100 623.0	100 777.5	100 923.6	100 1300.0	99 2755.5	99 19854.8
Exp ($\gamma=0.01$) $T0=0.01$	100 94.5	100 155.0	100 342.4	100 944.5	100 3842.8	100 18963.1
Exp ($\gamma=0.01$) $T0=1$	100 92.9	100 162.6	100 493.0	100 925.7	99 2017.6	99 16976.1
Exp ($\gamma=0.01$) $T0=100$	100 97.4	100 193.0	100 411.9	100 1024.4	98 4122.0	96 18207.5
Log $T0=0.01$	100 104.05	100 171.37	100 361.37	100 954.48	100 3285.4	99 20734
Log $T0=1$	100 350.0	100 512.9	100 893.9	100 5455.3	100 14410.8	0 -
Log $T0=100$	100 2764.1	86 18294.6	3 37474.7	0 -	0 -	0 -

Table 4: Number of successful runs out of 100 and average number of function evaluations for successful runs for the discrete 10-dimensional sinusoidal test problem.

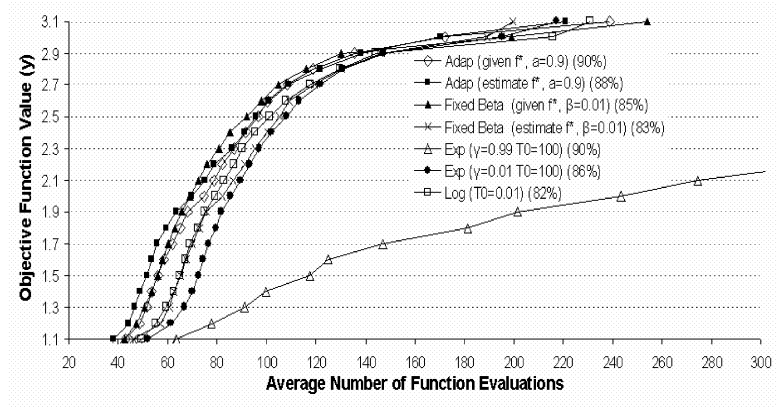


Figure 3: Average number of function evaluations v.s. function value for the continuous 6-dimensional Hartmann6 test problem.

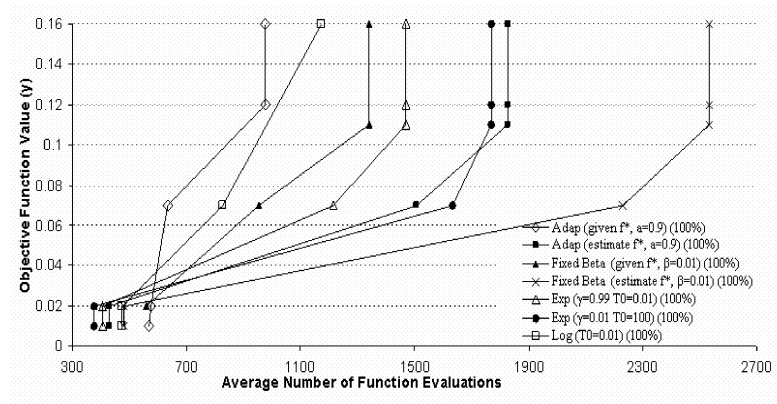


Figure 4: average number of function evaluations for successful runs for the discrete 6-dimensional Hartmann6 test problem.

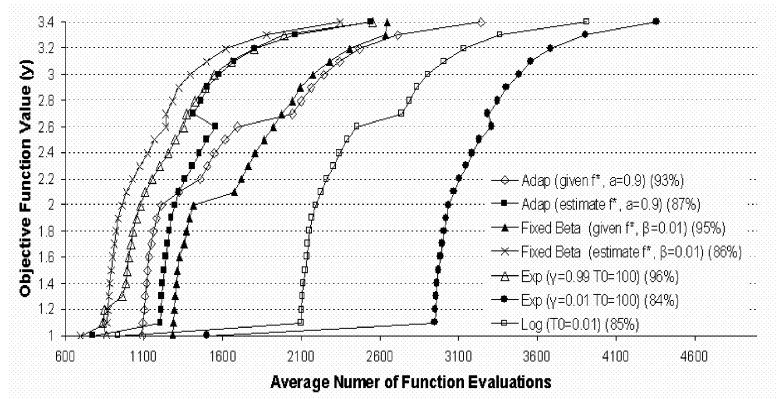


Figure 5: average number of function evaluations for successful runs for the continuous 10-dimensional sinusoidal test problem.

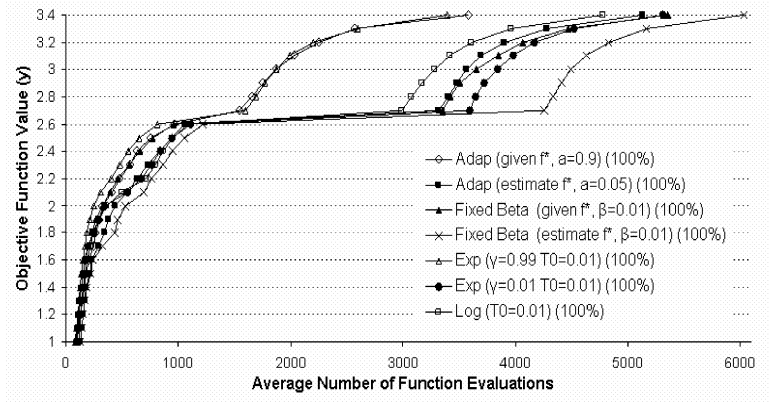


Figure 6: average number of function evaluations for successful runs for the discrete 10-dimensional sinusoidal test problem.

5 Summary and Conclusion

Simulated annealing is a class of sequential probabilistic search techniques for solving global optimization problems. The performance of simulated annealing is highly dependent on the choice of cooling schedule employed. In this paper, we consider an algorithm called adaptive search (AS) which is designed to model an idealized version of simulated annealing by assuming points can be sampled exactly according to a sequence of Boltzmann distributions. The paper focuses on analytically deriving cooling schedule strategies for AS applied to a general class of optimization problems over continuous and discrete domains. By choosing the temperature to guarantee an improvement with probability no less than $1 - \alpha$, the cooling schedule maintains the linear in complexity property for the expected number of sample points required by AS to solve this class of global optimization problems. Some numerical results demonstrate an effective implementation of the theoretical adaptive cooling schedule.

Appendix A

The following lemma is important for proving the results of Theorems 1, 4 and Lemma 3.

Lemma 4 For all $a, b \in \Re$ such that $b > a$ and $b > 0$, if $c \geq 0$, then

$$\frac{a+c}{b+c} \geq \frac{a}{b}.$$

Appendix B

Proof of Theorem 2

Proof. We first prove the result for continuous case, i.e.,

$$\pi_{h,T_k}(S_{h(X_k)}) \geq \frac{\int_{B_\theta} e^{h(x)/T_k} dx}{\int_{B_\rho} e^{h(x)/T_k} dx}.$$

Recall that

$$\pi_{h,T_k}(S_{h(X_k)}) = \frac{\int_{S_{h(X_k)}} e^{h(x)/T_k} dx}{\int_S e^{h(x)/T_k} dx}.$$

Therefore proving Theorem 2 is equivalent to proving

$$\frac{\int_{S_{h(X_k)}} e^{h(x)/T_k} dx}{\int_{B_\theta} e^{h(x)/T_k} dx} \geq \frac{\int_S e^{h(x)/T_k} dx}{\int_{B_\rho} e^{h(x)/T_k} dx}. \quad (17)$$

First we will prove that

$$\frac{v_n(B_\rho \setminus B_\theta)}{v_n(S \setminus S_{h(X_k)})} \geq \frac{v_n(B_\theta)}{v_n(S_{h(X_k)})}, \quad (18)$$

where $v_n(\cdot)$ is the n -dimensional volume of a set. The inequality (18) will be used to prove (17). According to the argument given in [25, Page 335], we have,

$$\frac{v_n(S_{h(X_k)})}{v_n(S)} \geq \frac{v_n(B_\theta)}{v_n(B_\rho)},$$

which is equivalent to

$$\frac{v_n(B_\rho)}{v_n(B_\theta)} - 1 \geq \frac{v_n(S)}{v_n(S_{h(X_k)})} - 1,$$

and considering the fact that $B_\theta \subseteq B_\rho$ and $S_{h(X_k)} \subseteq S$, we have

$$\frac{v_n(B_\rho \setminus B_\theta)}{v_n(B_\theta)} \geq \frac{v_n(S \setminus S_{h(X_k)})}{v_n(S_{h(X_k)})},$$

hence,

$$\frac{v_n(B_\rho \setminus B_\theta)}{v_n(S \setminus S_{h(X_k)})} \geq \frac{v_n(B_\theta)}{v_n(S_{h(X_k)})}. \quad (19)$$

Now consider the left-hand side of (17). We have,

$$\frac{\int_{S_{h(X_k)}} e^{h(x)/T_k} dx}{\int_{B_\theta} e^{h(x)/T_k} dx} = \frac{\left(\int_{S_{h(X_k)}} e^{h(x)/T_k} dx \right) \left(\int_{S_{h(X_k)}} e^{h(x)/T_k} dx + \int_{S \setminus S_{h(X_k)}} e^{f(X_k)/T_k} dx \right)}{\left(\int_{B_\theta} e^{h(x)/T_k} dx \right) \left(\int_{S_{h(X_k)}} e^{h(x)/T_k} dx + \int_{S \setminus S_{h(X_k)}} e^{f(X_k)/T_k} dx \right)}$$

$$= \frac{\int_{S_{h(X_k)}} e^{h(x)/T_k} dx + \int_{S \setminus S_{h(X_k)}} e^{f(X_k)/T_k} dx}{\int_{B_\theta} e^{h(x)/T_k} dx + \frac{\int_{B_\theta} e^{h(x)/T_k} dx}{\int_{S_{h(X_k)}} e^{h(x)/T_k} dx} v_n(S \setminus S_{h(X_k)}) e^{f(X_k)/T_k}.$$

According to the fact that $S_{h(X_k)} \subseteq B_\theta$ and applying Lemma 4.1 given in [23] with $T_k < T_\infty$, we have

$\frac{\int_{S_{h(X_k)}} e^{h(x)/T_k} dx}{\int_{B_\theta} e^{h(x)/T_k} dx} \geq \frac{v_n(S_{h(X_k)})}{v_n(B_\theta)}$. Therefore,

$$\frac{\int_{S_{h(X_k)}} e^{h(x)/T_k} dx}{\int_{B_\theta} e^{h(x)/T_k} dx} \geq \frac{\int_{S_{h(X_k)}} e^{h(x)/T_k} dx + \int_{S \setminus S_{h(X_k)}} e^{f(X_k)/T_k} dx}{\int_{B_\theta} e^{h(x)/T_k} dx + \frac{v_n(B_\theta)}{v_n(S_{h(X_k)})} v_n(S \setminus S_{h(X_k)}) e^{f(X_k)/T_k}},$$

and because of the fact that $\frac{v_n(B_\rho \setminus B_\theta)}{v_n(S \setminus S_{h(X_k)})} \geq \frac{v_n(B_\theta)}{v_n(S_{h(X_k)})}$ in inequality (19), we have

$$\begin{aligned} \frac{\int_{S_{h(X_k)}} e^{h(x)/T_k} dx}{\int_{B_\theta} e^{h(x)/T_k} dx} &\geq \frac{\int_{S_{h(X_k)}} e^{h(x)/T_k} dx + \int_{S \setminus S_{h(X_k)}} e^{f(X_k)/T_k} dx}{\int_{B_\theta} e^{h(x)/T_k} dx + \frac{v_n(B_\rho \setminus B_\theta)}{v_n(S \setminus S_{h(X_k)})} v_n(S \setminus S_{h(X_k)}) e^{f(X_k)/T_k}} \\ &= \frac{\int_{S_{h(X_k)}} e^{h(x)/T_k} dx + \int_{S \setminus S_{h(X_k)}} e^{f(X_k)/T_k} dx}{\int_{B_\theta} e^{h(x)/T_k} dx + v_n(B_\rho \setminus B_\theta) e^{f(X_k)/T_k}} \\ &= \frac{\int_{S_{h(X_k)}} e^{h(x)/T_k} dx + \int_{S \setminus S_{h(X_k)}} e^{f(X_k)/T_k} dx}{\int_{B_\theta} e^{h(x)/T_k} dx + \int_{B_\rho \setminus B_\theta} e^{f(X_k)/T_k} dx} \\ &= \frac{\int_S e^{h(x)/T_k} dx}{\int_{B_\rho} e^{h(x)/T_k} dx} \end{aligned}$$

Hence

$$\pi_{h, T_k}(S_{h(X_k)}) = \frac{\int_{S_{h(X_k)}} e^{h(x)/T_k} dx}{\int_S e^{h(x)/T_k} dx} \geq \frac{\int_{B_\theta} e^{h(x)/T_k} dx}{\int_{B_\rho} e^{h(x)/T_k} dx}.$$

Next, we prove the result for discrete case, i.e.,

$$\tilde{\pi}_{\tilde{h}, \tilde{T}_k}(\tilde{S}_{\tilde{h}(\tilde{X}_k)}) \geq \frac{\sum_{\tilde{x} \in (\tilde{B}_\theta \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k}}{\sum_{\tilde{x} \in (\tilde{B}_\rho \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k}}. \quad (20)$$

To prove the result, we first prove that

$$\frac{|\tilde{S}_{\tilde{h}(\tilde{X}_k)}|}{|\tilde{S}|} \geq \frac{|\tilde{B}_\theta \cap Z^n|}{|\tilde{B}_\rho \cap Z^n|}. \quad (21)$$

And then given the inequality (21), inequality (20) can be proved following the same procedure used for the continuous case.

Let \tilde{B} be a continuous set composed of the union of hypercubes surrounding all integer points in \tilde{S} , and let $\tilde{B}_{\tilde{h}(\tilde{X}_k)}$ be the continuous set composed of the union of hypercubes surrounding all integer points in $\tilde{S}_{\tilde{h}(\tilde{X}_k)}$, i.e.,

$$\tilde{B} = \{x \in \mathbb{R}^n : \text{Round}(x) \in \tilde{S}\}$$

$$\tilde{B}_{\tilde{h}(\tilde{X}_k)} = \{x \in \mathfrak{R}^n : \text{Round}(x) \in \tilde{S}_{\tilde{h}(\tilde{X}_k)}\}.$$

Since we assume that \tilde{S} is a discrete region over a hyperrectangle, according to the definition of \tilde{h} , the improving set $\tilde{S}_{\tilde{h}(\tilde{X}_k)}$ is also a discrete hyperrectangular region. Therefore,

$$\frac{|\tilde{S}_{\tilde{h}(\tilde{X}_k)}|}{|\tilde{S}|} = \frac{v_n(\tilde{B}_{\tilde{h}(\tilde{X}_k)})}{v_n(\tilde{B})}.$$

Now consider the four continuous sets, \tilde{B} , $\tilde{B}_{\tilde{h}(\tilde{X}_k)}$, $\tilde{B}_{\tilde{\theta}}$ and $\tilde{B}_{\tilde{\rho}}$. We know that \tilde{B} is a convex set, $\tilde{B}_{\tilde{h}(\tilde{X}_k)} \in \tilde{B}$, $\tilde{B}_{\tilde{\theta}}$ and $\tilde{B}_{\tilde{\rho}}$ are hyperrectangles with center \tilde{x}^* , and $\tilde{B}_{\tilde{h}(\tilde{X}_k)} \subseteq \tilde{B}_{\tilde{\theta}}$, $\tilde{B} \subseteq \tilde{B}_{\tilde{\rho}}$ and $\tilde{B}_{\tilde{\theta}} \subseteq \tilde{B}_{\tilde{\rho}}$. According to the argument given in [25, Page 335], we have,

$$\frac{v_n(\tilde{B}_{\tilde{h}(\tilde{X}_k)})}{v_n(\tilde{B})} \geq \frac{v_n(\tilde{B}_{\tilde{\theta}})}{v_n(\tilde{B}_{\tilde{\rho}})},$$

and

$$\frac{v_n(\tilde{B}_{\tilde{\theta}})}{v_n(\tilde{B}_{\tilde{\rho}})} = \frac{|\tilde{B}_{\tilde{\theta}} \cap Z^n|}{|\tilde{B}_{\tilde{\rho}} \cap Z^n|},$$

because $\tilde{B}_{\tilde{\theta}}$ and $\tilde{B}_{\tilde{\rho}}$ are defined such that the volume of each set equals the number of discrete points contained in the set. Therefore,

$$\frac{|\tilde{S}_{\tilde{h}(\tilde{X}_k)}|}{|\tilde{S}|} \geq \frac{|\tilde{B}_{\tilde{\theta}} \cap Z^n|}{|\tilde{B}_{\tilde{\rho}} \cap Z^n|}.$$

We have now proved equation (21). Following the same procedure used for the continuous case we could further prove the desired result for the discrete case in Theorem 2. ■

Appendix C

This appendix contains a lemma used in the proof of Theorem 4. Based on the definition of $\tilde{h}(x)$, the following lemma holds.

Lemma 5 *Given the current record value \tilde{X}_k , one has,*

$$\begin{aligned} \text{if } \lfloor \frac{\tilde{f}^* - f(\tilde{X}_k)}{\tilde{K}} \rfloor < 1, \quad \sum_{\tilde{x} \in (\tilde{B}_{\tilde{\theta}} \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k} &= e^{\tilde{f}^*/\tilde{T}_k}, \\ \text{otherwise,} \quad \sum_{\tilde{x} \in (\tilde{B}_{\tilde{\theta}} \cap Z^n)} e^{\tilde{h}(\tilde{x})/\tilde{T}_k} &\geq \int_0^{\tilde{\delta}} e^{(\tilde{f}^* - u\tilde{K})/\tilde{T}_k} 2n \cdot (2u)^{n-1} du, \end{aligned}$$

where $\hat{f}^* = \tilde{f}^* - 0.5\tilde{K}$ and $\tilde{\delta} = \frac{\hat{f}^* - f(\tilde{X}_k)}{\tilde{K}}$.

Proof. As defined in Theorem 2, the set $(\tilde{B}_{\tilde{\delta}} \cap Z^n)$ is an n -dimensional hypercube with center at \tilde{x}^* and the length of each side is $2(\tilde{f}^* - \tilde{f}(\tilde{X}_k))/\tilde{K}$, i.e.,

$$\tilde{B}_{\tilde{\delta}} \cap Z^n = \{\tilde{x} \in Z^n : \max_{i=1, \dots, n} (|\tilde{x}_i - \tilde{x}_i^*|) \leq (\tilde{f}^* - \tilde{f}(\tilde{X}_k))/\tilde{K}\}, \quad (22)$$

and because \tilde{x}^* must also be integer,

$$\tilde{B}_{\tilde{\delta}} \cap Z^n = \{\tilde{x} \in Z^n : \max_{i=1, \dots, n} (|\tilde{x}_i - \tilde{x}_i^*|) \leq \lfloor (\tilde{f}^* - \tilde{f}(\tilde{X}_k))/\tilde{K} \rfloor\}.$$

Obviously, if $\lfloor (\tilde{f}^* - \tilde{f}(\tilde{X}_k))/\tilde{K} \rfloor < 1$, there is only one integer point in $\tilde{B}_{\tilde{\delta}}$. Hence one has

$$\sum_{\tilde{x} \in \tilde{B}_{\tilde{\delta}} \cap Z^n} e^{\tilde{h}(\tilde{x})/\tilde{T}_k} = e^{\tilde{f}^*/\tilde{T}_k}.$$

For $\lfloor (\tilde{f}^* - \tilde{f}(\tilde{X}_k))/\tilde{K} \rfloor \geq 1$, let $m = \lfloor (\tilde{f}^* - \tilde{f}(\tilde{X}_k))/\tilde{K} \rfloor$, and for a given $j \in \{1, \dots, m\}$, define S_j , a subset of $\tilde{B}_{\tilde{\delta}} \cap Z^n$, as follows

$$S_j = \{\tilde{x} \in Z^n : \max_{i=1, \dots, n} (|\tilde{x}_i - \tilde{x}_i^*|) = j\},$$

i.e., S_j is a collection of lattice points contained on the surface of the box $[\tilde{x}_1^* - j, \tilde{x}_1^* + j] \times \dots \times [\tilde{x}_n^* - j, \tilde{x}_n^* + j]$.

According to the definition of \tilde{h} , one has $\tilde{h}(\tilde{x}) = \tilde{f}^* - j\tilde{K}$ for all $\tilde{x} \in S_j$. Therefore

$$\sum_{\tilde{x} \in \tilde{B}_{\tilde{\delta}} \cap Z^n} e^{\tilde{h}(\tilde{x})/\tilde{T}_k} = e^{\tilde{f}^*/\tilde{T}_k} + \sum_{j=1}^m (|S_j| e^{(\tilde{f}^* - j\tilde{K})/\tilde{T}_k}), \quad (23)$$

where $|S_j|$ represents the number of lattice points contained in the set S_j .

To calculate $|S_j|$, we first define the rounding region of lattice point. Let the box $B_{\tilde{x}} = [\tilde{x}_1 - 0.5, \tilde{x}_1 + 0.5] \times \dots \times [\tilde{x}_n - 0.5, \tilde{x}_n + 0.5]$ denote the rounding region of the lattice point \tilde{x} , i.e., $B_{\tilde{x}}$ is an n -dimensional hypercube of unit length with \tilde{x} being the center of the hypercube. Since $v_n(B_{\tilde{x}}) = 1$, one has

$$|S_j| = \sum_{\tilde{x} \in S_j} v_n(B_{\tilde{x}}) = v_n(\cup_{\tilde{x} \in S_j} B_{\tilde{x}}),$$

$$\cup_{\tilde{x} \in S_j} B_{\tilde{x}} = \{\tilde{x} \in \mathfrak{R}^n : j - 0.5 \leq \max_{i=1, \dots, n} (|\tilde{x}_i - \tilde{x}_i^*|) \leq j + 0.5\}.$$

Now considering two boxes $B_L = [\tilde{x}_1^* - j + 0.5, \tilde{x}_1^* + j - 0.5] \times \dots \times [\tilde{x}_n^* - j + 0.5, \tilde{x}_n^* + j - 0.5]$ and $B_U = [\tilde{x}_1^* - j - 0.5, \tilde{x}_1^* + j + 0.5] \times \dots \times [\tilde{x}_n^* - j - 0.5, \tilde{x}_n^* + j + 0.5]$, one has

$$v_n(\cup_{\tilde{x} \in S_j} B_{\tilde{x}}) = v_n(B_U \setminus B_L) = v_n(B_U) - v_n(B_L) = (2j + 1)^n - (2j - 1)^n,$$

where the second equality follows from the fact $B_L \subset B_U$. Hence

$$|S_j| = (2j+1)^n - (2j-1)^n. \quad (24)$$

Thus, by applying equation (24) to equation (23), we get that

$$\sum_{\tilde{x} \in \tilde{B}_{\tilde{\theta}} \cap Z^n} e^{\tilde{h}(\tilde{x})/\tilde{T}_k} = e^{\tilde{f}^*/\tilde{T}_k} + \sum_{j=1}^m ((2j+1)^n - (2j-1)^n) e^{(\tilde{f}^* - j\tilde{K})/\tilde{T}_k}.$$

Considering that

$$\begin{aligned} \int_{j-0.5}^{j+0.5} e^{(\tilde{f}^* - j\tilde{K})/\tilde{T}_k} \cdot 2n \cdot (2u)^{n-1} du &= e^{(\tilde{f}^* - j\tilde{K})/\tilde{T}_k} \int_{j-0.5}^{j+0.5} d(2u)^n \\ &= ((2j+1)^n - (2j-1)^n) e^{(\tilde{f}^* - j\tilde{K})/\tilde{T}_k}, \end{aligned}$$

and because $[\tilde{f}^* - \tilde{f}(\tilde{X}_k)]/\tilde{K} \geq 1$, one has

$$\sum_{\tilde{x} \in \tilde{B}_{\tilde{\theta}} \cap Z^n} e^{\tilde{h}(\tilde{x})/\tilde{T}_k} = e^{\tilde{f}^*/\tilde{T}_k} + \sum_{j=1}^m \left(\int_{j-0.5}^{j+0.5} e^{(\tilde{f}^* - j\tilde{K})/\tilde{T}_k} \cdot 2n \cdot (2u)^{n-1} du \right),$$

and because $\tilde{f}^* - j\tilde{K} \geq \tilde{f}^* - (u+0.5)\tilde{K} = \hat{f}^* - u\tilde{K}$ for all $u \in [j-0.5, j+0.5]$ and where $\hat{f}^* = \tilde{f}^* - 0.5\tilde{K}$,

one has

$$\begin{aligned} &\geq e^{\tilde{f}^*/\tilde{T}_k} + \sum_{j=1}^m \left(\int_{j-0.5}^{j+0.5} e^{(\hat{f}^* - u\tilde{K})/\tilde{T}_k} \cdot 2n \cdot (2u)^{n-1} du \right) \\ &= \int_0^{0.5} e^{\tilde{f}^*/\tilde{T}_k} \cdot 2n \cdot (2u)^{n-1} du + \int_{0.5}^{m+0.5} e^{(\hat{f}^* - u\tilde{K})/\tilde{T}_k} \cdot 2n \cdot (2u)^{n-1} du \end{aligned}$$

and apply the fact that $\tilde{f}^* > \tilde{f}^* - (u+0.5)\tilde{K} = \hat{f}^* - u\tilde{K}$ for all $u \in [0, 0.5]$, one has

$$\begin{aligned} &> \int_0^{0.5} e^{(\hat{f}^* - u\tilde{K})/\tilde{T}_k} \cdot 2n \cdot (2u)^{n-1} du + \int_{0.5}^{m+0.5} e^{(\hat{f}^* - u\tilde{K})/\tilde{T}_k} \cdot 2n \cdot (2u)^{n-1} du \\ &= \int_0^{m+0.5} e^{(\hat{f}^* - u\tilde{K})/\tilde{T}_k} \cdot 2n \cdot (2u)^{n-1} du \end{aligned}$$

and since $m+0.5 = \lfloor \frac{\tilde{f}^* - \tilde{f}(\tilde{X}_k)}{\tilde{K}} \rfloor + 0.5 \geq \frac{\tilde{f}^* - \tilde{f}(\tilde{X}_k)}{\tilde{K}} - 1 + 0.5$, one has

$$\geq \int_0^{\frac{\tilde{f}^* - \tilde{f}(\tilde{X}_k)}{\tilde{K}} - 0.5} e^{(\hat{f}^* - u\tilde{K})/\tilde{T}_k} \cdot 2n \cdot (2u)^{n-1} du$$

and setting $\tilde{\delta} = \frac{\tilde{f}^* - \tilde{f}(\tilde{X}_k)}{\tilde{K}} = \frac{\hat{f}^* - \tilde{f}(\tilde{X}_k)}{\tilde{K}} - 0.5$, yields the result,

$$\geq \int_0^{\tilde{\delta}} e^{(\hat{f}^* - u\tilde{K})/\tilde{T}_k} \cdot 2n \cdot (2u)^{n-1} du.$$

■

Appendix D

Proof of Lemma 1

Proof. We prove the lemma by analyzing the shape of the function $p_{\mathcal{M}}(z)$. According to the definition, z is a one-dimensional positive variable. It is easy to prove that $\lim_{z \rightarrow 0} p_{\mathcal{M}}(z) = 0$. Next let us look at the limit of $p_{\mathcal{M}}(z)$ as z goes to infinity,

$$\lim_{z \rightarrow \infty} p_{\mathcal{M}}(z) = (n-1)! - \lim_{z \rightarrow \infty} \sum_{i=0}^{n-1} \frac{(n-1)!}{i!} \frac{z^i}{e^z} - \lim_{z \rightarrow \infty} \mathcal{M} \frac{z^n}{e^z}.$$

Because $\frac{z^i}{e^z} \rightarrow 0$ as $z \rightarrow \infty$, for all i , we can see that

$$\lim_{z \rightarrow \infty} p_{\mathcal{M}}(z) = (n-1)!.$$

Now consider the derivative of $p_{\mathcal{M}}(z)$,

$$p'_{\mathcal{M}}(z) = \frac{dp(z)}{dz} = (1 - n\mathcal{M})z^{n-1}e^{-z} + \mathcal{M}z^n e^{-z}.$$

If $n\mathcal{M} \leq 1$, for z positive, one has $p'_{\mathcal{M}}(z) > 0$. In this case, we have,

$$(1) \quad \lim_{z \rightarrow 0} p_{\mathcal{M}}(z) = 0$$

$$(2) \quad \lim_{z \rightarrow \infty} p_{\mathcal{M}}(z) = (n-1)!$$

$$(3) \quad p'_{\mathcal{M}}(z) > 0$$

which implies that the function $p_{\mathcal{M}}(z)$ is monotonically increasing and concave as depicted in figure (1a).

Therefore the value of $p_{\mathcal{M}}(z)$ is positive for $z > 0$.

On the other hand, if $n\mathcal{M} > 1$, i.e., $n\mathcal{M} - 1 > 0$, we have,

$$p'_{\mathcal{M}}(z) \begin{cases} < 0 & \text{if } 0 < z < (n\mathcal{M} - 1)/\mathcal{M} \\ = 0 & \text{if } z = (n\mathcal{M} - 1)/\mathcal{M} \\ > 0 & \text{if } z > (n\mathcal{M} - 1)/\mathcal{M}. \end{cases}$$

According to the property of $p'_{\mathcal{M}}(z)$ for the case $n\mathcal{M} > 1$, and the fact that $\lim_{z \rightarrow 0} p_{\mathcal{M}}(z) = 0$ and $\lim_{z \rightarrow \infty} p_{\mathcal{M}}(z) = (n-1)! > 0$, one can draw the function shape of $p_{\mathcal{M}}(z)$, as shown in Figure (1b). Therefore, for $n\mathcal{M} > 1$, the equation $p_{\mathcal{M}}(z) = 0$ with $z > 0$ has a unique solution z^* .

The lower bound of z^* , i.e. $z^* \geq \frac{n\mathcal{M}-1}{\mathcal{M}}$, is immediate from the fact that $\lim_{z \rightarrow 0} p_{\mathcal{M}}(z) = 0$, $\lim_{z \rightarrow \infty} p_{\mathcal{M}}(z) = (n-1)! > 0$ and the property of $p'_{\mathcal{M}}(z) = 0$ at $z = (n\mathcal{M}-1)/\mathcal{M}$. ■

Appendix E

Proof of Lemma 2

Proof. According to Theorem 3, solving for T^* in $\frac{\int_{B_\theta} e^{h(x)/T_k} dx}{\int_{B_\rho} e^{h(x)/T_k} dx} = 1 - \alpha$ is equivalent to solving for z^* in $p_{\mathcal{M}}(z^*) = 0$ and setting $T^* = (f^* - f(X_k))/z^*$. Therefore, to prove that $L/(1-\varepsilon)$ is an upper bound on z^* , we prove an associated lower bound on T^* .

To establish the lower bound on T^* , for $0 < \varepsilon < 1$, we define a function $g : B_\rho \rightarrow \Re$ by

$$g(x) = \begin{cases} f^* - \varepsilon(f^* - f(X_k)) & \text{if } x \in B_{\hat{\varepsilon}}, \\ f(X_k) & \text{if } x \in B_\rho \setminus B_{\hat{\varepsilon}}, \end{cases}$$

where $B_{\hat{\varepsilon}} = \{x \in B_\rho : \|x - x^*\| < \hat{\varepsilon} = \varepsilon(f^* - f(X_k))/K\}$. Then $h(x) \geq g(x)$ on B_θ , but $h(x) = g(x)$ on $B_\rho \setminus B_\theta$. Also $B_{\hat{\varepsilon}} \subseteq B_\theta$. Following the same arguments in the proof of Theorem 1, one can show that

$$\frac{\int_{B_\theta} e^{h(x)/T_k} dx}{\int_{B_\rho} e^{h(x)/T_k} dx} \geq \frac{\int_{B_{\hat{\varepsilon}}} e^{g(x)/T_k} dx}{\int_{B_\rho} e^{g(x)/T_k} dx}.$$

Now consider $\frac{\int_{B_{\hat{\varepsilon}}} e^{g(x)/T_k} dx}{\int_{B_\rho} e^{g(x)/T_k} dx}$, we have

$$\begin{aligned} \frac{\int_{B_{\hat{\varepsilon}}} e^{g(x)/T_k} dx}{\int_{B_\rho} e^{g(x)/T_k} dx} &= \frac{\int_{B_{\hat{\varepsilon}}} e^{(f^* - \varepsilon(f^* - f(X_k)))/T_k} dx}{\int_{B_\rho \setminus B_{\hat{\varepsilon}}} e^{f(X_k)/T_k} dx + \int_{B_{\hat{\varepsilon}}} e^{(f^* - \varepsilon(f^* - f(X_k)))/T_k} dx} \\ &= \frac{v_n(B_{\hat{\varepsilon}}) \cdot e^{(f^* - \varepsilon(f^* - f(X_k)))/T_k}}{(v_n(B_\rho) - v_n(B_{\hat{\varepsilon}})) \cdot e^{f(X_k)/T_k} + v_n(B_{\hat{\varepsilon}}) \cdot e^{(f^* - \varepsilon(f^* - f(X_k)))/T_k}}. \end{aligned}$$

After algebraic manipulations, it can be seen that if we let

$$T^l = \frac{(1-\varepsilon)(f^* - f(X_k))}{L}$$

where

$$L = \ln \left(\frac{1-\alpha}{\alpha} \cdot \frac{v_n(B_\rho) - v_n(B_{\hat{\varepsilon}})}{v_n(B_{\hat{\varepsilon}})} \right)$$

then T^l satisfies

$$\frac{\int_{B_\theta} e^{h(x)/T^l} dx}{\int_{B_\rho} e^{h(x)/T^l} dx} \geq \frac{\int_{B_{\hat{\varepsilon}}} e^{g(x)/T^l} dx}{\int_{B_\rho} e^{g(x)/T^l} dx} = 1 - \alpha.$$

Since T^* is the solution to $\frac{\int_{B_\theta} e^{h(x)/T_k} dx}{\int_{B_\rho} e^{h(x)/T_k} dx} = 1 - \alpha$, and we have

$$\frac{\int_{B_\theta} e^{h(x)/T^l} dx}{\int_{B_\rho} e^{h(x)/T^l} dx} \geq \frac{\int_{B_\theta} e^{h(x)/T^*} dx}{\int_{B_\rho} e^{h(x)/T^*} dx},$$

we know

$$T^l \leq T^*$$

(also see [19, Proposition 3.9]). Thus T^l is a lower bound on T^* , and equivalently, $\frac{L}{1-\varepsilon}$ is an upper bound on z^* . ■

Proof of Lemma 3

Proof. According to Theorem 4, solving for \tilde{z}^* in $p_{\tilde{M}}(\tilde{z}) = 0$ is equivalent to solving for \tilde{T}^* in the equation

$$\frac{\int_0^{\tilde{\delta}} e^{(\hat{f}^* - u\tilde{K})/\tilde{T}_k} \cdot 2n \cdot (2u)^{n-1} du}{\int_0^{\tilde{\delta}} e^{(\hat{f}^* - u\tilde{K})/\tilde{T}_k} \cdot 2n \cdot (2u)^{n-1} du + \left(|\tilde{B}_{\tilde{\rho}} \cap Z^n| - (2\tilde{\delta})^n \right) e^{\tilde{f}(\tilde{X}_k)/\tilde{T}_k}} = 1 - \alpha, \quad (25)$$

and setting $\tilde{z}^* = (\tilde{f}^* - \tilde{f}(\tilde{X}_k))/\tilde{T}^*$, where $\tilde{\delta} = \frac{\hat{f}^* - \tilde{f}(\tilde{X}_k)}{\tilde{K}}$. Therefore, to prove that $\tilde{L}/(1 - \varepsilon)$ is an upper bound on \tilde{z}^* , we can equivalently prove an associated lower bound on \tilde{T}^* .

To establish the lower bound on \tilde{T}^* , we first define a function $\hat{h}(x)$ and sets \hat{S} and \tilde{G} so we can write Eq. (25) as

$$\frac{\int_{\tilde{G}} e^{\hat{h}(x)/\tilde{T}_k} dx}{\int_{\hat{S}} e^{\hat{h}(x)/\tilde{T}_k} dx} = \frac{\int_0^{\tilde{\delta}} e^{(\hat{f}^* - u\tilde{K})/\tilde{T}_k} \cdot 2n \cdot (2u)^{n-1} du}{\int_0^{\tilde{\delta}} e^{(\hat{f}^* - u\tilde{K})/\tilde{T}_k} \cdot 2n \cdot (2u)^{n-1} du + \left(|\tilde{B}_{\tilde{\rho}} \cap Z^n| - (2\tilde{\delta})^n \right) e^{\tilde{f}(\tilde{X}_k)/\tilde{T}_k}} = 1 - \alpha$$

where $\hat{S} = \{x \in \mathfrak{R}^n : \text{Round}(x) \in (\tilde{B}_{\tilde{\rho}} \cap Z^n)\}$, $\tilde{G} = \{x \in \hat{S} : \max_{i=1, \dots, n} (|x_i - \tilde{x}_i^*|) \leq (\hat{f}^* - \tilde{f}(\tilde{X}_k))/\tilde{K}\}$ and

$$\hat{h}(x) = \begin{cases} \hat{f}^* - \tilde{K} \max_{i=1, \dots, n} (|x_i - \tilde{x}_i^*|) & \text{if } x \in \tilde{G} \\ \tilde{f}(\tilde{X}_k) & \text{if } x \in \hat{S} \setminus \tilde{G} \end{cases}.$$

For $0 < \varepsilon < 1$, we now define a set \tilde{G}_ε and a function $\tilde{g}(x)$ as

$$\tilde{G}_\varepsilon = \{x \in \hat{S} : \max_{i=1, \dots, n} (|x_i - \tilde{x}_i^*|) \leq \hat{\varepsilon} = \varepsilon(\hat{f}^* - \tilde{f}(\tilde{X}_k))/\tilde{K}\}$$

$$\tilde{g}(x) = \begin{cases} \hat{f}^* - \varepsilon(\hat{f}^* - \tilde{f}(\tilde{X}_k)) & \text{if } x \in \tilde{G}_\varepsilon \\ \tilde{f}(\tilde{X}_k) & \text{if } x \in \hat{S} \setminus \tilde{G}_\varepsilon \end{cases}$$

so that

$$\frac{\int_{\tilde{G}} e^{\hat{h}(x)/\tilde{T}_k} dx}{\int_{\hat{S}} e^{\hat{h}(x)/\tilde{T}_k} dx} \geq \frac{\int_{\tilde{G}_\varepsilon} e^{\tilde{g}(x)/\tilde{T}_k} dx}{\int_{\hat{S}} e^{\tilde{g}(x)/\tilde{T}_k} dx}.$$

This is true because $\tilde{G}_\varepsilon \subseteq \tilde{G}$ and $\hat{h}(x) \geq \tilde{g}(x)$ for $x \in \tilde{G}$, and $\hat{h}(x) = \tilde{g}(x)$ for $x \in \hat{S} \setminus \tilde{G}$. Now we have

$$\begin{aligned} \frac{\int_{\tilde{G}_\varepsilon} e^{\tilde{g}(x)/\tilde{T}_k} dx}{\int_{\hat{S}} e^{\tilde{g}(x)/\tilde{T}_k} dx} &= \frac{\int_{\tilde{G}_\varepsilon} e^{(\hat{f}^* - \varepsilon(\hat{f}^* - \tilde{f}(\tilde{X}_k)))/\tilde{T}_k} dx}{\int_{\hat{S} \setminus \tilde{G}_\varepsilon} e^{\tilde{f}(\tilde{X}_k)/\tilde{T}_k} dx + \int_{\tilde{G}_\varepsilon} e^{(\hat{f}^* - \varepsilon(\hat{f}^* - \tilde{f}(\tilde{X}_k)))/\tilde{T}_k} dx} \\ &= \frac{v_n(\tilde{G}_\varepsilon) \cdot e^{(\hat{f}^* - \varepsilon(\hat{f}^* - \tilde{f}(\tilde{X}_k)))/\tilde{T}_k}}{(v_n(\hat{S}) - v_n(\tilde{G}_\varepsilon)) \cdot e^{\tilde{f}(\tilde{X}_k)/\tilde{T}_k} + v_n(\tilde{G}_\varepsilon) \cdot e^{(\hat{f}^* - \varepsilon(\hat{f}^* - \tilde{f}(\tilde{X}_k)))/\tilde{T}_k}}, \end{aligned}$$

where $v_n(\tilde{G}_\varepsilon) = (2\varepsilon \cdot \tilde{\delta})^n$ and $v_n(\hat{S}) = |\tilde{B}_\rho \cap Z^n| = |\tilde{S}|$. After algebraic manipulations, it can be seen that if

we let

$$\tilde{T}^l = \frac{(1 - \varepsilon)(\hat{f}^* - \tilde{f}(\tilde{X}_k))}{\tilde{L}},$$

where

$$\tilde{L} = \ln\left(\frac{1 - \alpha}{\alpha} \cdot \frac{|\tilde{S}| - (2\varepsilon\tilde{\delta})^n}{(2\varepsilon\tilde{\delta})^n}\right)$$

then \tilde{T}^l satisfies

$$\frac{\int_{\tilde{G}} e^{\hat{h}(x)/\tilde{T}^l} dx}{\int_{\hat{S}} e^{\hat{h}(x)/\tilde{T}^l} dx} \geq \frac{\int_{\tilde{G}_\varepsilon} e^{\tilde{g}(x)/\tilde{T}^l} dx}{\int_{\hat{S}} e^{\tilde{g}(x)/\tilde{T}^l} dx} = 1 - \alpha.$$

Since \tilde{T}^* is the solution to $\frac{\int_{\tilde{G}} e^{\hat{h}(x)/\tilde{T}_k} dx}{\int_{\hat{S}} e^{\hat{h}(x)/\tilde{T}_k} dx} = 1 - \alpha$, and we have

$$\frac{\int_{\tilde{G}} e^{\hat{h}(x)/\tilde{T}^l} dx}{\int_{\hat{S}} e^{\hat{h}(x)/\tilde{T}^l} dx} \geq \frac{\int_{\tilde{G}} e^{\hat{h}(x)/\tilde{T}^*} dx}{\int_{\hat{S}} e^{\hat{h}(x)/\tilde{T}^*} dx},$$

we know

$$\tilde{T}^l \leq \tilde{T}^*$$

(also see [19, Proposition 3.9]). Thus \tilde{T}^l is a lower bound on \tilde{T}^* , and equivalently, $\frac{\tilde{L}}{1 - \varepsilon}$ is an upper bound

on \tilde{z}^* . ■

Appendix F

Test Problem 1: 6-dimensional Hartmann problem over a continuous domain [19]

$$f(x) = \sum_{i=1}^4 c_i \exp\left(-\sum_{j=1}^6 a_{ij} \left(\frac{1}{j} x_j - p_{ij}\right)^2\right),$$

$$\text{s.t.} \quad 0 \leq x_j \leq j, \text{ for } j = 1, \dots, 6,$$

where $c_1 = 1$, $c_2 = 1.2$, $c_3 = 3$, $c_4 = 3.2$,

$$\begin{pmatrix} a_{11} = 10 & a_{12} = 3 & a_{13} = 17 & a_{14} = 3.5 & a_{15} = 1.7 & a_{16} = 8 \\ a_{21} = 0.05 & a_{22} = 10 & a_{23} = 17 & a_{24} = 0.1 & a_{25} = 8 & a_{16} = 14 \\ a_{31} = 3 & a_{32} = 3.5 & a_{33} = 1.7 & a_{34} = 10 & a_{35} = 17 & a_{36} = 8 \\ a_{41} = 17 & a_{42} = 8 & a_{43} = 0.05 & a_{44} = 10 & a_{45} = 0.1 & a_{46} = 14 \end{pmatrix}$$

$$\begin{pmatrix} p_{11} = 0.1312 & p_{12} = 0.1696 & p_{13} = 0.5569 & p_{14} = 0.0124 & p_{15} = 0.8283 & p_{16} = 0.5886 \\ p_{21} = 0.2329 & p_{22} = 0.4135 & p_{23} = 0.8307 & p_{24} = 0.3736 & p_{25} = 0.1004 & p_{16} = 0.9991 \\ p_{31} = 0.2348 & p_{32} = 0.1451 & p_{33} = 0.3522 & p_{34} = 0.2883 & p_{35} = 0.3047 & p_{36} = 0.6650 \\ p_{41} = 0.4047 & p_{42} = 0.8828 & p_{43} = 0.8732 & p_{44} = 0.5743 & p_{45} = 0.1091 & p_{46} = 0.0381 \end{pmatrix}$$

The global optimum $f^* = 3.32$ was determined numerically, and an estimated upper bound of the Lipschitz constant is $K \leq 1320.52$. The stopping rule is: either reach maximal number of function evaluations (1,500) or find a function value f such that $(f^* - f)/f^* \leq 0.01$.

Test Problem 2: 6-dimensional Hartmann problem over a discrete domain (modified directly from the continuous problem)

$$f(x) = \sum_{i=1}^4 c_i \exp \left(- \sum_{j=1}^6 a_{ij} \left(\frac{1}{10^j} x_j - p_{ij} \right)^2 \right),$$

$$\text{s.t.} \quad 0 \leq x_j \leq 10j, \text{ for } j = 1, \dots, 6,$$

where c_i , a_{ij} and p_{ij} are the same as in the continuous problem. The global optimum $f^* = 0.166$ was determined numerically, and an estimated upper bound of the Lipschitz constant is $\tilde{K} \leq 1320.52$. The stopping rule is: either reach the maximal number of function evaluations (30,000) or find f^* .

Test Problems 3 and 4: 10-dimensional Sinusoidal function over continuous and discrete domains [24]

$$\text{Minimize} \quad f(x) = -2.5 \prod_{i=1}^{10} \sin(x_i) - \prod_{i=1}^{10} \sin(5(x_i))$$

$$\text{s.t (over a continuous domain)} \quad 0 \leq x_i \leq 180, \text{ for } i = 1, \dots, 10,$$

$$\text{or s.t (over a discrete domain)} \quad 0 \leq x_i \leq 180, \text{ and } x_i \text{ integer valued, for } i = 1, \dots, 10.$$

The global optimum is $f^* = 3.5$ for both the continuous and discrete problems, an estimated upper bound of the Lipschitz constant for the continuous problem is $K \leq 23.72$, and an estimated upper bound of the Lipschitz constant for the discrete problem is $\tilde{K} \leq 7$. The stopping rule for the continuous problem is: either reach the maximal number of function evaluations (50,000) or find a function value f such that $(f^* - f)/f^* \leq 0.01$. The stopping rule for the discrete problem is: either reach the maximal number of function evaluations (50,000) or find f^* .

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