Enhancements on Reproduction of Spatial Variability with Multi-Objective Simulated Annealing

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ABSTRACT: Simulated Annealing (SA) has been increasingly used in the reproduction of spatial variability. In this research, SA was used to improve output of direct sequential simulation method as initial solution. SA algorithm mainly consists of four parts: objective (cost) function, transition (perturbation) mechanism, acceptance criterion and cooling schedule. The objective function was expressed as a multiple criteria minimisation problem in terms of deviations of semi-variogram and histogram of new solution from those of current solution. The approach was demonstrated on a chromites ore deposit. The results showed that SA could be used to reproduce the spatial variability.

1 INTRODUCTION

SA is a stochastic method for solving large combinatorial minimisation problems (Lundy and Mees, 1986, Laarhoven and Aarts, 1987, Eglese, 1990, Pres *et. al.*, 1992, Ansari and Hou, 1997). The method is based on the principle of stochastic relaxation. The method has an analogy in thermodynamics, specifically with the way that liquids freeze and crystallise or metal cools and anneals.

Suppose that a cost function in many variables is to be minimised. A simple, iterative, local search could be performed to find the minimum cost. During the local search process, an initial solution is given and then a new solution is selected at random. If the cost of the new solution is smaller than that of the current solution, the current solution is replaced by the new solution. Unfortunately, a local search may get stuck at local minima. Let / : $X \rightarrow R$ be a function to be minimised over X, where X is a finite, but very large, set. A neighbourhood $N(x)$ cX is associated with each element x £ X. Iterations can be defined by first selecting a starting point and then repetitively selecting y e $N(x)$ and comparing successive values. SA allows the choice of y to be governed by the following stochastic rule: the first y e $N(x)$ is selected with probability q_{xy}, then y is accepted with probability:

$$p_{xy}(T) = \min\left\{1, e^{-\frac{f(y)-f(x)}{t}}\right\} \quad (1)$$

where 7* is a parameter known as temperature, x is the current solution, y is the new solution.

2 PROBLEM SPECIFIC DECISIONS

2.1 Cost / **objective function**

The reproduction of stochastic image is expressed as an optimisation problem, which can be solved by multi-objective SA. In this research, two objectives are introduced. Firstly, to reproduce the same spatial dispersion (Eq. 2). Secondly, to reproduce the same histogram as the true values (Eq. 3).

Jti = minimisation of deviation from value of the target semi-vanogram at lags

$$\pi_1 = Min \sum_{i=1}^{l} \frac{[\gamma(h_i) - \hat{\gamma}(h_i)]^2}{[\gamma(h_i)]^2} \quad (2)$$

where $y(\backslash)$ is value of expected semi-variogram at lag h, and $f(h,)$ is value of experimental semi-variogram at lag h, after new transition.

Given that behaviour of model of semi-variogram is more reliable near origin, the division of square of the semi-variogram model gives more weights at each lag.

π_2= minimisation of deviation from target cumulative histogram at each interval

$$\pi_2 = Min \sum_{j=1}^{J} \left[G_j - \hat{G}_j\right]^2 \quad (3)$$

where G_j is value of expected cumulative histogram at interval y and $\hat{G}$, is cumulative distribution of simulated realization after new transition.

Objective function:

$$Min\ \pi = \pi_1 + \pi_2$$

$$Min \sum_{i=1}^{I} \frac{[\gamma(h_i) - \hat{\gamma}_0(h_i)]^2}{[\gamma(h_i)]^2} + \sum_{j=1}^{J} \left[G_j - \hat{G}_j\right]^2 \quad (4)$$

However, the objective functions have different units. Therefore, the solution may be dominated by other solutions that lead to the algorithm being dependent on one objective. This problem is handled small modification in acceptance criterion.

2.2. Perturbation Mechanism

In transition mechanism possible locations are selected in a certain order. As known, when a location is selected at random it is possible to accept some uphill moves before the local optimum is selected. Therefore, the local optimum may never be attained. This mechanism also prevents to consider for a second time before all possible locations are tried once. In this research conditional distributions have been extracted from ordinary kriging weights. The sum of the kriging weights assigned to data of any given class is interpreted as the conditional probability of this class (Rao and Journel, 1997).

2.3. Initial solution

In this research direct sequential simulation was used as initial solution. The conditional distributions could be of any type as long as their means and variances are determined by simple kriging (Journel, 1994). The implicit random function model is no longer Gaussian and may be difficult to identify *a priori,* but the properties of the implicit random function can be observed in the simulated realisations. This kind of generalisation preserves the prior covariance matrix and leads to an important theoretical extension of the sequential simulation paradigm. Thus, original data values can be used in simulation without data transformation. This is called direct sequential simulation. Given a stationary random function *Z(u),* not necessarily Gaussian, and *N* original data, $\{Z(u_\alpha) = z(u_\alpha), \alpha = 1,...,N\}$, the direct sequential simulation algorithm is as follows:

1. Define a random path through all nodes to be simulated,
2. Build the" cumulative conditional distribution function of $Z(u_i)$ given the *N* original data and all previously simulated values at each node,
3. Draw a realisation from the estimated ccdf. This realisation becomes a conditioning datum for all subsequent nodes
4. Loop until all *K* nodes are visited.

The direct sequential simulation produced the smoothed random field. In addition, as the numbers of location being simulated and of objectives increase, only SA can be prohibitively difficult because of computer time.

3 GENERIC DECISIONS

3.1. Acceptance criterion

The percentage deviation is calculated for each solution instead of the difference between new and current solutions as shown in the Equation 6:

$$AC = p_{yx}(T) = min\left\{1, e^{-\sum_{i=1}^{iobj}(\lambda_i d_i)}\right\} \quad (5)$$

Where:

$$d = \left(\frac{f_i(y) - f_i(x)}{f_i(x)}\right) \text{ and } \sum_{i=1}^{iobj} \lambda_i = 1 \quad (6)$$

If the new solution is accepted, it becomes the current solution and is noted as a potentially non-dominated (PN) point. The current solution is compared with previously noted potential PN points. If the current solution dominates any PN solution, this PN solution is removed from the PN points file. If a dominated solution is chosen by the acceptance criteria, the comparison procedure is not applied. This solution will be removed to prevent solutions becoming stuck in local optima.

3.2. Cooling schedule

Although SA is a simple process, the selection of the annealing parameters is not simple because of possibility of stuck at local optima and the operational restrictions such as execution time.

r*+;=a7"/t was used for the decrement function firstly (Kirkpatrick *et. al.,* 1983), where «is accepted as 0.80-0.95. This decrement form reduces the temperature very rapidly and most of the running time is spent at low temperatures. In this research, a more gradual process was used (Dowsland, 1993). Every time a move is accepted the system cools according to the function $T \leftarrow T/(1+\beta T)$, and every time a move is rejected the system is heated according to the function $T \leftarrow T/(1-\alpha T)$. If $\beta = ka$ the system will need to go through k heating iterations to balance one cooling. If the ratio of rejected moves to accepted moves is greater than k, the system heats up and vice versa. Thus, this schedule theoretically tends to converge to a situation in which the ratio is about *k*. This was also used as stopping (termination) criterion, *k* should be governed by the size of the neighborhoods around these minima. Therefore, sufficient number of iterations was allowed around these minima, *k* is separating factor that gives a measure of required ratio of reduction amount at accepted transitions to increasing amount at rejected transitions. In this research it is planned in such a way that 99 out of 100 transitions are rejected. β and *a* are chosen as 0.01500 and 0.00015, respectively.

In order to reduce execution time, an initial temperature is calculated before running the algorithm in the following way:

$$T \approx \frac{(f_{new} - f_{current})^{(+)}}{\ln\left(\frac{n_2}{n_2 A - n_1(1-A)}\right)} \qquad (7)$$

Where;

fnew-fmrrem is the average difference in cost over the n_2 cost increasing transitions, n_t is the number of cost-decreasing transitions, «2 is the number of cost-increasing transitions, *A* is the required acceptance ratio - the ratio between the number of accepted transitions and the number of proposed transitions at the given temperature.

k value is desired as 200 in the case study. Since annealing algorithm has also been used in combination with direct sequential simulation, this ratio is adequate. The direct sequential simulation generates a sub-optimal solution that then becomes the starting solution for SA. Initial temperature was selected as 35.0 to yield the required ratio.

4 ENHANCEMENTS ON SA STRUCTURE

4.1 Quick calculation of cost function

In SA most of running time was spent for calculating new cost function in each transition. Given mat the vast numbers of transitions are implemented, the computer time required may be prohibitively long since calculations of histogram and semi-variogram should be repeated in each transition. Therefore, histograms are updated locally. As for semi-variogram, a new value replaces with old value. Contribution of old value to semi-variogram is subtracted at corresponding lag and is added to the contributions of the new value.

4.2 Storing best solution

As has been known, SA may accept worse solution in final transition. Therefore, it is possible to find worse solution as final solution in the end of annealing. In addition, It was remarked that the SA algorithm did not rely on a strong convergence over time with this modification (Glover and Greenberg, 1989). If the best solution found so far is storaged, it will be guarantee to retain the best solution. This is not computationally expensive.

5. CASE STUDY

A case study has been conducted on a chromite data set to demonstrate the algorithm developed during this research.

The initial data comprised a set of 27 drillholes, the cores from which had been assayed for Cr_2O_3. A three-dimensional block model was created by direct sequential simulation the three grades for each block. Blocks are 4m (EW) x 4m (NS) x 3m on a 50 (EW) x 50 (NS) x 20 grid. This provided a total of 50 000 blocks.

Model statistics are inferred from sample information, which are assumed to represent population parameters. A stochastic realization should reproduce the declustered sample histogram and tiie semi-variogram model, and should coincide with data values at their locations. Figure 1 showed histogram and semi-variogram of 205 core samples. Figure 2 showed histogram and semi-variogram of 50 000 simulated values obtained from direct sequential simulation. As has been seen, there was no exact match with histogram and semi-variogram of data. This sub-optimal reproduction was then submitted to the SA algorithm. The algorithm was implemented

for four million transitions. As the algorithm has been designed for multi-criteria optimization problems, there are generally more than one optimal solution (non-dominated or Pareto optimality). In the case study, the program has yielded three random fields in the end of execution of algorithm. Table 1 summarizes these fields. Final reproduction has the same semi-variogram as the true values and the same distribution as the true values.

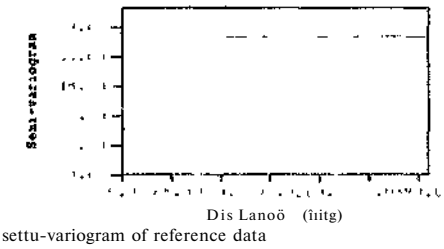

Figure 1. Histogram and settu-variogram of reference data

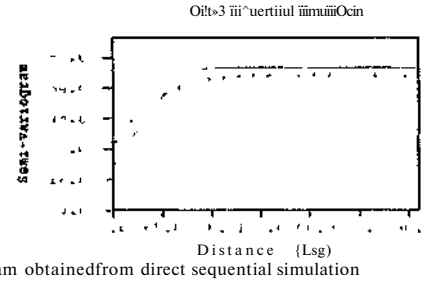

Figure 2 Histogram and semi-variogram obtainedfrom direct sequential simulation

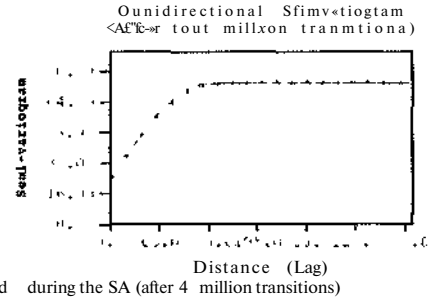

Figure 3 Histograms and semi-venograms obtained during the SA (after 4 million transitions)

Table 1. Non-dominated results fo • two objectives

	Objective					Objective 2	
	Co	c,	C-,	ai	ai	Mean	St.Dev
Sample	23.80	37.71	13.59	119.41	155.24	37.52	8 6239
Field 1	23 88	37.48	13.58	119 03	155 37	37 53	8 6217
Field 2	23 81	37.62	13.64	! 19.87	155.81	37.59	8.6277
Field 3	23 85	37.49	13.52	118.91	154.40	37.50	8.6235

6. CONCLUSIONS

As SA with enhancements proceeded, exact reproduction was obtained Implementation m the selected temperature decrement, selection of locations m certain order during transition mechanism and storing best solution so fai produced good ıesults m shorter time The program yielded three nondominated fields Selection among these repioduc tions depends upon preferences of decision maker These preferences could be incorporated into algorithm directly Multi-objective SA ıs very powerful technique for reproduction of same spatial dispersion and dıstıibutıon However, the approach needs extensive experimentation to find the parameters of cooling schedule

7 KAYNAKLAR

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