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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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Abstract

Geological modeling is the primary task of any exploratory geological investigation, and it is performed even during the mine development. In the study area, the Serra dos Quintos Formation hosts banded iron formations represented by assorted itabirites. The database used in this work was exploited from a geological databank which was structured to gather data and information depicted from an exhaustive exploratory drilling program. A survey was performed throughout the entire databank to collect the available thickness data values (measured in meters) from drill core logs that intersected the itabirite. Since structural heterogeneities can occur within these rocks, this study aims to identify such features. Geostatistical estimation and simulation methods were employed to map folded itabiritic beds based on thickness data accurately. Kriging estimators are often used for practical reasons; however, sometimes, the estimates can be smoothed and do not represent the entire original data range. Simulation algorithms can yield several stochastic images, but local accuracy cannot always be guaranteed. Simulated annealing was performed by adjusting the global statistics and preserving the local accuracy. We demonstrated that the banded iron formations' thicker areas might correspond to the antiform fold as the dominant tectonic feature in the study area. Finally, we show that the simulated thickness map discloses the thicker mineralized spots. Meanwhile, the thinner ones may unveil intrinsic structural heterogeneities mainly observed at the limbs of the Bonito fold, where intensive deformation within the itabiritic layer was higher than expected. Concerning the mining issues, information obtained from the simulated thickness map could provide ancillary data to improve mining planning in the study area.

Keywords: Itabirites; Conditional simulation; Serra dos Quintos Formation

Resumo

O modelamento geológico é tarefa primordial em qualquer investigação geológica, tanto na fase exploratória quanto durante o desenvolvimento da mina. Neste trabalho é apresentada uma abordagem simples relacionada ao mapeamento geoestatístico de recursos minerais, relativa à espessura do corpo mineralizado. A Formação Serra dos Quintos aloja formações ferríferas bandadas representadas por tipos variados de itabirito. A base de dados utilizada neste trabalho foi obtida a partir de um banco de dados geológicos que foi estruturado para armazenar dados e informações oriundas de um extenso programa de sondagens na área. Um levantamento foi executado em todo o banco de dados com o objetivo de coletar valores de espessura (em metros) em perfis de sondagem que interceptaram os itabiritos. Tendo em vista que heterogeneidades estruturais nestas rochas possam ocorrer, objetivou-se realizar um modelamento geoestatístico para, possivelmente, identificá-las. Para mapear rochas itabiríticas dobradas, baseando-se em dados precisos de espessura, foram empregados métodos de estimação e simulação geoestatística. 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; porém, a precisão local nem sempre pode ser garantida. O método *simulated annealing* foi utilizado no ajustamento das estatísticas globais e preservação da precisão local. Como resultado, observa-se 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. O mapa de espessuras simuladas revelou setores mais espessos e aqueles mais delgados que podem indicar heterogeneidades estruturais intrínsecas, preferencialmente observadas nos flancos da dobra do Bonito. Isto sugere a existência de zonas localizadas onde a deformação pode ter sido mais intensa do que o esperado. Com relação ao aspecto do aproveitamento mineral, o mapa simulado de espessura das rochas itabiríticas pode prover informações que auxiliarão no incremento do planejamento da lavra.

Palavras-chaves: Itabiritos; Simulação condicional; Formação Serra dos Quintos

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1 Introduction

Mineral resource evaluation is often performed by estimating grades and tonnages, which is fundamental to the economic feasibility of mining projects. Hence, exploratory drilling programs must yield the appropriate data for geological modeling. This approach must include operational drilling data, lithostratigraphic intervals, structural features, and geotechnical parameters. Geophysical profiling, hydrological and structural measurements can be associated sources of data. The integration of databases from different sources is the basis for three-dimensional modeling, which includes many approaches to geological problems, mainly for estimating the geometry of ore bodies. Volumetric methods can 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 occur, can be integrated into the model (Mallet 2002).

Geostatistical evaluation, a mineral resource assessment tool, may be classified as a particular 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 mining science and technological progress. Estimation methods can aid in determining metal grade values and evaluating the uncertainty attached to estimates (Journel & Huijbregts 1978).

The study area is located at the Bonito mine, Northeastern Brazil (Figure 1), where low-grade iron ore is constrained by the banded iron formations (itabirites), which were previously studied by Barbosa (2013), Fonteles et al. (2019a) and Fonteles et al. (2020). The regional mapping works by Van Schmus et al. (2003), and Angelim, Medeiros and Nesi (2006) recognized the BIF rocks as a relevant lithotype in the Serra dos Quintos Formation owing to their geological significance. As shown in Figure 2A, the itabirites stand in the landscape as an elevation form reaching 415 meters high.

We aim to identify unexpected local structural features in folded strata. Some simulation algorithms such as the simulated annealing method have on its core the assumptions of constraining physical phenomena and may provide the means of geomathematical identification of such structures. Hence, this study shall not be as conclusive as a 3D geological model. Mapping the mineralized thickness may yield quicker information concerning the most interesting spots with a 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.

Mineralized thickness values can change from one spot to another at the mine site due to structural constraints. Predicting and establishing thickness patterns in such situations can be tricky due to its spatial variability. Although spatial interpolation algorithms are available and some are currently applied to geological issues, geostatistical methods can overcome uncertainty drawbacks and predict variance errors regarding the estimation techniques.

The first step of this investigation is to evaluate how estimation methods (based on the assumption of local accuracy) can give the responses in terms of spatial variability and estimates. Alternatively, we must consider other ways when the estimation outcomes are insufficient 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.

Geostatistical estimation and simulation methods were employed to achieve the goal proposed in this study. Although the "best" approach to reach the expected results is not the primary goal 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, Emery & Madani 2015).

In this study, a geostatistical map of folded BIF rocks based on thickness is presented. Although three-dimensional (3D) geological modeling provides comprehensive lithological information, and thickness modeling can be more able to enhance specific embedded structural features without any cutting-edge modeling techniques. Meanwhile, increasing the knowledge of where the BIF-hosted ore is more expressively deformed can be crucial for mining planning.

2 Geological Setting of the Study Area

2.1 Lithostratigraphy

As part of a significant 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, Medeiros and Nesi (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 assemblage of itabirites (proto-iron ore types) previously studied by Barbosa (2013), Fonteles et al. (2019a), Fonteles, Pereira and Veríssimo (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 (Sá 1984). 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.

2.2 Tectonic Framework

In the northern region of Patos shear zone, i.e., the Northern Borborema Province, the first noticeable deformation event (D_1/D_2) is referred to as the Brasiliano orogeny with WNW thrusts associated with isoclinal folding and penetrative subhorizontal or mylonitic foliation (S_2) (Figure 2D). This event is succeeded by transcurrent tectonics (D_3) 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 D_2 phase are present in the Bonito mine establishing 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).

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 rights 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 Fe_2O_3 grades. Hematitic itabirites, magnetitic itabirites, and martitic itabirites represent BIF types with a 44.61% Fe_2O_3 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 (Figure 3).

The data analyses were executed using the Geostatistical Modelling Software (GeoMS – CMRP 2000), and the spatial database management was handled using ESRI ArcGIS® 10.1.

3.2 Geostatistical Applied Methods

This section will not present a comprehensive exposition of the theory of geostatistical modeling owing to its widespread knowledge. Instead, a summary of some methods used in this study will be given.

3.2.1. Spatial Variance Analysis and Estimation Tool

According to the classic theory and practice presented by Matheron (1963, 1965), Journel and 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.

Kriging estimators form an extensive set 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.

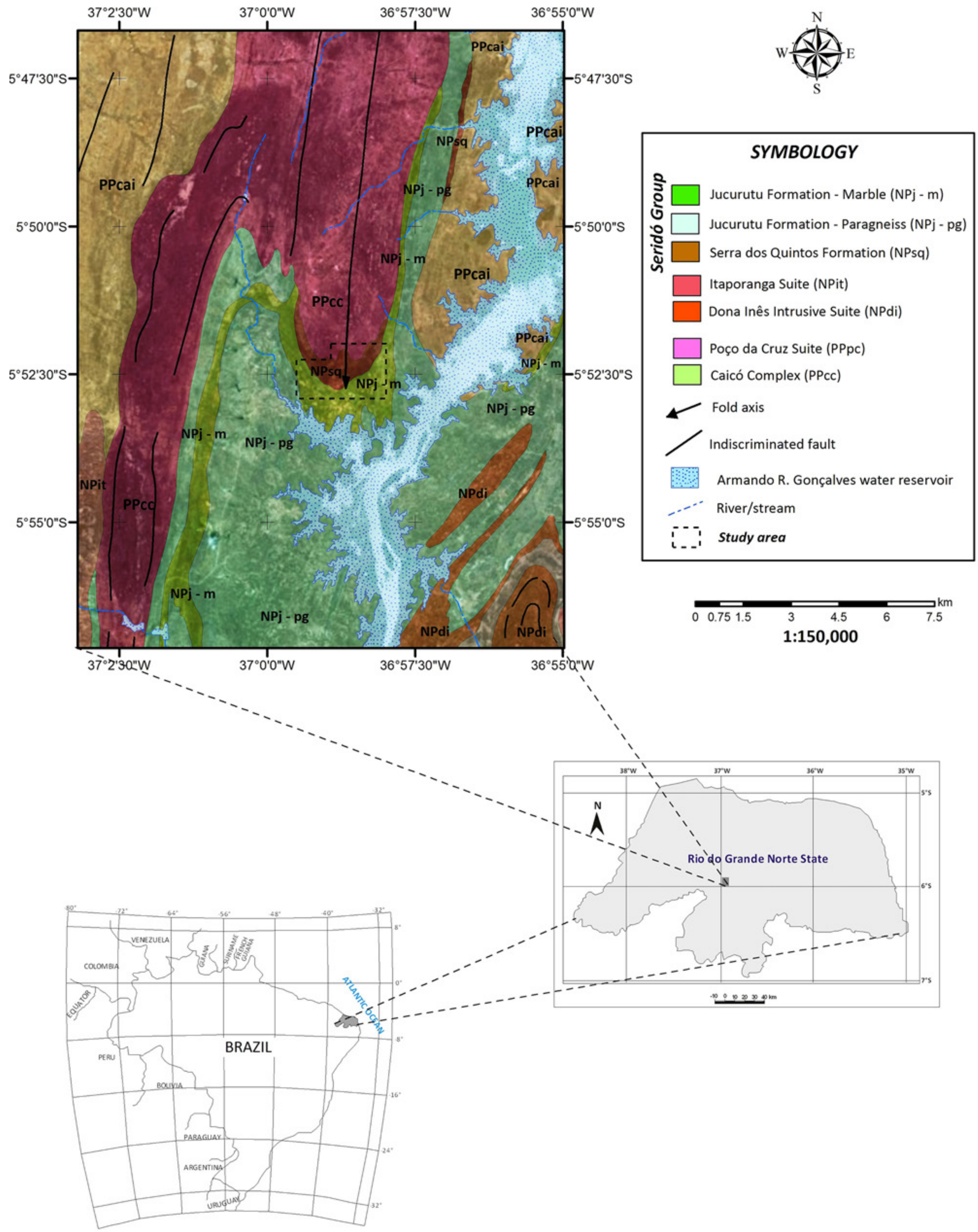


Figure 1 Simplified geological map of the study area (Adapted from Angelim et al. 2006).

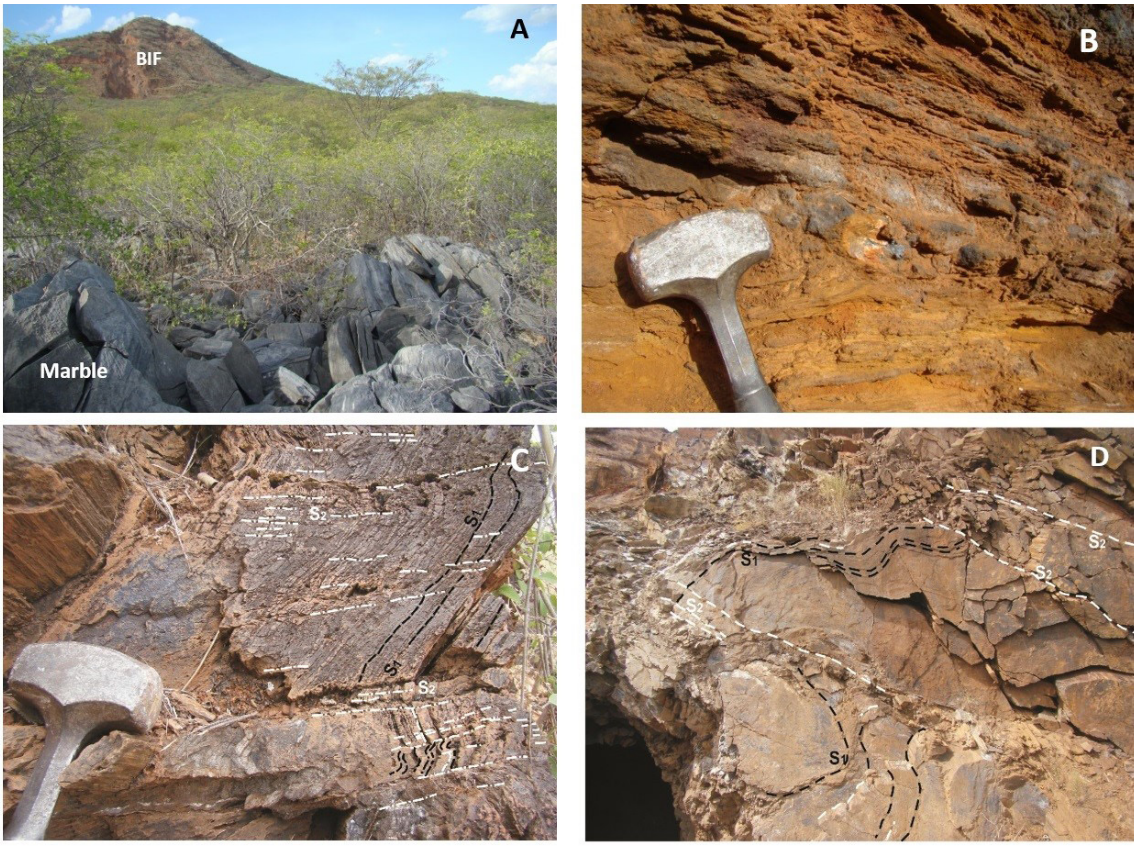


Figure 2 A. BIFs are seen in the most elevated terrains at the mining site, whereas marble is displayed as gray massive folded rocks in the first plan; B. Hematitic itabirite outcropped at the higher grounds corresponding to the hinge of the Bonito antiform; C and D. Folded BIF rocks exhibit the field relations of S_1/S_2 foliations. (Photo A was adapted from Barbosa 2013).

Table 1 Fe2O3 mean grades of the selected BIF types.

BIF type	Fe_2O_3 mean grade (%)
Hematitic itabirite	46.32
Magnetitic itabirite	37.45
Martitic itabirite	40.68

Additionally, an estimation variance measure is available despite some criticism 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 sum up 1 (Boufassa & Armstrong 1989; Goovaerts 1997).

The primary criticism of kriging estimation is related to obvious smoothing issues when the original extreme values of the data range are underestimated or overestimated. Many authors have addressed these problems (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. Its effectiveness, however, 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, various 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 until the system reaches its "freezing point" (Kirkpatrick, Gellat & Vecchi 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 image (3-D model) is eventually perturbed by random swapped pair or sets of values. SA requires a convergence criterion explicitly by the gradual decrease in temperature (Boltzmann's distribution parameter). The final "annealed" image, e.g., stochastic realization, is generated when the swapping stops (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 4). 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 more extended spatial continuity through that direction than its orthogonal component (300º Az). This pattern is crucial in defining the ellipsoid search parameters in kriging and simulation procedures (Figure 5).

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

$$\begin{cases} \gamma(h)_{30\,Az} = 3.35 + 404.94\left[1.5\left(\frac{h}{374.94}\right) - 0{,}5\left(\frac{h}{374.94}\right)^3\right], if\ h < 374.94m \\ \gamma(h)_{30\,Az} = 408.29,\ \ if\ h \geq 374.94m \end{cases}$$

$$\begin{cases} \gamma(h)_{300\,Az} = 41.88 + 365.55\left[1.5\left(\frac{h}{171.21}\right) - 0{,}5\left(\frac{h}{171.21}\right)^3\right], if\ h < 171.21m \\ \gamma(h)_{300\,Az} = 410.43,\ \ if\ h \geq 171.21m \end{cases}$$

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.

A minimum of four points and a maximum of eight were selected within the search radii to minimize edge effects. Furthermore, the geological contact between the BIF and other rocks was used as a graphical mask avoiding the unnecessary extrapolation far beyond the geological boundaries of the BIF in the 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 the unknown mean and second-order stationarity hypothesis (Figures 6 and 7). As stated by Isaaks and Srivastava (1989), the cross-validation test precedes the OK estimation and yields the initial figures showing how the estimation procedures are or are not suitable (Figure 6).

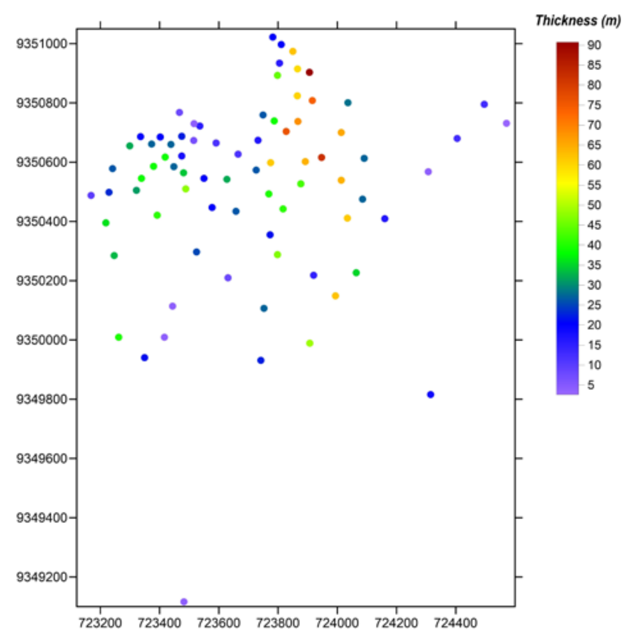
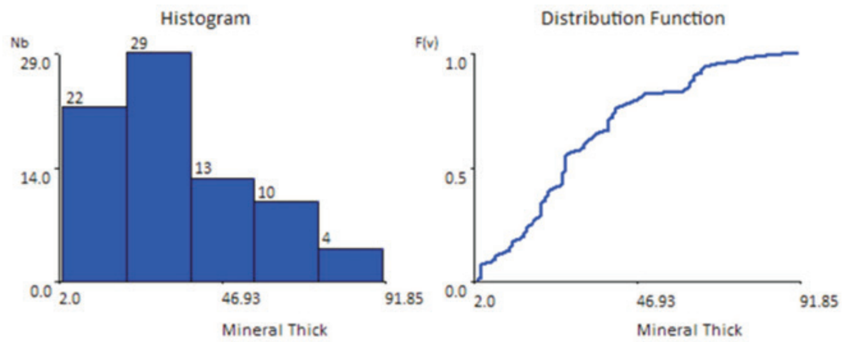


Figure 3 Map showing the location of the data points.

4.3 Geostatistical Conditional Simulation

The simulated annealing (SA) technique was applied to adjust the global data accuracy to the local exactitude to overcome the smoothing issues due to OK estimation. 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 reduced factor of 0.01 from the initial temperature ($T_0 = 1$) during 250,000 iterations. Increasing the number of iterations did not show any improvements in the final simulated image.



N	Mean	Median	Min.	P_{25}	P_{75}	Max.	Variance	Coef. Var.
78	32.00	27.00	2.00	17.00	41.00	91.85	442.72	0.66

Figure 4 Histogram cumulated and the distribution function plot.

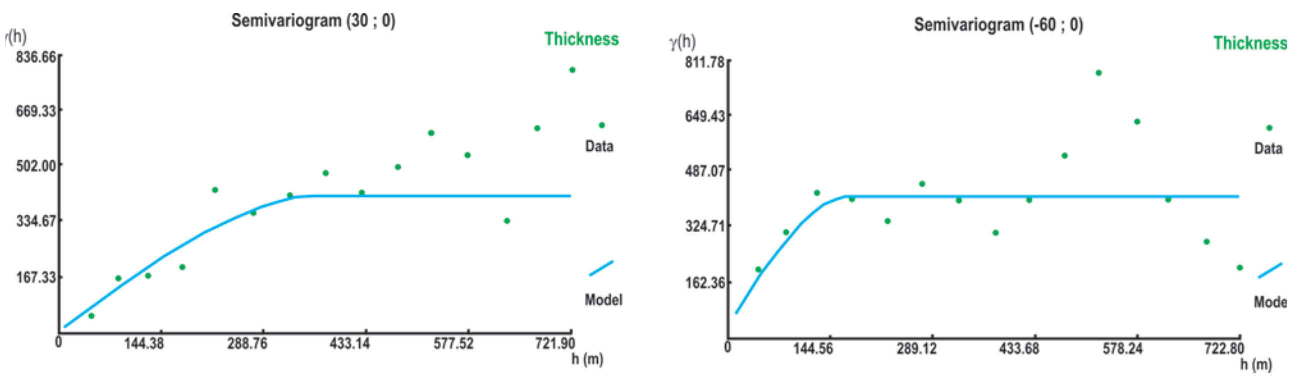


Figure 5 Modeled experimental semivariograms on the orthogonal directions.

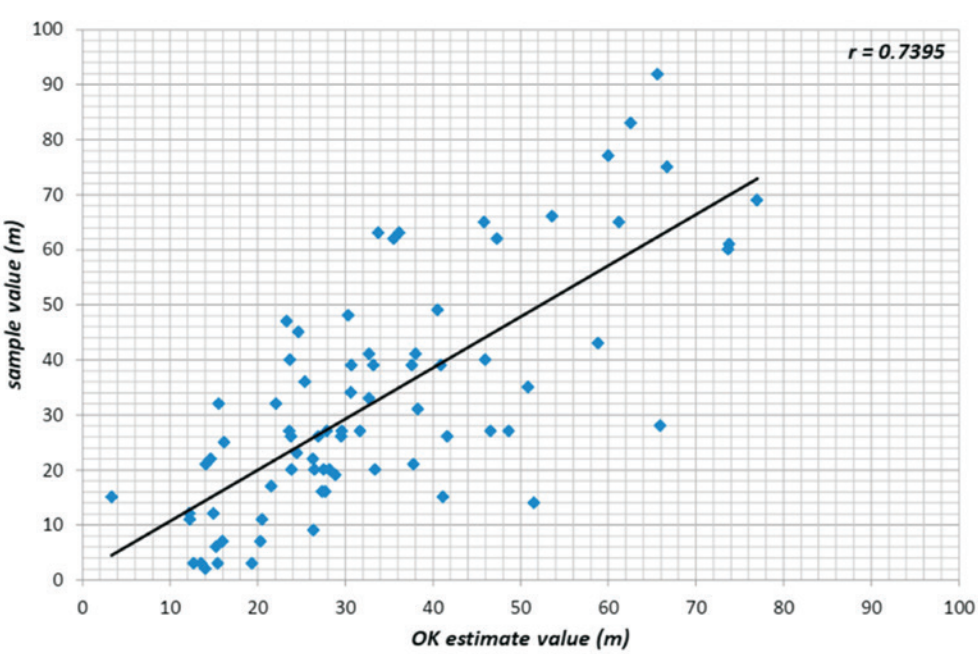


Figure 6 Cross-validation scattergram for OK estimates.

The spherical adjusted models denote the objective functions which were applied to reach convergence. The BIF thickness map was produced as an annealed image concealing the original sample data to the simulated data (Figure 8).

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 in the prior variographic exploratory analysis (see section 4.1). According to Leuangthong, Mclennan and Deutsch (2004), the SA data histogram was obtained and indicated that not all descriptive statistics were reproduced (Table 2; Figures 9 and 10).

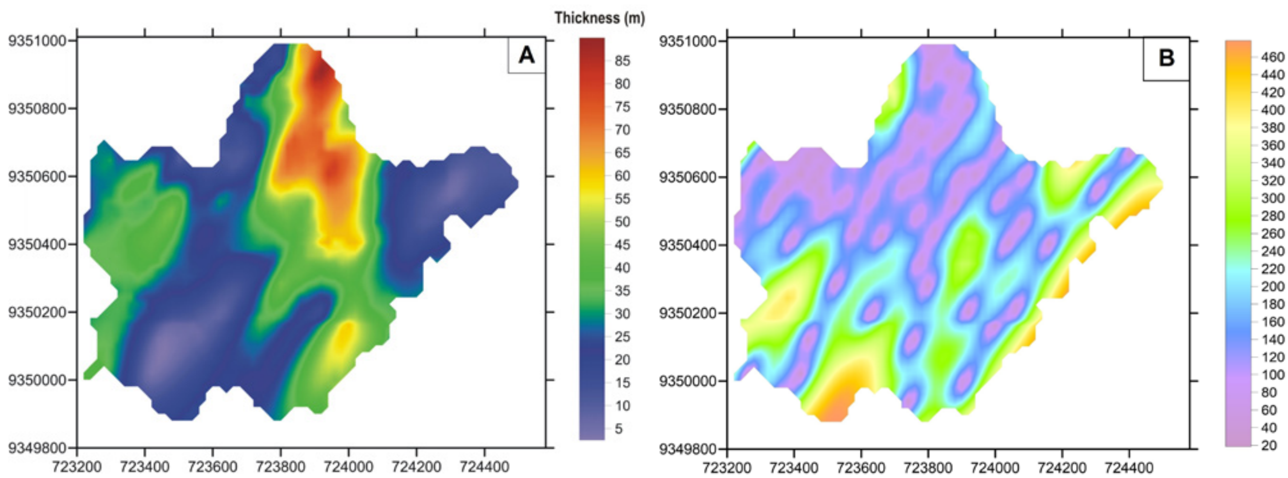


Figure 7 A. OK estimates map and; B. estimation variance map.

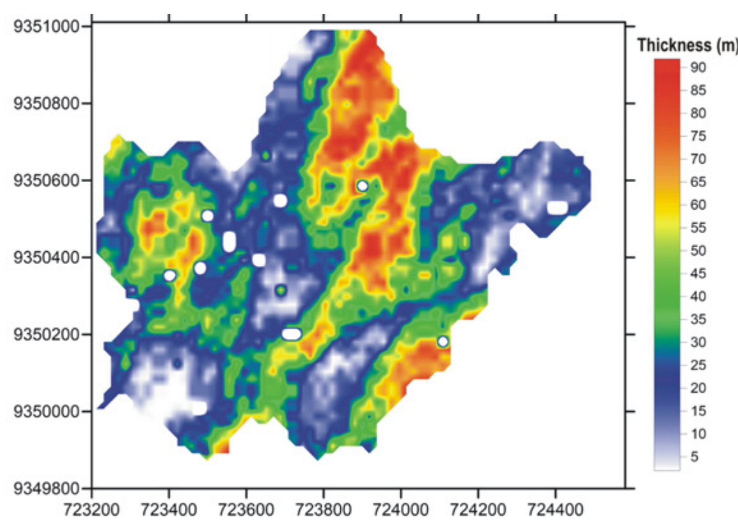


Figure 8 Thickness map produced as an image on SA simulation. The white spots are related to those nodes which were not able to be simulated.

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

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

*P_{25} - 25%; P_{75} - 75%; C.V. - coefficient of variation

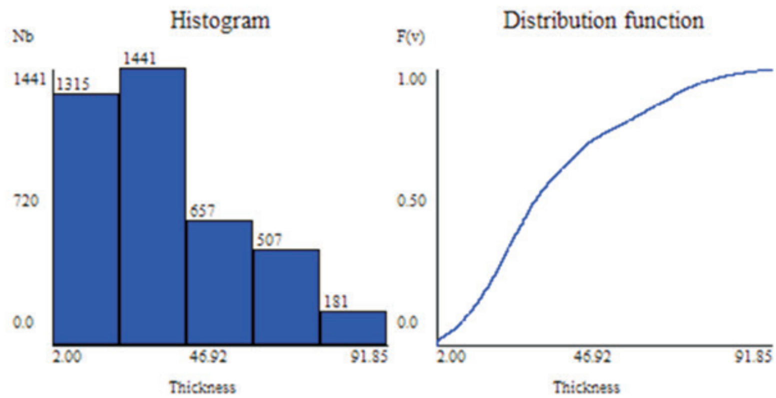


Figure 9 Conditional histogram and distribution function of simulated BIF thickness data in the study area reproduced by simulated annealing.

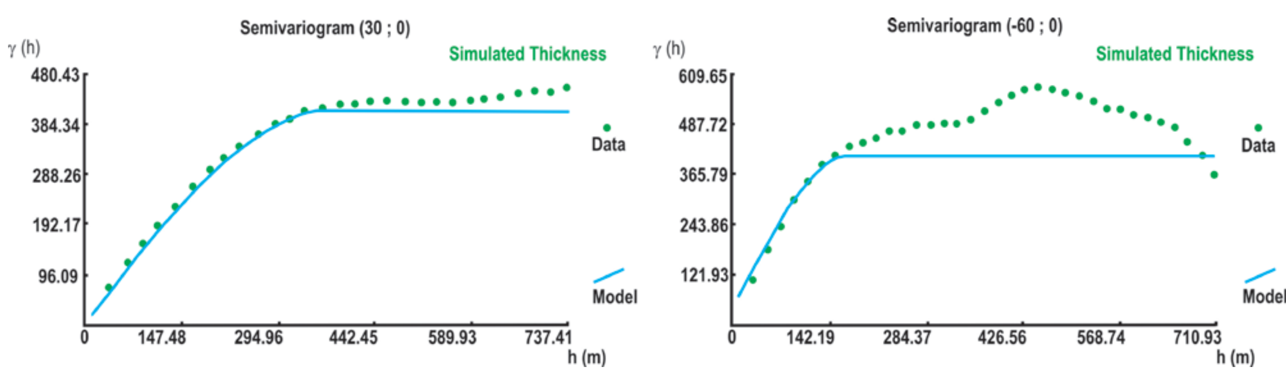


Figure 10 Modeled semivariograms of simulated mineralized thickness values by simulated annealing method.

5 Discussion

The positively skewed histogram has revealed a possible data trend. In the first round of geostatistical analysis of the BIF thickness, the OK method was applied. The high nugget effect on semivariograms contributes to smooth kriging estimates, following the second-order stationarity model for natural phenomena. 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 6 for reference).

OK estimates, as clearly reported by Boufassa & Armstrong (1989) and Yamamoto (2000, 2008), are smoothed (Table 2). In this case, some theoretical semivariogram models were tested (spherical, exponential, and Gaussian) to obtain less smoothed estimates 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 with 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 algorithm mathematically forces the entire process by constraining the local data (original data values) to match the local simulated values on their grid positions.

The primary statistical features were acceptably reproduced using an equal direction component weighting improved the stochastic simulation. Furthermore, the scheme used allowed the local raw data to be perturbed (Deutsch & Cockerham, 1994). The upgraded stochastic image exhibited the thicker mineralized BIF rocks that match an antiform's fold axis region heading south (Figure 11).

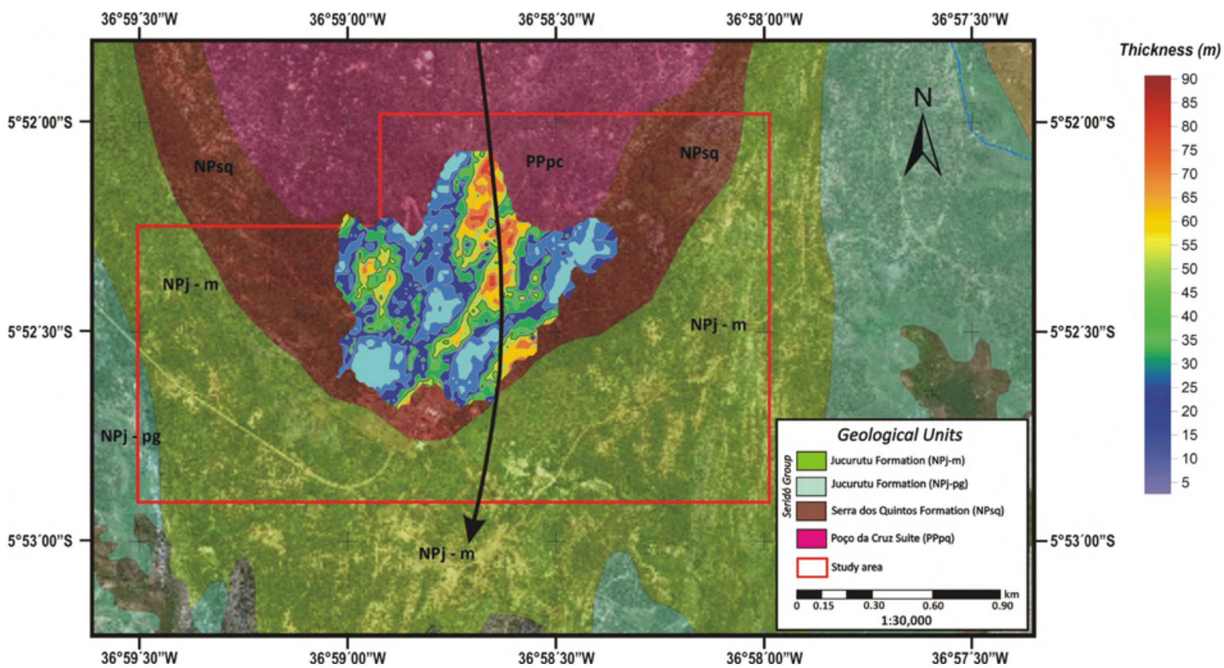


Figure 11 The simulated thickness map positioned at the Serra dos Quintos Formation. The geometric space was constrained to the geological boundaries of the geological unit of interest. The black arrow heading south refers to the Bonito fold axis. Simplified geological map based on Angelim, Medeiros and Nesi (2006).

In this study, SA simulation was presumed to reproduce the intrinsic structural heterogeneities within the itabirite. The isopach map provided by OK estimation (see Figure 7A for reference) unveils not only smoothed estimates but a forced smoothed thickness surface. Although the primary volcano-sedimentary BIF rocks could form an extensive lithological layer with a uniform thickness within the basin, it is crucial to consider the deformational events, imposing compressional strain and squeezing the itabiritic layer locally.

The simulated thinner spots – with thickness values below 25 m revealed how the assumed structural heterogeneities could be interpreted as intrinsic features of the Bonito fold's limbs (Figures 8 and 11).

6 Conclusions

Spatial thickness assessment indicated that estimation methods such as OK could be applied first in modeling procedures. 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, since 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 11) in the hinge of the Bonito fold. Jiafu, Fu and Yu (1987), when studying some Precambrian BIFs in South China, also observed such a situation. Despite the small area of the mining site, the folded BIF rocks may match a compressional area formed during the most intense phase of the overthrusting of the Seridó Group.

Instead of a smoothed image-map provided by the OK estimator, the simulated thickness image-map was interpreted, possibly reproducing intrinsic structural heterogeneities within the itabiritic rocks. Due to the SA core algorithm, the achieved unsmoothed image can disclose thinner mineralized zones where the itabiritic layer was probably more deformed at the limbs of the Bonito fold. Regarding mining issues, the simulated map of the BIF thickness can aid how to identify the most voluminous rock sectors. This ancillary information could improve the decision-making in mining planning.

Fonteles et al. (2020) proposed a typological model for itabirites from the Bonito mine. The thickness data is part of the exhaustive primary database. However, owing to the complex typological associations within the BIF rocks, identifying the most significant BIF-type within the thicker spots could not be demonstrated. It is worth mentioning that no fieldwork was executed during the investigation. Thus, no structural survey was performed to reinforce the geomathematical interpretation.

Finally, not only at the study area, the spatial modeling of thickness attribute can be used to identify spots of interest but also in other geological settings such as weathered rock masses, gold-bearing rocks at shear zones, coal seams in fold zones, etc. (Ayalew, Reyk & Busch 2002; Grijp & Minnitt 2015; Cao et al. 2018).

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Helano Regis da Nóbrega Fonteles: conceptualization; formal analysis; methodology; validation; writing-original draft; writing – review and editing; visualization. **César Ulisses Vieira Veríssimo:** formal analysis; methodology; validation; writing-original draft; funding acquisition; supervision; visualization; other contribution (field data).

Conflict of interest

The authors declare no potential conflict of interest.

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