Dear Editor,

We, the authors, would like to take this opportunity to express our appreciation to the reviewers for their helpful comments, which have aided us significantly in improving our manuscript. According to the suggestions, we have thoroughly revised our manuscript, and its final version is enclosed. Point-by-point responses to the comments are tracked in the following text addressing all the observations and suggestions.

Geostatistical mapping of folded itabiritic rocks of the Bonito mine, Northeastern Brazil

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**Geostatistical mapping of folded itabiritic rocks of the Bonito mine,**

**Northeastern Brazil**

Mapeamento geoestatístico de rochas itabiríticas dobradas da Mina do Bonito,

Nordeste do Brasil

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**Resumo**

Avaliação de recursos minerais é a tarefa primordial em qualquer investigação geológica exploratória e é executada durante o desenvolvimento da mina. Uma abordagem simples no mapeamento geoestatístico de recursos minerais relativa à espessura mineralizada é apresentada. A Formação Serra dos Quintos aloja formações ferríferas representadas por variados tipos de itabirito. Para mapear rochas itabiríticas dobradas, baseando-se em dados precisos de espessura, métodos de estimação e simulação geoestatística foram empregados. Os métodos de krigagem são frequentemente utilizados por razões práticas. Contudo, algumas vezes as estimativas podem ser suavizadas e não representar toda a amplitude original dos dados. Métodos de simulação podem fornecer várias imagens estocásticas. Entretanto, a precisão local nem sempre pode ser garantida. O método *simulated annealing* foi utilizado no ajustamento das estatísticas hglobais e preservação da precisão local. Por fim, ficará demonstrado que as áreas mais espessas das formações ferríferas bandadas (itabiritos) podem corresponder a uma dobra antiformal como a feição tectônica dominante na área de estudo.

**Palavras-chaves:** Itabiritos; simulação condicional; Formação Serra dos Quintos.

**Abstract**

Mineral resource evaluation is the primary task of any exploratory geological investigation and is performed even during the mine development. A simple approach for the geostatistical mapping of mineral resource pertaining to mineralized thickness is presented. The Serra dos Quintos Formation hosts iron formations represented by assorted itabirites. To map folded itabiritic rocks based on thickness data accurately, geostatistical estimation and simulation methods were employed. Kriging methods are often used for practical reasons; however, sometimes the estimates can be smoothed and do not represent the entire original data range. Simulation methods can yield several stochastic images. However, local accuracy cannot always be guaranteed. Simulated annealing was performed by adjusting the global statistics and preserving the local accuracy. Finally, we demonstrated that the banded iron formations’ thicker areas may correspond to the antiform fold as the dominant tectonic feature in the study area.

**Keywords:** Itabirites; conditional simulation; Serra dos Quintos Formation.

**1 Introduction**

Mineral resource evaluation is often performed by estimating grades and tonnages. It is fundamental to the economic feasibility of mines. Hence, exploratory drilling programs must yield the appropriate data for geological modeling. This must include operational drilling data, lithological/stratigraphic intervals, structural descriptive features, and geotechnical parameters. Another source of data can be associated, e.g. geophysical profiling, hydrological and structural measurements.

Geological modeling includes many approaches to geological problems. The most typical would be the geometry of ore bodies. Volumetric methods are applied to create tridimensional shapes with an emphasis on distinguishing each lithological type individually. The ore bodies can be referred to as an individual lithological type or as a separated lithology. Structural features such as fractures, fault planes, and shear zones, if they exist, can be integrated into the model (Mallet, 2002).

Geostatistical evaluation, a mineral resource assessment tool, may be classified as a special case of geological modeling. The theory presented by Matheron (1963,1965), which is based on the pioneering study by Krige (1951) on South African mines, exhibits a complete applied statistical innovation for addressing mining geology problems. The concepts of spatially dependent variance and ore grade estimation procedures have contributed to the progress in mining science and technology. Estimation methods were developed to determine metal grade values and evaluating the uncertainty attached to estimates (Journel & Huijbregts, 1978).

The main goal of this study is to enhance the geometric feature of the mineralized thickness (as geological feature) and to discuss its geological significance in terms of structural control. Hence, this study shall not be as conclusive as a 3D geological model. Meanwhile, mapping the mineralized thickness may yield quicker information concerning the most interesting mining spots with known metal grade range in a mining site. The 2-D model to be generated is an isopach map that will depict the different thickness’ zones throughout the study area.

The first step of this investigation is to evaluate how estimation methods (that are based on the assumption of local accuracy) can give the responses in terms of spatial variability and estimates. Alternatively, we must consider other methods when the estimation outcomes are not sufficient to describe the regionalized variable of interest. The second step is related to how local accuracy can be embraced by other geostatistical methods (such as the stochastic simulation methods) building a geospatial model depicting the mineralized thickness of BIF rocks in the study area.

The study area is located at Bonito mine, Northeastern region of Brazil. Low-grade iron ore constrained by the banded iron formations (itabirites) that have been previously studied by Barbosa (2013), Fonteles *et al.* (2019), and Fonteles *et al.* (2020) was the target of this research. Regional mapping works by Van Schmus *et al.* (2003) and Angelim *et al.* (2006) recongnized the the BIF rocks as a relevant lithotype in the Serra dos Quintos Formation owing to its geological significance (See Figure 2 for reference).

To achieve the goal proposed in this study, geostatistical estimation and simulation methods were employed. Although the “best” method to reach the expected results is not the primary aim of this study, few experiments must be performed to improve the analytical tasks involved (Boufassa & Armstrong, 1989; Deutsch, 1992; Journel, 1994; Goovaerts, 1998; Soares, 2001; Paravarzar *et al.* 2015).

In this study, a geostatistical map of folded BIF rocks based on thickness is presented. When using the mineralized thickness as a regionalized variable, we here approach a mining attribute of the BIF rocks within the geological formation of interest (in this case, the Serra dos Quintos Formation). Although three-dimensional (3D) geological modeling provides comprehensive lithological information, thickness modeling can be more able to enhance specific embedded structural features without any cutting-edge modeling techniques.

**2 Geological setting of the study area**

**2.1 Lithostratigraphy**

As part of a major geotectonic feature (Borborema Province, NE Brazil), the geological setting of the Bonito mine is defined by the Poço da Cruz Suite that is composed of augen leuco-gneiss with quartz-monzonitic to granitic composition rocks overlapped by the Seridó Group, described by Angelim *et al.* (2006) as a metasedimentary sequence formed by the following units: Serra dos Quintos Formation (BIFs, marble, ferruginous quartzite, amphibolite, and schist), Jucurutu Formation (primarily paragneiss, marble, quartzite, iron formations and metaconglomerate), Equador Formation (muscovite-quartzite) and Seridó Formation (feldspathic mica schist) (Figure 2). The BIF rocks of the Serra dos Quintos Formation gather an assembly of itabirites (proto-iron ore types) previously studied by Barbosa (2013), Fonteles *et al.* (2019a), Fonteles *et al.* (2019b) and, Fonteles *et al.* (2020).

Earlier studies performed during the 1980s suggest a poly-orogenetic evolution model explaining the collage and tectonic evolution of the Borborema Province, Northeastern Brazil. However, on the grounds of structural surveys (Caby *et al.*, 1991, 1995; Hackspacher *et al.*, 1997) and geochronological research (Van Schmus *et al*., 2003), the deformational history of the Seridó Group has been ascribed to a monocyclic evolution model developed throughout three primary events under the same metamorphic conditions during the Brasiliano/Pan-African orogeny.

According to Hackspacher *et al.* (1997), the tectono-metamorphic history can be summarized by a transitional and progressive deformation from a primary thrust in a syn-collisional regime to a secondary and local strike-slip regime, both in similar metamorphic conditions.

Figure 1Simplified geological map of the study area (Adapted after Angelim *et al.* 2006).

**2.2 Tectonic framework**

In the northern region of Patos shear zone, i.e. the Northern Borborema Province, the first noticeable deformation event (D1/D2) is referred to as the Brasiliano orogeny with WNW thrusts associated with isoclinal folding and penetrative subhorizontal or mylonitic foliation (S2) (Figure 2). This event is succeeded by transcurrent tectonics (D3) that created a vertical or mylonitic foliation (S3) related to expressive dominant dextral transpressional shear zones in the NE-SW direction generating positive flowers structures. Hackspacher *et al.* (1997) suggested that the thrust regime occurred between 650 and 580 Ma, whereas the strike-slip regime was developed from 580 to 500 Ma.

The subhorizontal foliations associated with the D2 phase are present in the Bonito Mine establishes an expressive antiformal fold with an N-S axial plane and dip-direction heading south. The itabirites are positioned at the central sector whereas the marble of the Jucurutu Formation surrounds the external border of the great fold (See Figure 1 for reference).

Figure 2(**a**) BIFs are seen in the most elevated terrains at the mining site whereas marble is displayed in the first plan as gray massive folded rocks. (**b**) Hematitic itabirite outcropped at the higher grounds corresponding to the hinge of the Bonito antiform. (**c,d**) Folded BIF rocks exhibit the field relations of S1/S2 foliations. (Photo 2a was adapted from Barbosa, 2013).

**3 Materials and methods**

3.1 Thickness data

The database used in this study was exploited from a geological databank that has been structured to gather data and information depicted from an exhaustive exploratory drilling program at the study area executed by the mineral right’s owner, MHAG Mineração e Serviços S/A company. A survey was performed throughout the entire databank to extract the available thickness data values (measured in meters) from drill core logs that intersected the BIF rocks (itabirites) pertained to the Serra dos Quintos Formation (Figure 1). Based on the typological model proposed by Fonteles *et al.* (2020), three BIF types were pre-selected owing to their Fe2O3 grades. Hematitic itabirites, magnetitic itabirites, and martitic itabirites represent BIF types with 44.61% Fe2O3 mean grade (Table 1).

It is noteworthy that not all drilling boreholes have reached the mineralized strata owing to the geological setting of the study area. Therefore, from 126 drilling cores, we could analyze 78 that constitute the BIF types of interest.

|  |  |
| --- | --- |
| BIF type | Fe2O3 mean grade (%) |
| Hematitic itabirite | 46.32 |
| Magnetitic itabirite | 37.45 |
| Martitic itabirite | 40.68 |

Table 1– Fe2O3 mean grades of the selected BIF types

The data analyses were executed using the Geostatistical Modelling Software (GeoMS - CMRP/IST) and the spatial database management was handled using ESRI ArcGIS® 10.1.

Figure 3 Map showing location of the data points.

**3.2 Geostatistical applied methods**

In this section, a comprehensive exposition of the theory of geostatistical modeling owing to its wide-spread knowledge will be not presented. Instead, a summary of some methods used in this study will be presented.

*3.2.1. Spatial variance analysis and estimation tool*

According to the classic theory and practice presented by Matheron (1963, 1965), Journel & Huijbregts (1978), and Goovaerts (1997), variographic analysis is a simple and powerful tool for spatial dispersion assessment based on the averaged quadratic difference between two points in *R* space. Experimental semivariograms alone are insufficient to describe spatial phenomena, thus, adjusted theoretical models will yield structural parameters for estimation methods, widely known as kriging. The experimental semivariogram is, thus, expressed by

|  |  |
| --- | --- |
|  | (1) |

for estimation of the spatial variance between two points (*xi*and *xi+h*) separated from each other by the experimental Euclidean distance *h*. The structural parameters for variogram modeling are obtained by adjusting a theoretical model to the experimental semivariogram (Figure 4).

Figure 4 Some usual theoretical semivariogram models. (Source: https://www.aspexit.com/en/variogram-and-spatial-autocorrelation/)

Kriging estimators form an extensive ensemble of linear and nonlinear interpolators to address stationary and nonstationary phenomena (Krige, 1951; Deutsch & Journel, 1992). Some of them were developed to address Gaussian, multi-Gaussian, and non-Gaussian distribution functions. In addition to the interpolated values, an estimation variance measure is available despite some criticism that emerged concerning the usefulness of such a measure (Yamamoto, 2000; 2008).

Among the linear interpolators, ordinary kriging (OK) can be considered the most used method hitherto. Based on the OK theory, the phenomenon to be investigated is second-order stationary but its mean is assumed unknown. Thus, neighboring kriging weights are set to total to 1 (Boufassa and Armstrong, 1989; Goovaerts, 1997). Estimation of an unknown value *z\*(x0)* by OK is given by

|  |  |
| --- | --- |
|  | (2) |

where *λi* is the ith weight obtained by equation system resolution related to the experimental semivariogram modeling and *z(xi)* is the ith spatial data point used in the estimation process. The OK system is based on the unknown global mean, hence, the estimates are constrained by kriging weights summation:

|  |  |
| --- | --- |
|  | (3) |

and the OK variance is, thus, expressed by

|  |  |
| --- | --- |
|  | (4) |

where *C* is the spatial covariance and *µ* is the Lagrange operator that mathematically stabilizes the OK equation system.

The primary criticism of kriging estimation is related to smoothing issues that are obvious when the original extreme values of the data range are underestimated and/or overestimated. Many authors have addressed these problems over the years (Journel, 1974; Journel & Huijbregts, 1978; Boufassa & Armstrong, 1989; Deutsch & Journel, 1992; Yamamoto, 2008). Nonetheless, this interpolation method continues to be applied in several geological situations.

*3.2.2. Geostatistical simulation*

Stochastic simulation has been applied to Earth Sciences problems since the 1970s, however, its effectiveness has always relied on the computational capacity of the machines of that time. Geostatistical simulation methods have evolved along with the kriging methods and exhibit the same appeal, but with different purposes (Journel, 1974). Currently, assorted options of simulation algorithms have been developed and become available to users through private-use and freeware computational programs since the 1990s.

Simulated Annealing (SA) as a stochastic simulation method differs from other simulation techniques far owing to the particular solution given to a problem related to thermal interaction between particles through a numerical implementation of an optimization technique (Metropolis *et al.* 1953). The “annealing” model was developed by comparing the melting process of a single crystal and subsequently reducing the temperature to control its annealing that can be monitored by stages until the system reaches its “freezing point” (Kirkpatrick *et al.,* 1983). Geman & Geman (1984) extended the concept of SA to restore degraded images by applying Bayesian and Markovian statistics.

The SA algorithm instructs the creation of a 3-D model by thermal perturbation that imputes random values obtained from a histogram at each data location. The next step is related to the objective function (O) that is described as the average squared difference between the semivariogram of the simulated image [γ\*(h)] and the previous semivariogram model [γ(h)] for each stochastic realization achieved:

|  |  |
| --- | --- |
|  | (5) |

The image (3-D model) is eventually perturbed by swapping a pair or sets of values, randomly. SA requires a convergence criterion explicitly by the gradual decrease in temperature (parameter of the Boltzmann’s distribution). When swapping stops, the final “annealed” image, e.g. stochastic realization, is generated (Deutsch, 1992; Deutsch & Cockerham, 1994; Goovaerts, 1998).

**4. Results of geostatistical modeling**

4.1. Exploratory analysis

Exploratory data analysis revealed a positively skewed pattern histogram (Figure 5). Spatial variance patterns were explored through variographic analysis to model the sample spatial dependency, considering the lag spacing of 50 m. The process went through several interactive attempts to find valid variographic structures. After that, two experimental directional semivariograms were obtained capturing spatial variance structures related to 30º Az and 300º Az (or -60, by software default). The 30º Az structure shows a longer data spatial continuity through that direction compared with its orthogonal component (300º Az). This pattern is crucial in the definition of the ellipsoid search parameters in kriging and simulation procedures (Figure 6).

Figure 5 Histogram cumulated and the distribution function plot.

Spherical models were adjusted to the experimental semivariograms and represented by the following equations:

Figure 6Adjusted experimental semivariograms on the orthogonal directions.

4.2. Estimating the BIF thickness

The irregular sample spacing shows that some sectors were more densely drilled than others (Figure 3). An average sample distance of 49 m was measured to aid the estimation/simulation gridding design. Thus, the size of the square grid spacing was set to 20 m × 20 m. The moving search ellipsoid was configured to consider the variographic anisotropic range. Thus, 4,101 blocks were estimated.

To minimize edge effects, a minimum of four points and a maximum of eight were selected within the search radii. Furthermore, the geological contact between the BIF and other lithologies was used as a graphical mask avoiding the unnecessary extrapolation far beyond the geological boundaries of the BIF in Serra dos Quintos Formation (See Figure 1 for reference).

The first round of geostatistical modeling was initiated with ordinary kriging (OK) estimation. OK estimates were processed based on unknown mean and second-order stationarity (Figures 8 and 9). The cross-validation test, as stated by Isaaks & Srivastava (1989), precedes the OK estimation and yields the initial figures showing how the estimation procedures whether are or are not suitable (Figure 7).

Figure 7Cross-validation scattergram for OK estimates.

Figure 8OK estimates map (a) and estimation variance map (b).

4.3. Geostatistical conditional simulation

To overcome the smoothing issues due to OK estimation, Simulated Annealing (SA) was applied to adjust the global data accuracy to the local exactitude. Following the basic idea of the method, an initial image (the training image) was perturbed by swapping two data pairs at a constant temperature with a reduce factor of 0.01 from the initial temperature (T0 = 1), during 250,000 iterations. A further number of iterations did not show any improvements in the final simulated image.

The objective functions that were applied to reach convergence are denoted by the spherical adjusted models. The BIF thickness map was produced as an annealed image concealing the original sample data to the simulated data (Figure 9).

Figure 9Thickness map produced as an image on SA simulation. The white spots are related to those nodes which were not able to be simulated.

To validate the SA simulated image, we constructed new semivariograms to assess the spatial variance of this stochastic realization. The search window was the same as that used in the prior variographic exploratory analysis (see section 4.1). As suggested by Leuangthong *et al.* (2004), the SA data histogram was obtained and indicated that not all descriptive statistics were reproduced (Table 2; Figures 10 and 11).

Figure 10Conditional histogram and distribution function of simulated BIF thickness data in the study area reproduced by simulated annealing.

Figure 11Adjusted semivariograms of simulated mineralized thickness values by simulated annealing method.

|  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- |
| **Data source** | **Mean** | **Median** | **Min.** | **P*25***\* | **P*75***\* | **Max.** | **Variance** | **C.V.**\* |
| Thickness | 32.00 | 27.00 | 2.00 | 17.00 | 41.00 | 91.85 | 442.72 | 0.66 |
| OK | 28.32 | 25.94 | 2.50 | 18.83 | 34.46 | 89.97 | 213.99 | 0.52 |
| SA | 32.45 | 27.13 | 2.00 | 17.20 | 44.52 | 91.85 | 424.09 | 0.63 |

\*P25 - 25%; P75 - 75%; C.V. - coefficient of variation

Table 2Comparative statistical summary of the estimation and simulation output data.

**5 Discussion**

The positively skewed histogram has revealed a possible data trend. In the first round of geostatistical analysis of the BIF thickness, OK method was applied. In the second-order stationarity model for natural phenomena, the high nugget effect on semivariograms tends to contribute to smooth kriging estimates. The cross-validation test unveiled that the correlation between thickness’ sample values and their estimates suffers from a considerable dispersion in the scattergram (See Figure 7 for reference).

OK estimates, as clearly reported by Boufassa & Armstrong (1989) and Yamamoto (2000; 2008), are smoothed (Table 2). In this particular case, some theoretical semivariogram models were tested (spherical, exponential, and Gaussian) to obtain less smoothing estimation results such that the spherical model yielded the best fit. Gaussian models were interactively adjusted to the experimental semivariogram. From these attempts, unrealistic negative kriged thickness values emerged. The exponential model provided slightly smoother estimates than the spherical model.

Kriging variance values represent minimized squared differences that tend to increase in sectors with low sampling (Journel, 1974; Yamamoto, 2000). Lower kriging variance values are closely associated to sampled spots; conversely, the higher ones are related to the unsampled sites.

SA allows for the simulation of a quenching process where one pair of data points at one time is swapped until the number of iterations is reached. The entire process is mathematically forced by the algorithm constraining the local data (original data values) to match the local simulated values on their grid positions.

Once the primary statistical features were acceptably reproduced, using an equal direction component weighting improved the stochastic simulation. Furthermore, the scheme used allowed for the local raw data to be perturbed (Deutsch & Cockerham, 1994). The upgraded stochastic image exhibited the thicker mineralized BIF rocks that match to a fold axis region of an antiform heading south. (Figure 12).

Figure 12 BIF thickness map. The geometric space was constrained to the geological boundaries of the Serra dos Quintos Formation (NPsq). The black arrow heading south refers to an antiform fold axis. Simplified geological map based on Angelim *et al.* (2006).

**6 Conclusions**

Spatial thickness assessment indicated that estimation methods such as OK could be applied as a first step in the modeling process. OK variance values revealed a measure of uncertainty in some areas, primarily those with low sampling spots. The smoothing effect related to these estimation methods cannot be avoided without any post-processing technique (Yamamoto, 2008; Zhao *et al.* 2014).

The SA method was not performed unconditionally, inasmuch as the goal of this study was to map the thickness surface so accurately as possible. Hence, the stochastic simulation represented both global statistics of the target histogram and local data honoring.

The BIF thickness map assembled by stochastic simulation provided a clear delimitation of the thicker areas that may correspond to the most deformed strata of the BIF within the Serra dos Quintos Formation in the Bonito Mine (Figure 12) in the hinge of the Bonito Fold. Tang *et al.* (1987) when studying some Precambrian BIFs in South China also observed such a situation. Similarly, Cao *et al.* (2018) studied the deformation on folded coal seams in Northwest China. Despite the small area of the mining site, the folded BIF rocks may match a compressional area that was formed during the most intense phase of the overthrusting of the Seridó Group.

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