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# Optimum design with multimodal simulated annealing strategies

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## Abstract

Strategies for locating multiple relative optima in a multimodal optimization problem using multiple-point simulated annealing are proposed. Two strategies incorporated with multiple-point simulated annealing are developed to increase the capabilities of locating more relative optima in a nonconvex design space. Balance strategy involves the use of a balance function that evaluates the degree of design spreading over the entire design space and create a corresponding direction bias in the subsequent design-change process. Bounce strategy evaluates the degree of design crowding and aims to push designs away from the crowd center by creating a direction bias in the next design-change process. Both strategies are evaluated on a number of illustrative multimodal problems.

## Introduction

The basic idea of simulated annealing (SA) was originated by Metropolis *et al* [1] in 1953 who proposed a Monte Carlo method in which a sequence of states of solid was generated according to *Metropolis Procedure* so as to simulate the evolution to thermal equilibrium of a solid for a fixed temperature. Kirkpatrick *et al* [2,3] and Cerny [4] successfully applied simulated annealing to combinatorial optimization problems and since then simulated annealing has been applied to diverse engineering problems, more extensively to VLSI design problems [5] and circuit placement problems [6]. Simulated annealing based on statistical mechanics is categorized as a stochastic search method and is analogous to the natural energy minimization process as found in melt metal during a controlled temperature dropping schedule. A design change with an increased internal energy (objective function value) is probabilistically acceptable in a simulated annealing. This unique character provides the search with the ability to escape from a valley with a local optimum and accordingly SA is a global optimization method in nature. More detailed description on simulated annealing can be found in the work by van Laarhoven and Aarts [7].

As the number of relative optima in the design space increases, the chances of locating a true global optimum by using a regular simulated annealing algorithm is reduced. In order to improve the opportunity of finding global optimum in a complex multimodal design problem, sequential or parallel simulated annealing algorithms can be used [8,9]. These works mostly relate to the use of multiple processors with parallel computing techniques. For a regular multipoint simulated annealing, the information of multiple designs during the simulated annealing process has not been well utilized to further increase the search efficiency and effectiveness. Two strategies which use the information of design distributions in a given temperature to create adjusted biases on the determination of subsequent design-change process are described in the next section.

## New strategies in multipoint simulated annealing

During a simulated annealing process, a new design of $n$-dimension will be determined by $n$ random numbers. For a given temperature $T$, the maximum move step toward the positive-axis and negative-axis directions is $\Delta x(T)$, $\Delta y(T)$, etc. Equal probabilities are assigned to positive- and negative-axis directions. A random number ranged between 0.0 and 1.0 for each dimension will match to a move step between $-\Delta x(T)$ and $\Delta x(T)$. For example, a random number of 0.7 will simultaneously determine the move direction, positive $x$-direction, and the move step, $(0.7-0.5)/(1.0-0.5)\Delta x(T)$ or $0.4\Delta x(T)$. Two strategies introduced here work to create a direction bias for each dimension according to design distribution patterns. A normal probability for a design to move toward each positive-axis direction, saying x-axis direction, is 0.5. Biases can add this probability to 1.0 or reduce it to as less as 0.0. The probability of moving toward (positive) x-direction as 0.0 means the move will be toward negative x-direction and the move step is $\Delta x(T)$ multiplied by the random number.

### Balance strategy

The purpose of the balance strategy is to create a pressure which will make multiple design points to search more evenly in the design space. Balance strategy can be applied according the following steps:

Step 1: calculate the center of each axis and the centroid of designs in each axis as referenced in Figure 1.

$$x_c = \frac{x_\ell + x_u}{2} \tag{1}$$

$$x_d = \sum_{i=1}^{4} x_i / 4 \tag{2}$$

where $x_c$ is the center of defined range in $x$-axis,
$x_l$ is the lower bound of $x$-axis,
$x_u$ is the upper bound of $x$-axis,
$x_i$ is $x$-coordinate of $i$-th design,
$x_d$ is the centroid of designs in $x$-axis.

Step 2: determine the balance-adjusted probability, $P_x$, for designs to move toward positive $x$-direction in a given temperature.

$$P_x = \begin{cases} 2d / D, & (-\frac{D}{4} < d < \frac{D}{4}) \\ 0.5, & (d \geq \frac{D}{4}) \\ -0.5, & (d \leq -\frac{D}{4}) \end{cases} \tag{3}$$

$$(-0.5 \leq P_x \leq 0.5)$$

where $D$ is the distance between lower and upper bounds, $D = x_l - x_u$,
$d$ is the distance between is the center of defined range in $x$-axis and the centroid of designs in $x$-axis, $d = x_d - x_c$.

Step 3: calculate the actual probability for designs to move toward the positive $x$-direction.

$$C_x = 0.5 + P_x \tag{4}$$

For an $m$-point simulated annealing is being executed, the actual probability for all $m$ designs to move toward the positive $x$-direction has to be calculated $n$ times if the design space consists of $n$ design variables. From Equations (3) and

(4), it is noted that if the centroid of designs is closer to either bounds than to the center of an axis ($d \geq D/4$ or $d \leq -D/4$), all designs will be forced to move toward either negative $x$-direction ($d \geq D/4$) or positive $x$-direction ($d \leq -D/4$).

Although balance strategy helps maintain the centroid of designs to close to the center of the design space, symmetric design clusters as represented by triangles or squares shown in Figure 2 can not be prevented. Multiple designs still form a crowd and ability to discover extremes located apart is therefore reduced. Bounce strategy will serve to prevent designs from clustering together.

**Bounce strategy**

The basic idea of bounce strategy is to assume that an imaginary elastic spring of length $R$ exists for each design. As the distance between any two designs is less than the spring length $R$, the spring will be deflected and an extending force will be applied on each design so as to push two designs away. The procedure to use bounce strategy consists of the following three steps:

Step 1: Calculate the deflection of the imaginary spring as one foreign design falls into the territory of an interrupted design as shown in Figure 3,

$$d = R - r \tag{5}$$

where $d$ represents the deflection of the imaginary spring,
$R$ represents the length of the imaginary spring,
$r$ is the distance between two contacted designs.

Step 2: Calculate the bounce-adjusted probability for the foreign design to move toward positive direction of each axis.

$$P'_x = \frac{x_f - x_k}{r} E \qquad (-0.5 < P'_x < 0.5) \tag{6}$$

$$P'_y = \frac{y_f - y_k}{r} E \qquad (-0.5 < P'_y < 0.5) \tag{7}$$

where $P'_x$: the bounce-adjusted probability for the foreign design to move toward positive $x$-direction,
$P'_y$: the bounce-adjusted probability for the foreign design to move toward positive $y$-direction,
$x_f$, $y_f$, $x_k$, and $y_k$ are $x$, $y$ coordinates for the foreign design and the design being interrupted,
$E$ represents the internal energy created by deflection $d$, $E = kd^2/2$,

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$k$ represents the spring constant, $k = 1 / R^2$.

Step 3: Calculate the actual probability for designs to move toward each positive-axis direction.

$$C'_x = 0.5 + P'(x) \tag{8}$$

$$C'_y = 0.5 + P'(y) \tag{9}$$

If the balance strategy and the bounce strategy are both adopted, the actual probability for designs to move toward each positive-axis direction is as follows:

$$C''_x = 0.5 + P_x + P'_x \tag{10}$$

$$C''_y = 0.5 + P_y + P'_y \tag{11}$$

Although actual values of $C''_x$ and $C''_y$ can be greater than 1.0 or less than 0.0 according to Equations (10) and (11), actual probabilities for a design to move toward each positive-axis direction is restricted between 0.0 and 1.0.

## Illustrative Examples

For all experiments in Example 1 and 2, the maximum move steps in each dimension according to different temperature ranges are defined in Table 1. Starting temperature is 50 and the ending temperature is $8\times10^{-7}$. A temperature dropping rate is 0.99 applied after each design change is accepted.

Table 1. Maximum move step in each dimension for all simulated annealing algorithms.

| Temperature | T>20 | T>10 | T>1 | T>0.01 | T>0.001 | lower T |
|---|---|---|---|---|---|---|
| Maximum move step | 0.8 | 0.5 | 0.2 | 0.1 | 0.08 | 0.05 |

Example 1: Two strategies are tested in an unconstrained Himmeblau's function which comprises four local/global minima of an equal value 0.0. The function contour and the three-dimensional diagram of Himmeblau's function is shown in Figure 2 and 4. Four randomly generated initial designs are used in all multi-point simulated annealing processes. A regular simulated annealing is used to serve as the performance reference against the simulated annealing with the balance and bounce strategies. Each simulated annealing algorithm will be executed fifteen times in order to reduce the sampling errors introduced by random numbers in the stochastic optimization. In the first experiment, regular SA(SA), SA with balance strategy(SA+Ba), SA with bounce strategy(SA+Bo), SA with both balance and bounce strategy(SA+Ba+Bo) are performed with the same temperature reducing schedule. Performances of 15 runs of four different

SA algorithms are shown in Table. 2. With two new strategies, SA located more extremes and less optima are located repeatedly.

Table 2. Performance of four SA algorithms.

| | SA | SA+Ba | SA+Bo | SA+Ba+Bo |
|---|---|---|---|---|
| total number of optima located | 36 | 49 | 41 | 49 |
| average number of optima located | 2.40 | 3.27 | 2.73 | 3.27 |

Example 2: In the second experiment, the same four SA algorithms are tested with five types of initial design formation. Four initial design formations consist of all four randomly generated designs restricted in the first quadrant, the second quadrant, the third quadrant, the fourth quadrant of the design space. The fifth formation requires that one design is randomly generated in each of four guadrants. The purpose of this experiment aims to evaluate new strategies in the circumstances where initial designs are not evenly distributed. Average performances of 15 runs of four different SA algorithms in each initial design formation are shown in Table. 3. Although it can be seen that the performance trend of SA algorithms is quite consistent with the first experiment, most cases show that SA with both balance strategies is less sensitive to the distribution of initial designs than the regular SA.

Table 3. Total number of extremes located by four algorithms with various patterns of initial designs.

| | SA | SA+Ba | SA+Bo | SA+Ba+Bo |
|---|---|---|---|---|
| 1st quadrant | 32 | 50 | 39 | 46 |
| 2nd quadrant | 31 | 45 | 36 | 48 |
| 3rd quadrant | 38 | 42 | 45 | 52 |
| 4th quadrant | 36 | 46 | 45 | 50 |
| one in each quadrant | 42 | 46 | 42 | 53 |
| random* | 36* | 49* | 41* | 49* |

*cited from the first example

Example 3: The third problem involves the design of a lap joint between two steel plates in which the rivet size and the number and arrangement of the rivet pattern are considered as design variables. The configuration of the plates and the rivets is shown in Figure 5. The number of rows parallel to side AB is represented by an integer variable $x_1$ with permissible values between 1 and 32. The number of the rivets in each row $x_2$ is an integer variable and was allowed to assume values between 1 and 128. The diameter $x_3$ of all rivets was assumed to be the same, and is chosen from a commercially available set. The objective of this optimization was to maximize the efficiency of the joint, defined as the ratio of the strength of joint to the strength of the plate. Stress concentrations

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due to the close placement of any two rivets were avoided by the imposition of two linear constraints. Detailed description of this problem can be found in a previous publication [10]. This problem consists of 12 relative maxima with two of them are next to each other. A regular SA with 11 randomly generated initial designs is performed 15 times so was the simulated annealing with both balance and bounce strategies. Maximum move steps in each dimension according to different temperature ranges are defined in Table 4. Starting temperature is 50 and the ending temperature is $8\times10^{-7}$ with a temperature dropping rate of 0.985. Performances of 15 runs of two SA algorithms are shown in Table. 5. Two strategies increased the number of relative optima located.

Table 4. Maximum move step in each dimension for all simulated annealing algorithms.

| Temperature | T>1.0 | T>0.1 | T>0.001 | lower T |
|---|---|---|---|---|
| Max. move step in $x_1$ | 2 | 2 | 1 | 1 |
| Max. move step in $x_2$ | 3 | 2 | 2 | 1 |
| Max. move step in $x_3$ | 2 | 1 | 1 | 1 |

Table 5. Comparison of performance of two SA algorithms.

| | SA | SA+Ba+Bo |
|---|---|---|
| total number of optima located | 65 | 98 |
| average number of optima located | 4.33 | 6.53 |

## Concluding Remarks

Balance strategy and bounce strategy are useful tools for a multipoint simulated annealing for increasing the chances of locating the global optimum and elevating the ability of locating more local optima. Both strategies are simple and can be easily implemented to a regular SA with improved effectiveness.

## Acknowledgments

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## References

1. Metropolis, N., Rosenbluth, A., Rosenbluth, M., Teller A. and Teller, E., Equation of State Calculations by Fast Computing Machines, *Journal of Chem. Physics*, 1953, **21**, 1087-1092.

2. Kirkpatrick, S., Gelatt Jr., C.D. and Vecchi, M.P. Optimization by Simulated Annealing, *IBM Research Report* RC 9355, 1982.
3. Kirkpatrick, S., Gelatt Jr., C.D. and Vecchi, M.P. Optimization by Simulated Annealing, *Science*, 1983, **220**, 671- 680.
4. Cerny, V., Thermodynamical Approach to the Traveling Salesman Problem: An Efficient Simulated Algorithm, *Journal of Optimization Theory and Applications*, 1985, **45**, 41-51.
5. Carter, H.W., Computer-Aided Design of Integrated Circuits, *Computer*, 1986, **19**, 19-36.
6. Rothman, S., Circuit Placement by Simulated Annealing at IBM, Presented at Workshop on Stat. Physics in Engineering and Biology, Lech, July 1986.
7. Aarts, E.H.L. and van Laarhoven, P.J.M., *Simulated Annealing: Theory and Applications*, Wiley, New York, 1987.
8. Catoni, O., Rates of Convergence for Sequential Annealing: A Large Deviation Approach, *Simulated Annealing: Parallelization Techniques*, Edited by Azencott, R., John Wiley & Sons, 1992, 25-35.
9. Azencott, R., Parallel Simulated Annealing: An Overview of Basic Techniques, *Simulated Annealing: Parallelization Techniques*, Edited by Azencott, R., John Wiley & Sons, 1992, 37-46.
10. Lin, C.Y. and Hajela, P., Genetic Algorithms in Optimization Problems with Discrete and Integer Design Variables, *Journal of Engineering Optimization*, 1992, **19**, 309-327.

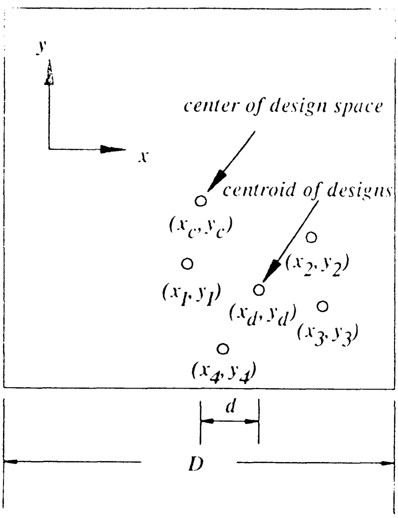


Figure 1: Distribution of 4 designs in a 2-D space.

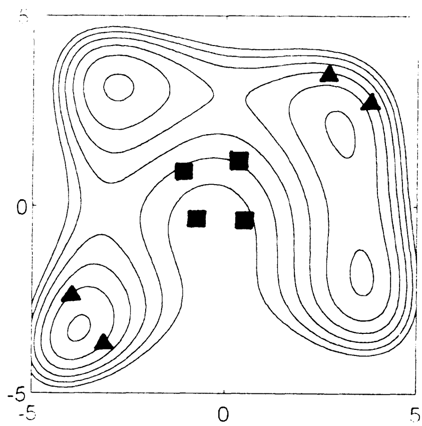


Figure 2: Design clusters in a 2-D design space.

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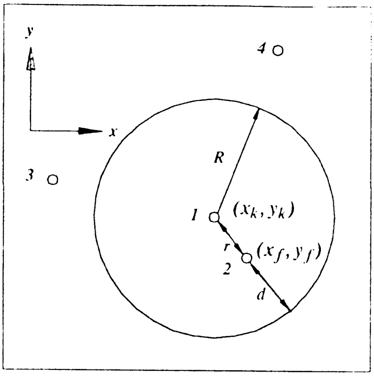
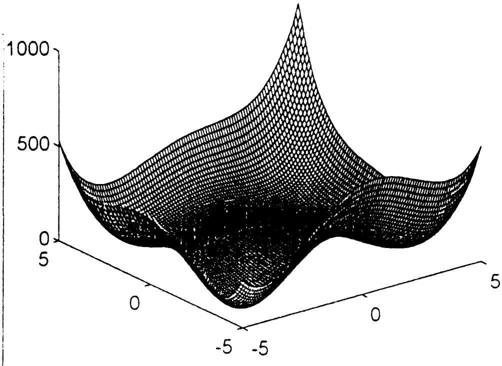



Figure 3: Two designs connected by an imaginary spring.




$$f(x,y) = (x^2 + y - 11)^2 + (x + y^2 - 7)^2$$

Figure 4: 3-D diagram of Himmeblau's function.

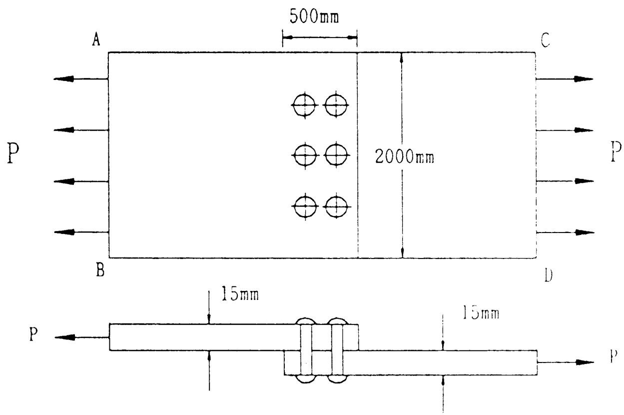



Figure 5: Geometric configuration of rivted plates.