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Boreholes plans optimization methodology combining geostatistical simulation and simulated annealing

Marisa Pinheiro[a,*], Xavier Emery[b,c], Ana Maria A.C. Rocha[d], Tiago Miranda[a], Luís Lamas[e]

[a] ISISE, University of Minho, Azurém, 4800-058 Guimarães, Portugal
[b] Department of Mining Engineering, University of Chile, Avenida Tupper 2069, Santiago, Chile
[c] Advanced Mining Technology Center, University of Chile, Avenida Beauchef 850, Santiago, Chile
[d] Algoritmi Research Centre, University of Minho, Azurém, 4800-058 Guimarães, Portugal
[e] Portuguese National Laboratory for Civil Engineering - LNEC, Lisboa, Portugal

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ABSTRACT

Nowadays, the prospection plans have the difficult task of ensuring a more complete and rich characterization of the rock mass for the purpose of optimizing costs and increasing safety in geotechnical projects. Currently, boreholes location and depth are mainly defined based on experience and know-how of professionals, as such, it is user-dependent. Hence, there is a lack of methodologies to help the decision-makers in defining the optimal location of boreholes (with relevant information). Therefore, this paper presents a methodology based on the use of geostatistical conditional simulation allied to a stochastic global optimization algorithm (Simulated Annealing) to develop optimized boreholes plans comparing a uni-objective and a multi-criteria optimization approaches. In this work, the optimized location is considered the one that minimizes uncertainty translated by either the average local variance or the average width of 95% probability intervals of simulated values at unsampled locations. This methodology was applied using preliminary information obtained from previously executed boreholes using as variable the empirical rock mass classification system, Rock Mass Rating, in a Chilean deposit.

1. Introduction

Rock mass prospection, mainly regarding boreholes, involves very high costs. Moreover, due to the frequently large spacing between boreholes and the fragmentary nature of the obtained data, considerable uncertainties affect the geotechnical models, mostly in highly heterogeneous rock masses. Currently, boreholes location and depth are mainly defined based on experience and *know-how* of professionals, as such, it is user-dependent. Therefore, the search for more rational ways of planning the borehole locations, as they can provide higher quality data and decrease the uncertainties, is of utmost importance, essentially in large geotechnical projects.

Usually, the time and money available for rock mass model construction is very short. The geotechnical prospection plans in large geotechnical works are generally divided into two phases: the initial phase where a preliminary and confined characterization is carried out, and a second phase where the number of executed boreholes, as well as laboratory and *in situ* tests, are significantly higher. Thus, the proposed methodology can be applied in the second phase, using the preliminary information obtained from the initial phase. This methodology intends to fill the existing gap of consolidated methodologies for this purpose, and to help professionals to optimize the boreholes position in the second phase of the prospection works by giving them information regarding the borehole quantity and depth.

In this search, a few existing methodologies for boreholes optimization combining different types of algorithms, in which the goal consists in minimizing a wide range of uncertainty measures obtained by using geostatistical techniques, were found. In detail, McBratney et al. (1981), Scheck and Chou (1983), Olea (1984) and Englund and Heravi (1994) presented methodologies to minimize the sampling requirements necessary to predict a regionalized variable at a specific level of accuracy based on the maximum or on the average standard kriging error as a global index of sampling efficiency. Subsequently, Marchant and Lark (2006) developed an approach to optimize the sampling scheme used to identify the spatial continuity (variogram) of the variable of interest. The goal was to understand what type of sampling scheme could result in more accurate variograms to use in further simulations and, consequently, reduce the sampling costs. In each phase the information from previous phases is used to generate new information and to decide if a new phase is required. As an objective

* Corresponding author.
E-mail address: marisamotapinheiro@gmail.com (M. Pinheiro).

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function, the authors minimized the developed expression to evaluate the uncertainty of variogram parameter estimation (sill, range, nugget, etc.). Van Groenigen et al. (1999, 2000) and Brus and Heuvelink (2007) presented more complex methodologies using the Simulated Annealing optimization algorithm to find the pattern for new samples that minimizes the average kriging variance. Soltani and Hezarkhani (2009, 2013b) also proposed a simulated annealing methodology, which aims to maximize the kriging variance reduction, calculated after dividing the kriging variance obtained from the initial samples with the kriging variance obtained with new additional boreholes. The same authors published a related work (Soltani and Hezarkhani, 2013a), this time combining the simulated annealing algorithm and an objective function to assess the value information that additional boreholes will bring for the deposit characterization, based on the range of reliability of each individual block resulting from its prediction. Similarly, Soltani et al. (2011) proposed the use of a genetic algorithm instead of simulated annealing, and the average kriging variance as the objective function to minimize.

These statements lead to the identification of a limitation in optimal boreholes sampling strategies, mostly because the use of kriging only results in a single outcome for the random field and the obtained uncertainty metrics (kriging variance and related metrics) do not reflect the local variability of the regionalized variable under consideration, such as proportional and regressive effects, i.e., a local dispersion that depends on the local mean value (Chilès and Delfiner, 2012). Thus, the replacement of kriging by geostatistical simulation that results in several outcomes (realizations) and, consequently, in a greater uncertainty reduction and accuracy in the spatial variability quantification of a random field, is a way to overcome the aforementioned limitation.

As previously mentioned, the proposed methodology will work as a helping tool in supporting the decision-maker when defining the prospection plans. To establish this methodology, it is necessary to combine two important techniques: the geostatistical simulation of the geotechnical variable of interest, conditionally to the available preliminary information, and an optimization algorithm known as simulated annealing (SA). The methodology can be divided into three major steps: first, preliminary information, i.e. geotechnical information resulting from preliminary boreholes, is required; second, the data should allow performing geostatistical simulation to obtain the objective functions needed in the optimization process; and the third and last step culminates by performing the optimization with SA. As a result of this optimization, it is possible to extract the optimal position for additional boreholes, the gain in terms of geotechnical details and the minimum depth of each borehole. It is worth mentioning that the methodology is of easy use and presents considerably low pre- and post-processing times.

The paper is organized as follows. The general global optimization algorithm and the developed methodology to optimize boreholes plans are presented in Sections 2 and 3, respectively. A case study is then described in Section 4, with a short introduction of the data and a presentation of the results of geostatistical simulation. In Section 5, the optimization results are presented considering uni- and multi-criteria approaches. Discussion and conclusions follow.

2. Simulated annealing

In the metallurgical industry, a thermal process named annealing aims to forge iron in order to minimize the energy spent to cool and freeze the metal. Then, the metal is heated to a maximum temperature able to change its physical properties (creating a particle disorder) and followed by slow cooling to guarantee that the final configuration of the solid is structurally superior. Simulated annealing (SA) (Kirkpatrick et al., 1983) is an iterative algorithm to solve combinatorial optimization problems inspired in this process in order to find a balanced state for each temperature, this way minimizing the internal energy of the process. In engineering problems, the use of SA has been increasing once it is an alternative to gradient-based methods or other local classical methods that can be trapped in local optima.

This algorithm starts by randomly generating a solution at each iteration, the so-called new solution (j) that emerges after random changes in the parameters that generate the previous solution (i). Then, in the case of facing a minimization problem, SA compares the objective function (OF) values for each solution. On the one hand, if $OF_j \leqslant OF_i$, solution j is automatically accepted and assumed as the temporary best solution. Under these conditions, the algorithm jumps to another iteration and new solutions are generated. On the other hand, if $OF_j > OF_i$ there is a possibility to accept solution j, even if it is a "worse" solution than solution i. By allowing these controlled uphill moves to counter the downhill moves, the algorithm is forced towards the global minimum that sometimes can be found near the worst solutions. This selection is made through the calculation of an acceptance probability (P_{accept}) that depends on a temperature parameter that decreases in a slow rhythm to avoid, once again, the algorithm to be trapped into a local minimum:

$$P_{accept} = \begin{cases} 1 & OF_j \leqslant OF_i \\ e^{\frac{-\Delta O}{T}} & otherwise \end{cases} \quad (1)$$

where in ΔO represents the difference between the OF values in the states i and j ($\Delta O = OF_j - OF_i$) and T is the control temperature. In the case of lower temperature values, the probability of accepting worse solutions is also lower, allowing SA to converge.

As previously mentioned, the initial temperature to start the process must be high enough to allow SA exploring all the space of solutions. However, during the process, the temperature is progressively reduced until a threshold value defined by the user. This cooling should be slow in order to avoid rushing the stopping criteria of the algorithm, e.g.:

$$T_j = \alpha \times T_i \quad (2)$$

where T_i represents the temperature value assumed when solution i is generated and α represents the cooling constant, whose value ranges from 0.70 to 0.99 for a fast and slow cooling, respectively (Aarts and Korst, 1989).

Besides the previously mentioned parameters, others should be defined:

- A perturbation or transition kernel, which indicates the mechanism used to generate a new solution to be tested given a current solution.
- A maximum number of allowed moves for each temperature value. This number translates the number of times that SA generates new solutions before decreasing the temperature. Once reached this maximum number of moves, the temperature is decreased using the aforementioned cooling process. Additionally, the maximum number of accepted solutions given the same temperature value must also be defined.
- A stopping criterion: this criterion can be defined based on one or more key parameters. Many authors stop SA by defining a final value for the temperature, while others add more criteria to the process (Yang, 2010; Brus and Heuvelink, 2007; Hernandez and Emery, 2009). In the present case, the stopping criterion will be composed by a temperature, an iteration number and a maximum number of rejections within a given temperature state. The latter will allow stopping the algorithm if no progress is shown.

3. Proposed methodology

3.1. Overview

In spite of the decreasing uncertainty associated with the rock mass geotechnical model, as the number of executed boreholes increases, it seems essential to optimize the number and cost of the boreholes in the prospection plans, as the location and depth of these boreholes