A Simulated Annealing Algorithm with Constant Temperature for Discrete Stochastic Optimization

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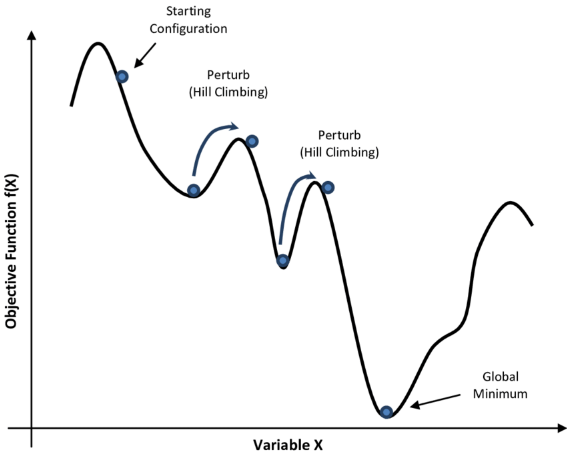
Original Simulated Annealing Algorithm



Original Simulated Annealing Algorithm

Algorithm

PROCEDURE SIMULATED ANNEALING

```
begin
    INITIALIZE;
    M := 0;
    repeat
        repeat
            PERTURB(config. i → config. j,ΔC_ij);
            if ΔC_ij ≤ 0 then accept else
                if exp(−ΔC_ij/c) > random[0,1) then accept;
            if accept then UPDATE(configuration j);
        until equilibrium is approached sufficiently closely;
        c_{M+1} := f(c_M);
        M := M + 1;
    until stop criterion = true (system is 'frozen');
end.
```

Original Simulated Annealing Algorithm

- Most studies have focused on determining an appropriate annealing schedule
- $T_k = \frac{C}{ln(1+k)}, \forall k \in N$
- The convergence depends on C, but C is generally unknown in practice
- Assuming that the objective function values can be evaluated exactly.
- Using the state that is visited by the algorithm in iteration k as the estimated optimal solution in that iteration

Modified Simulated Annealing Algorithm

- estimates of the objective function values will be used throughout since exact objective function values are not available
- the state that is visited most often by the algorithm (divided by a normalizer)
- the state that has the best average estimated objective function value
- not require the Markov chain generated by our algorithm to converge to the set of global optimal solutions
- not restrict the temperature to decrease to 0 (more aggressive)

Formulation

The discrete stochastic optimization problem can be presented as

$$\min_{x \in \varphi} f(x) = \min_{x \in \varphi} E[h(x, Y_x)]$$

where Y_x is a r.v. Denote φ^* as the set of global optimal solutions.

DEFINITION 1. For each $x \in \mathcal{S}$, there exists a subset $N(x)$ of $\mathcal{S} \backslash \{x\}$, which is called the set of neighbors of x.

ASSUMPTION 1. *For any $x, x' \in \mathcal{S}$, x' is reachable from x; i.e., there exists a finite sequence $\{n_i\}_{i=0}^{l}$ for some l, such that $x_{n_0} = x$, $x_{n_l} = x'$, and $x_{n_{i+1}} \in N(x_{n_i})$, $i = 0, 1, 2, \ldots, l-1$.*

Let $R': \mathcal{S} \times \mathcal{S} \to [0, \infty)$ be a function and for all $x \in \mathcal{S}$, define $D(x) = \sum_{x' \in \mathcal{S}} R'(x, x')$ and

$$R(x, x') = \frac{R'(x, x')}{D(x)}, \tag{4}$$

The 1st Approach

Assumptions

ASSUMPTION 2. *Let the transition probability* $R(x, x')$ *be defined as in Equation* (4) *and let* N *satisfy Definition* 1. *Then we assume that:*

1. $R' : \mathcal{S} \times \mathcal{S} \to [0, \infty)$ *satisfies* $R'(x, x') > 0 \Leftrightarrow x' \in N(x)$, *and*
2. $R'(x, x') = R'(x', x)$, *for each* $x, x' \in \mathcal{S}$.

ASSUMPTION 3. *The feasible region* $\mathcal{S}$ *is a finite set containing at least two states and the set of all global optimal solutions* $\mathcal{S}^*$ *is a proper subset of* $\mathcal{S}$.

The 1st Approach
Assumptions

ASSUMPTION 4. *The temperature T is a positive (constant) real number.*

ASSUMPTION 5. *Let $\{L_k\}$ be a sequence of positive integers such that $L_k \to \infty$ as $k \to \infty$.*

The 1st Approach

Lemma 1. (Andradóttir (1995), Lemma 3.1). *Suppose that* $\{D_k\}$ *is a nonhomogeneous Markov chain with a finite state space* $\mathcal{S}$ *and with* $P\{D_{k+1} = d \mid D_0, \ldots, D_k\} = P_k(D_k, d)$ *for all* $d \in \mathcal{S}$ *and* $k \in \mathbb{N}$, *where* $P_k(x, x') \to P(x, x')$ *as* $k \to \infty$ *for all* $x, x' \in \mathcal{S}$ *and* P *is an irreducible and aperiodic Markov matrix. If* $g: \mathcal{S} \to \mathbb{R}$, *then*

$$(1/K)\Sigma_{k=1}^{K} g(D_k) \to \Sigma_{d \in \mathcal{S}} \pi_d g(d)$$

a.s. as $K \to \infty$, *where* π *is the steady-state distribution corresponding to* P.

The 1st Approach

Notations:

- X_k: the current state after k iterations
- $V_k(x)$: the number of times the Markov chain $\{X_k\}$ has visited state x in the first k iterations for all $x \in \varphi$
- X_k^*: the state that maximizes $\frac{V_k(x)}{D(x)}$, where $D(x)$ is the normalizer

The 1st Approach
Algorithm

Parameters: R, N, T, $\{L_k\}$.

Step 0: *Select a starting point* $X_0 \in \mathcal{S}$. *Let* $V_0(X_0) = 1$ *and* $V_0(x) = 0$, *for all* $x \in \mathcal{S}$, $x \neq X_0$. *Let* $k = 0$ *and* $X_k^* = X_0$.

Step 1: *Given* $X_k = x$, *choose* $Z_k \in N(x)$ *such that* $P[Z_k = z \mid X_k = x] = R(x, z)$ *for all* $z \in N(x)$, *where* $N(\cdot)$ *is defined in Definition* 1 *and* $R(\cdot, \cdot)$ *is given in Equation* (4).

Step 2: *Given* $X_k = x$ *and* $Z_k = z$, *generate independent, identically distributed, and unbiased observations* $Y_z(1)$, $Y_z(2), \ldots, Y_z(L_k)$ *of* Y_z *and* $Y_x(1), Y_x(2), \ldots, Y_x(L_k)$ *of* Y_x. *Compute* $\hat{f}_{L_k}(x)$ *and* $\hat{f}_{L_k}(z)$ *as follows:*

$$\hat{f}_{L_k}(s) = \frac{1}{L_k} \sum_{i=1}^{L_k} h(s, Y_s(i)) \quad \text{for } s = x, z. \qquad (5)$$

Step 3: *Given* $X_k = x$ *and* $Z_k = z$, *generate* $U_k \sim U[0, 1]$, *and set*

$$X_{k+1} = \begin{cases} Z_k & \text{if } U_k \leq G_{x,z}(k), \\ X_k & \text{otherwise,} \end{cases}$$

where

$$G_{x,z}(k) = \exp\left[\frac{-[\hat{f}_{L_k}(z) - \hat{f}_{L_k}(x)]^+}{T}\right]. \qquad (6)$$

Step 4: *Let* $k = k + 1$, $V_k(X_k) = V_{k-1}(X_k) + 1$, *and* $V_k(x) = V_{k-1}(x)$, *for all* $x \in \mathcal{S}$, $x \neq X_k$. *If* $V_k(X_k)/D(X_k) > V_k(X^*_{k-1})/D(X^*_{k-1})$, *then let* $X^*_k = X_k$; *otherwise let* $X^*_k = X^*_{k-1}$. *Go to Step* 1.

The 1st Approach

Transition Probability Matrices

$$P_k\left(x, x'\right) = P\left\{X_{k+1} = x' \mid X_k = x\right\}$$
$$= \begin{cases} R\left(x, x'\right) P\left\{U_k \leq G_{x,x'}(k)\right\} & \text{if } x' \in N(x), \\ 1 - \sum_{y \in N(x)} P_k(x, y) & \text{if } x' = x, \\ 0 & \text{otherwise} \end{cases}$$

$$P(x, x')$$

$$= \begin{cases} R(x, x') \exp\left[\dfrac{-[f(x') - f(x)]^+}{T}\right] & \text{if } x' \in N(x), \\ 1 - \sum_{y \in N(x)} P(x, y) & \text{if } x' = x, \\ 0 & \text{otherwise,} \end{cases} \tag{8}$$

and let π_x be defined as follows:

$$\pi_x = \frac{D(x) \exp\left[\dfrac{-f(x)}{T}\right]}{\sum_{x' \in \mathcal{S}} D(x') \exp\left[\dfrac{-f(x')}{T}\right]} \tag{9}$$

Proposition 2

Under Assumptions 1 through 3, the transition probability matrix P given in Equation (8) is irreducible and aperiodic and has stationary distribution π, where π is a vector whose entries π_x are given in Equation (9).

The 1st Approach

Proposition 2

PROOF. The proof of irreducibility follows directly from Assumptions 1 and 2 and Equation (8). The proof that π is the stationary distribution of P can be found in Proposition 3.1 in Mitra et al. (1986). To prove aperiodicity, note that by Assumption 3, $\mathcal{S}^* \neq \mathcal{S}$, so by Assumption 1 there exist $x^* \in \mathcal{S}^*$ and $x \in N(x^*)$ with $f(x^*) < f(x)$. Therefore, from the definition of P given in Equation (8) and the definition of R given in Equation (4), $P(x^*, x^*) > 0$ and therefore, P is aperiodic. □

Proposition 3

Suppose that Assumptions 4 and 5 are satisfied and that φ is finite. Then $P_k(x, x') \to P(x, x')$ as $k \to \infty$ for all $x, x' \in \varphi$, where the Markov matrices P_k and P are given in Equations (7) and (8), respectively

The 1st Approach

Proposition 3

Proof:

$$
\begin{aligned}
&\lim_{k\to\infty} P_k\left(x,x'\right)\\
=&R\left(x,x'\right)\lim_{k\to\infty} E\left[\exp\left[\frac{-\left[\hat{f}_k\left(x'\right)-\hat{f}_k(x)\right]^+}{T}\right]\right]\\
=&R\left(x,x'\right) E\left[\lim_{k\to\infty}\exp\left[\frac{-\left[\hat{f}_k\left(x'\right)-\hat{f}_k(x)\right]^+}{T}\right]\right]\\
=&R\left(x,x'\right) E\left[\exp\left[\frac{-\left[f\left(x'\right)-f(x)\right]^+}{T}\right]\right]=P\left(x,x'\right)
\end{aligned}
$$

Theorem 4

Under Assumptions 1 through 5 , the sequence $\{X_k^*\}$ generated by Algorithm 1 converges almost surely to the set φ^* (in the sense that there exists a set A such that $P(A) = 1$ and for all $\omega \in A$, there exists $K_\omega > 0$ such that $X_k^*(\omega) \in \varphi^*$ for all $k \geq K_\omega$).

Proof: By Lemma 1 (let $D_k = X_k$ for all $k \in \mathbb{N}$ and $g(d) = I_{\{d=x\}}$ for all $d \in \varphi$), we have that

$$\frac{V_k(x)}{kD(x)} = \frac{1}{D(x)} \times \frac{1}{k} \sum_{i=0}^{k} I_{\{X_i=x\}} \rightarrow \frac{\pi_x}{D(x)} \quad \text{a.s. as } k \rightarrow \infty$$

for all $x \in \varphi$, where $V_k(x), x \in \varphi$. It is clear that $\pi_x > 0$ for all $x \in \varphi$ so that Equation (9) yields

$$\frac{\pi_y / D(y)}{\pi_x / D(x)} = \exp\left[\frac{-[f(y) - f(x)]}{T}\right]$$

for all $x, y \in \varphi$. Therefore, $\pi_y/D(y) \leq \pi_x/D(x)$ if and only if $f(y) \geq f(x)$. This shows that

$$arg \max_{x \in \varphi} \frac{\pi_x}{D(x)} = \varphi^*$$

The 2rd Approach

- This variant uses the same mechanism for moving around the state space as Algorithm 1 but a different approach for estimating the optimal solution.
- Selecting the state with the best average estimated objective function value obtained from all the previous estimates to be the estimated optimal solution

Assumption 5': $\{L_k\}$ is a sequence of positive integers satisfying $lim_{k \to \infty} L_k = L \leq \infty$

The 2rd Approach

Algorithm

Parameters: R, N, T, $\{L_k\}$.

Step 0: *Select a starting point* $X_0 \in \mathcal{S}$. *For all* $x \in \mathcal{S}$, *let* $A_0(x) = 0$ *and* $C_0(x) = 0$. *Let* $k = 0$ *and* $X_k^* = X_0$.

Step 1: *Identical to Step* 1 *of Algorithm* 1.

Step 2: *Given* $X_k = x$ *and* $Z_k = z$, *generate independent, identically distributed, and unbiased observations* $Y_z(1), Y_z(2), \ldots, Y_z(L_k)$ *of* Y_z *and* $Y_x(1), Y_x(2), \ldots, Y_x(L_k)$ *of* Y_x. *Compute* $\hat{f}_{L_k}(x)$ *and* $\hat{f}_{L_k}(z)$ *as in Equation* (5) *for* $s = x, z$. *Let* $C_{k+1}(s) = C_k(s) + L_k$ *and* $A_{k+1}(s) = A_k(s) + L_k\hat{f}_{L_k}(s)$ *for* $s = x, z$. *Moreover, let* $C_{k+1}(x') = C_k(x')$ *and* $A_{k+1}(x') = A_k(x')$ *for all* $x' \in \mathcal{S}$, $x' \neq x, z$.

Step 3: *Identical to Step* 3 *of Algorithm* 1.

Step 4: *Let* $k = k + 1$ *and select* $X_k^* \in \arg\min_{x\in\mathcal{S}} A_k(x)/C_k(x)$ (*use the convention* $0/0 = +\infty$). *Go to Step* 1.

Theorem 5

Suppose that Assumptions 1, 2, 3, 4 and 5' are satisfied , the sequence $\{X_k^*\}$ generated by Algorithm 2 converges almost surely to the set φ^* (in the sense that there exists a set A such that $P(A) = 1$ and for all $\omega \in A$, there exists $K_\omega > 0$ such that $X_k^*(\omega) \in \varphi^*$ for all $k \geq K_\omega$).

Proof:

(i) $L = \infty$

$P_k \to P$, P is irreducible and aperiodic and has the stationary distribution π. Since φ is finite, $\pi_x > 0$ for all $x \in \varphi$.

By Lemma 1, $\frac{V_k(x)}{k} \to \pi_x > 0$ a.s. as $k \to \infty$ for for all $x \in \varphi$

$\Rightarrow V_k(x) \to \infty$ as $k \to \infty$ for for all $x \in \varphi$. Clearly, $C_k(x) \geq V_k(x) - 1$

$\Rightarrow C_k(x) \to \infty$a.s. as $k \to \infty$ for for all $x \in \varphi$

$\Rightarrow \frac{A_k(x)}{C_k(x)} \to f(x)$ a.s. as $k \to \infty$ for for all $x \in \varphi$

Proof:

(ii) $L < \infty$, $P_k(x, x') \to P'(x, x')$

Firstly, we show that P' is irreducible

$$P'(x, x') = P\{X_{k+1} = x' \mid X_k = x\}$$

$$= \begin{cases} R(x, x')p'_{x,x'} & x' \in N(x), \\ 1 - \Sigma_{y \in N(x)} P'(x, y) & \text{if } x' = x, \\ 0 & \text{otherwise,} \end{cases} \quad (11)$$

$p'_{x,x'} = E[\exp[-[\hat{f}(x') - \hat{f}(x)]^+/T]]$, and $\hat{f}(s) = (1/L) \Sigma_{i=1}^{L} h(s, Y_s(i))$ for $s = x, x'$.

By Jensen's inequality, we have that

$$p'_{x,x'} \geq \exp\left[\frac{-1}{T} E[\hat{f}(x') - \hat{f}(x)]^+\right]$$

$$\geq \exp\left[\frac{-1}{T} E[\,|\hat{f}(x')| + |\hat{f}(x)|\,]\right]$$

$$> 0,$$

Then, we show that P' is aperiodic

$$
\begin{aligned}
& P'(x, x) = 0, \ \forall x \in \mathcal{S} \\
& \Leftrightarrow \sum_{x' \in N(x)} P'(x, x') = 1, \ \forall x \in \mathcal{S} \\
& \Leftrightarrow E\left[\exp\left[\frac{-[\hat{f}(x') - \hat{f}(x)]^{+}}{T} \right] \right] = 1, \\
& \quad \forall x \in \mathcal{S}, x' \in N(x) \\
& \Leftrightarrow \exp\left[\frac{-[\hat{f}(x') - \hat{f}(x)]^{+}}{T} \right] = 1 \text{ a.s.}, \\
& \quad \forall x \in \mathcal{S}, x' \in N(x) \\
& \Leftrightarrow \hat{f}(x') - \hat{f}(x) \le 0 \text{ a.s.}, \ \forall x \in \mathcal{S}, x' \in N(x) \\
& \Leftrightarrow \hat{f}(x') = \hat{f}(x) \text{ a.s.}, \ \forall x \in \mathcal{S}, x' \in N(x) \\
& \Leftrightarrow \hat{f}(x') = \hat{f}(x) \text{ a.s.}, \ \forall x, x' \in \mathcal{S} \\
& \Leftrightarrow f(x') = f(x), \ \forall x, x' \in \mathcal{S}.
\end{aligned}
$$

Since this contradicts Assumption 3, we have shown that P' is aperiodic.

Since $P_k \to P'$ as $k \to \infty$, where P' is irreducible and aperiodic and P' has a stationary distribution r, with $r_x > 0$ for all $x \in \mathcal{S}$, by Lemma 1, $V_k(x)/k \to r_x > 0$ a.s. as $k \to \infty$ for all $x \in \mathcal{S}$. This implies that $V_k(x) \to \infty$ a.s. as $k \to \infty$ for all $x \in \mathcal{S}$. The rest of the proof is similar to the proof for the case $L = \infty$. $\square$

Comparison

- Algorithm 2 will converge to the set of global optimal solutions to the optimization problem more rapidly than Algorithm 1
- Algorithm 2 is expected to obtain a good estimate of the optimal solution quickly. Since Algorithm 2 selects the state in φ that has the best objective function value among the states that have been visited by the algorithm so far to be the estimate of the optimal solution.

Thanks!