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Geostatistical modelling of a coal seam for resource risk assessment

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Abstract

The evaluation of a coal seam for profitable extraction requires the estimation of its thickness and quality characteristics together with the spatial variability of these variables. In many cases the only data available for the estimation are from a limited number of exploration and feasibility drill holes. Spatial variability can be quantified by geostatistical modelling, which provides the basis for estimation (kriging). In cases where the spatial variability of the seam thickness and quality characteristics have a significant impact on how the coal is extracted and stored, geostatistical simulation may be preferable to geostatistical kriging methods. In this paper we present solution to the resource risk assessment problem. We consider the propagation of the uncertainty in semi-variogram model parameters to the spatial variability of the coal variables and we deal with the non-stationarity observed in many coals seams (which is often related to

the depositional basin shape) in a simple but efficient way. The methodology is illustrated with a coal seam from North-westhern Spain

Key words

Simulation, maximum likelihood, confidence region, thickness, probability sampling

1. Introduction

One of the most significant contributors to the total risk in the evaluation of a coal-mining project is the uncertainty of the resource tonnage and quality characteristics, often called the resource risk (see, for example, Sobczyk, 2010). The depositional and tectonic history of basin coal deposits is a significant determinant of the spatial variability of the thickness and quality characteristics of constituent coal seams and may have a major impact on the accuracy of coal resource estimates and, ultimately, on the investment risk. The thickness of a coal seam determines the total resource tonnage and the quality parameters (calorific value, ash content and total sulphur content) determine the coal price.

There are several ways in which geostatistics can improve coal seam resource estimation (Larkin, 2011):

- Estimation of coal seam thickness and overburden volumes.
- Estimation of coal seam quality parameters.
- Provision of confidence limits on these estimations.
- Optimisation of drilling: determining where to place additional drill holes and determining the minimum drill hole spacing for the classification of resources as measured, indicated or inferred[1].

[1] We use the Australasian Joint Ore Reserves Committee (JORC) code for reporting exploration results, mineral resources and ore reserves (http://www.jorc.org/pdf/jorc2004print_v2.pdf).

- Simulation of mining operations to achieve a particular objective such as minimizing the variability of the quality characteristics of mined or stock-piled product so as, for example, to meet sales contract specifications.

Although kriging has been used extensively to address most of these problems (Noppé, 1994, Demirel et al., 2000; Watson, 2001) it has two important drawbacks. Firstly, although kriging is distribution-free and provides the estimation variance as a measure of the uncertainty of the estimates, a distribution must be assumed to provide confidence limits for the estimates; in addition, the estimates are correlated as are the measures of uncertainty. The usual approach is to assume a Gaussian (Normal) distribution because of its simplicity but other more suitable alternatives can be found at the expense of increased computing time. Secondly, kriging provides estimated values of the coal seam variables that have less variability than the real values, i.e., the estimated values are smoother than reality.

Geostatistical simulation is a well-established technique (e.g., Journel and Huijbregts, 1978; Remy et al. 2009) that can be used to generate realisations that reproduce the spatial variability of coal seam parameters. In applications, a set of simulated realisations is used to assess the impact of the spatial uncertainty of the variables of interest (e,g., thickness, coal quality variables). The simulation, however, is based on a semi-variogram model that is estimated from the relatively sparse, available data and thus the model itself is uncertain. The uncertainty of the semi-variogram model can be quantified by assessing the uncertainty of the semi-variogram model parameters and considering a set of likely model parameters. This quantification provides a means of propagating the uncertainty in the semi-variogram model parameters into the uncertainty of the estimated coal seam variables (Pardo-Igúzquiza and Chica-Olmo, 2008).

The consequence of many depositional mechanisms, such as alluvial fans that have in-filled basins, is a directional thickening or thinning of a seam; tectonic mechanisms, such as rifting or differential subsidence, can have similar consequences. In geostatistical terminology the systematic increase or decrease of seam thickness in one or more directions is termed a drift or trend, which must be accounted for in estimation and simulation. The two common ways of accommodating drift in estimation and simulation are explicit modelling and the use of intrinsic random functions (Wackernagel, 1999) although, as we expound in the following section, there is a more parsimonious solution.

2. Methodology

The estimation of coal tonnage and coal quality is based on the available data, which, at the resource estimation stage is usually limited to exploration and feasibility drill holes. The significant advantage of geostatistical methods over other methods (e.g., polygonal, inverse of distance) of estimating resources and reserves is that they are probabilistic. The outcome of a probabilistic process (estimation or simulation) is a random field of spatially variable values. Two decisions must be taken in any applied geostatistical study:

- whether the variable of interest (e.g., thickness) can be considered second-order stationary (Myers, 1989) or there is a trend that must be modelled; and
- how a semi-variogram model can be estimated from the data.

With respect to the first question, mean coal seam thickness often exhibits a trend that reflects the geological origin of the coal from sediment deposition within a basin or sub-basins and the effects of differential subsidence, or other mechanisms, on those basins. In principle, a non-stationary model is the most appropriate for estimation in such cases.

However, coal resources are usually estimated from data from exploration and feasibility drill holes, on a more or less regular grid, that provide good coverage of the area of interest; in such cases the estimation of resources is similar to an interpolation problem. In this situation, Journel and Rossi (1989) have shown that a stationary model within a local search window gives very similar results to those obtained from a non-stationary model in which the drift is explicitly included. The presence of sufficient data, regularly distributed over the area of interest, has the double effect of conditioning and screening. Conditioning implies that, even if a stationary model is used within a local search window, the global drift is implicitly introduced into the final fields (whether estimated or simulated). Screening implies that, at an unsampled location, the closest neighbours are the most informative and influential values, in both kriging and simulation, and they screen the effect of neighbours that are further away from the location at which a value is to be estimated or simulated.

With respect to the second question, visual fitting is very common in mining applications largely because competent resource estimator can take into account his/her own knowledge of the geology and structure of the deposit to interpret the behaviour of the semi-variogram (e.g., nugget effect, anisotropy, zonal effect). However, when a semi-variogram model is estimated from a small number of data, the semi-variogram model parameters have an associated uncertainty that must be assessed and included in estimation or simulation. Thus a parametric approach, such as maximum likelihood estimation, is more appropriate because it provides the uncertainty of the parameters of the semi-variogram model that is fitted to the calculated values (Pardo-Igúzquiza, 1998).

The semi-variogram parameter estimates are obtained as the values that minimize the negative log-likelihood function (ℓ) given by (Kitanidis, 1983):

$$\ell(\boldsymbol{\theta},\sigma^2;\hat{\beta},\mathbf{z}) = \frac{n}{2}\ln(2\pi) + \frac{n}{2}\ln(\sigma^2) + \frac{1}{2}\ln|\mathbf{Q}| + \frac{1}{2\sigma^2}[(\mathbf{z}-\boldsymbol{\beta})'Q^{-1}(\mathbf{z}-\boldsymbol{\beta})'] \tag{1}$$

where, $\boldsymbol{\theta}' = (r_0, a)$ is the vector of correlogram parameters: the nugget/variance ratio and the range respectively. σ^2 is the variance parameter.. $\mathbf{Q} = \mathbf{Q}(r_0, a)$ is the $n \times n$ correlation matrix, which depends r_0 and a.

$\hat{\beta}$ is the estimated global mean and $\mathbf{z}' = (z(\mathbf{u}_1), z(\mathbf{u}_2), ..., z(\mathbf{u}_n))$ is the $1 \times n$ vector of n spatial data with the general element $z(\mathbf{u}_i)$ being the i^{th} data value at the spatial location $\mathbf{u}_i = \{x_i, y_i\}$.

$\boldsymbol{\beta}' = (\hat{\beta}, \hat{\beta}, ..., \hat{\beta})$ is the $1 \times n$ vector with all elements equal to the global mean, which is estimated as:

$$\hat{\beta} = (\mathbf{1}'\mathbf{Q}^{-1}\mathbf{1})\mathbf{1}'\mathbf{Q}^{-1}\mathbf{z}. \tag{2}$$

$\mathbf{1}' = (1,1,...,1)$ is a $1 \times n$ vector of ones.

The maximum likelihood estimates, $\hat{\boldsymbol{\theta}}^* = \{\hat{\boldsymbol{\theta}}, \sigma^2\}$, of the semi-variogram parameters, $\boldsymbol{\theta}$ and σ^2, are the values that minimize the NLLF $\ell(;)$ in Equation (1).

One way of providing confidence regions (that is, sets of parameter values that have a given probability of being the true parameter values) is by using likelihood regions (sets of parameters which the NLLF is smaller than a given threshold) and the likelihood ratio statistic (Kalbfleisch, 1979):

$$D(\boldsymbol{\theta}^*) = -2\ln\frac{\ell(\hat{\boldsymbol{\theta}}^*)}{\ell(\boldsymbol{\theta}^*)} \tag{3}$$

That is,

$$D(\boldsymbol{\theta}^*) = 2[\ell(\boldsymbol{\theta}^*) - \ell(\hat{\boldsymbol{\theta}}^*)] \tag{4}$$

where $D(\boldsymbol{\theta}^*)$ is the likelihood ratio statistic; $\ell(\boldsymbol{\theta}^*)$ is the NLLF value for a set of arbitrary covariance parameters $\boldsymbol{\theta}^*$; $\ell(\hat{\boldsymbol{\theta}})$ is the NLLF value for the set of ML covariance parameter estimates $\hat{\boldsymbol{\theta}}$.

It can be shown that for large *n*, $D(\boldsymbol{\theta}^*)$ is approximately chi-square distributed with *p* degrees of freedom (McCullagh and Nelder, 1989):

$$D(\boldsymbol{\theta}^*) \approx \chi_p^2 \qquad (5)$$

where the symbol $\approx$ denotes "distributed as", χ_p^2 is the chi-square distribution with *p* degrees of freedom where *p* is the number of covariance parameters.

Hence, for example, an approximate 75% confidence interval for the three parameters (*p* = 3) (nugget variance, variance and range) is defined by the set of parameters with NLLF satisfying the criterion:

$$\ell(\boldsymbol{\theta}^*) < \ell(\hat{\boldsymbol{\theta}}^*) + \frac{1}{2}(4.108). \qquad (6)$$

An application is presented in the following case study.

3. Case study

The case study is from an area in the North-West of the Iberian Peninsula (Galicia, Figura1A-B) in which there are several basins along dextral strike-slip fault zones (Figure 1C) developed as a consequence of a Cenozoic North-South shortening (Santanach et al. 1988). The As Pontes (A Coruña province) is the most northerly of these basins and is the best known because of a recently depleted brown lignite deposit.

The As Pontes basin (Figure 1C-D) has an ellipsoidal shape with a NW-SE (N140-160ºE) orientation, with a major axis of 7 km, a variable width of 1.5 km to 2.5 km and a sedimentary fill of up to 300 m of thickness (Figure 1D). The substratum outcrops in the margins and is composed of gneiss, philites, schist, quartzites and meta-arkoses from the Hercynian orogeny.

The basement contact is irregular and, in places, ancient earth movements of the contact have formed a border that divides the basin into two sub-basins (Figure 1D, Barcelar et al., 1988). The structure of the As Pontes basin can be used to deduce the importance of the N-S shortening during the Tertiary in NW Galicia that gave rise to the generation of two systems of dextral strike faults in the NW-SE direction (Ferrús Piñol, 1994).

The data are from 80 exploration drill holes in a 30 km^2 lignite deposit in the As Pontes basin. Figure 2 shows the 80 data and the limits of an area o interest of 22 km^2, within which the mean coal seam thickness is to be estimated for small panels of 50 × 50 m. The experimental semi-variogram for seam thickness is shown in Figure 3 and the model fitted by eye using a graphical fitting program is a spherical model with nugget variance 3 m^2, partial sill 25 m^2 and range 4128 m, which can be written using the notation:

$$\gamma(h) = 3 + 25\text{Sph}(h;4128) \tag{7}$$

where $A + B\text{Sph}(h;C)$ is a spherical semi-variogram model with nugget variance *A*, partial sill *B* and range *C*. Thus the sill or total variance is *A*+*B*.

The model estimated by maximum likelihood is:

$$\gamma(h) = 4 + 23\text{Sph}(h;4460) \tag{8}$$

Although the maximum likelihood estimates of the parameters are very similar to those estimated by visual fitting, maximum likelihood has the advantage of providing estimates of the uncertainty of the parameters as is shown below.

The ordinary kriging map estimated using the semi-variogram model given in Equation (7) is given in Figure 4. The calculated resources (in volume) from the kriging map are of 2.48 × 10^8 m^3 or 248 million cubic metres. However, there is an associated uncertainty as given in Figure 5 by the kriging error (square root of the kriging estimation variance). It is difficult to use this uncertainty map jointly for the whole deposit because the kriging error estimates are correlated. In the worst case scenario the thickness is assumed to be overestimated for the whole deposit and thus two times the standard deviation (kriging error) is discounted to each estimate. This yields a total estimated resource of 1.66×10^8 m^3. This is a naïve and unrealistic estimate because kriging is globally unbiased and thus many kriging estimates will sometimes underestimate and sometimes overestimate. If each kriging estimate is discounted by only one standard deviation, the total estimated resource is 2.07×10^8 m^3, which is closer to the original estimates but still not an effective way of evaluating uncertainty.

We will use geostatistical simulation for assessing the uncertainty first by assuming that the estimated semi-variogram has no uncertainty and then assuming that the semi-variogram is uncertain.

We will use sequential Gaussian simulation (Deutsch and Journel, 1992), which requires the following steps:

1) Calculate the normal scores of the original data.
2) Calculate the semi-variogram of the normal scores and infer a semi-variogram model.
3) Generate the Gaussian conditional simulation by sequential Gaussian simulation.
4) Back-transform the Gaussian conditional simulation to original units (metres of thickness).

The normal scoring transform (Pardo-Igúzquiza et al., 1992) is shown in Figure 6 in which the tails of the transform have also been modelled.

The semi-variogram model fitted to the experimental semi-variogram of the normal scores is shown in Figure 7 and the semi-variogram model fitted to these values is:

$$\gamma(h) = 0.1 + 0.9\mathrm{Sph}(h;3360) \tag{9}$$

A realisation of a conditional simulation of the thickness random field is shown in Figure 8. A comparison of the simulation with the kriging estimated field in Figure 4, clearly shows that the spatial variability in the simulation is larger than that of the estimated field. In fact, the simulation reproduces the observed variability by reproducing the semi-variogram model fitted to the experimental semi-variogram values. The total resource calculated from the simulation in Figure 8 is 2.45×10^8 m^3. However, this is only one of the thousands of realisations that could be generated.

In this study, 200 realisations were generated and for each realization the total resources were calculated; the histogram (Figure 9) of these values represents the uncertainty of the estimated resources. The 95% confidence interval for the total resources is $[2.41 \times 10^8, 2.59 \times 10^8]$ m^3.

The uncertainty of the resource estimates, represented in Figure 9, has been calculated assuming that the semi-variogram is known with certainty. However, as the semi-variogram has been estimated from the experimental data, there is an additional uncertainty associated with the fitted model. This uncertainty is readily quantified by the method discussed above. The value of the negative log-likelihood function at the minimum is $\ell(\hat{\boldsymbol{\theta}}^*) = 83.132$, and the set of parameters $\{r_0, a, \sigma^2\}$, such that $\ell(\boldsymbol{\theta}^*) < 85.186$, is a 75% confidence region for those semi-variogram parameters.

The negative log-likelihood function as a function of $\{r_0, a\}$ is shown in Figure 10 in which the 75% confidence region is highlighted.

The parameter space $\{r_0, a, \sigma^2\}$ has been discretized with steps of 0.05 for the nugget/variance ratio in the interval [0,1]; 700 m for the range in the interval [1000,15000] and 0.1 for the variance in the range [0.6,2.6]. On the basis of this discretization, there are 268 models of triplets $\{r_0, a, \sigma^2\}$ that lie inside the 75% confidence region. These models do not have the same probability and some are more likely than others. To account for these differences the probabilities are normalised so that they sum to 1.0 and each model is included as many times as indicated by its normalised probability (i.e., probability sampling in which, for example, a model with a normalised probability of 0.35 comprises 35% of the total simulated resource). A total of 869 simulations were used. The histogram of the total resource is shown in Figure 11. The 95% confidence interval for the total resource is $[2.39 \times 10^8, 2.62 \times 10^8]$ m^3, which is slightly higher than the same interval calculated under the assumption that the semi-variogram is known with certainty. However, the probability that the total resource will be greater than 2.5×10^8 m^3, is 0.41 when the uncertainty of the semi-variogram parameters is ignored and 0.53 when the uncertainty of the semi-variogram parameters is propagated into the simulated realisations. In other words, whilst there is no significant difference in the mean resource (approximately the mid-point of the respective confidence intervals assuming a symmetrical distribution) for the two sets of simulations, the difference in the two distributions (as a consequence of different variances) is sufficient to generate significantly different resource estimates above selected thresholds or cut-offs.

4. Discussion and conclusions

Geostatistics is a standard means of estimating coal resources from exploration and feasibility drilling. The quantification of spatial variability in the form of the semi-variogram model is the basis of the probabilistic approach provided by geostatistics, a significant advantage of which is that it is amenable to uncertainty evaluation. Although kriging has, for some time, been the standard technique for spatial estimation in mining applications, it is not adequate for global uncertainty analysis of a complete coal deposit and the consequent evaluation of resource risk. This is because the kriging estimation variances of the estimated panels are correlated. Geostatistical simulation is an alternative to estimation that provides a means of quantifying uncertainty and resource risk.

In simulation, the uncertainty of the variable of interest (in the case treated here, the thickness of a coal seam) is taken into account by simulating a large number of realisations of a random function model using the estimated semi-variogram. In a standard simulation approach, it is assumed that the semi-variogram is known with certainty but, as it has been estimated from relatively sparse data, the semi-variogram parameters are uncertain. We have used maximum likelihood to evaluate the uncertainty of the semi-variogram and to provide confidence regions with specified probability coverage. Probabilities are assigned to semi-variogram parameters and probability sampling is applied in which each model is selected according to its probability. This approach achieves two objectives: it accounts for the uncertainty of thickness values at unsampled locations and it accounts for the uncertainty of the semi-variogram model parameters.

In the case study presented here, for the specific coal deposit, sampling density and spatial variability of seam thickness, the differences in the total volume of resources, with and without the quantification of semi-variogram uncertainty, is small but the consequence of selecting from the distribution of possible resources (e.g., the probability that the true resource will exceed a specified value) is significant. This illustrates a general principle: the estimated (kriged) total resource and the mean simulated resource (approximately the mid-points of the respective confidence intervals for symmetrical distributions), with and without the semi-variogram uncertainty, will not differ significantly but the distributions of the two simulations will differ as a consequence of the different variances. Similarly, selecting panel values above a specified threshold or cut-off from the set of estimated (kriged) panel thicknesses or from any set of simulated panel thicknesses will yield different results. In particular, applying cut-offs to the estimated (kriged) panel thicknesses for panel sizes significantly less than the mean drilling or sampling grid will yield meaningless results because of the significant smoothing effect, which increases as the panel size decreases.

In general, the outcome from the simulations with and without semi-variogram uncertainty will depend on the deposit and the amount of data available for resource estimation. Evaluation of this source of uncertainty is critical in resource risk assessment even if it is ultimately found in a particular case that there is no practical difference between resource estimates obtained by ignoring or including semi-variogram uncertainty.

In the work presented here we have provided a general, integrated approach to the quantification of resource risk. We consider that the inclusion of semi-variogram uncertainty, which is a function of deposit geology, spatial variability of resource variables and the amount and locations of data, to be an essential component of best practice in the quantification of resource risk.

Acknowledgements

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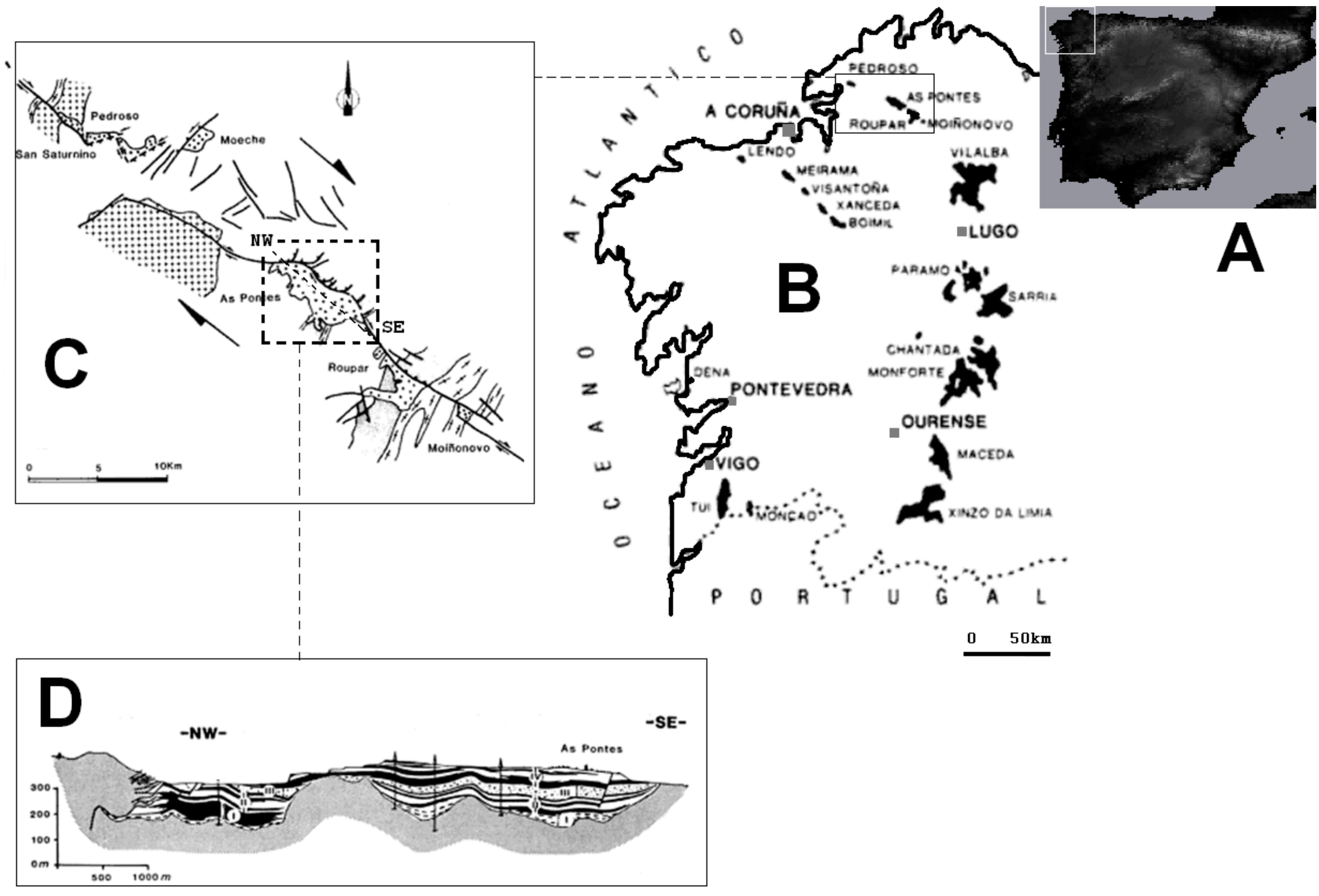


Figure 1. Location of the As Pontes deposit in Galicia, North-western Spain (A) as one of the Tertiary basins in Galicia (B) in relation to dextral slip fault zones (C). The irregular basement surface divides the basin into two sub-basins (D).

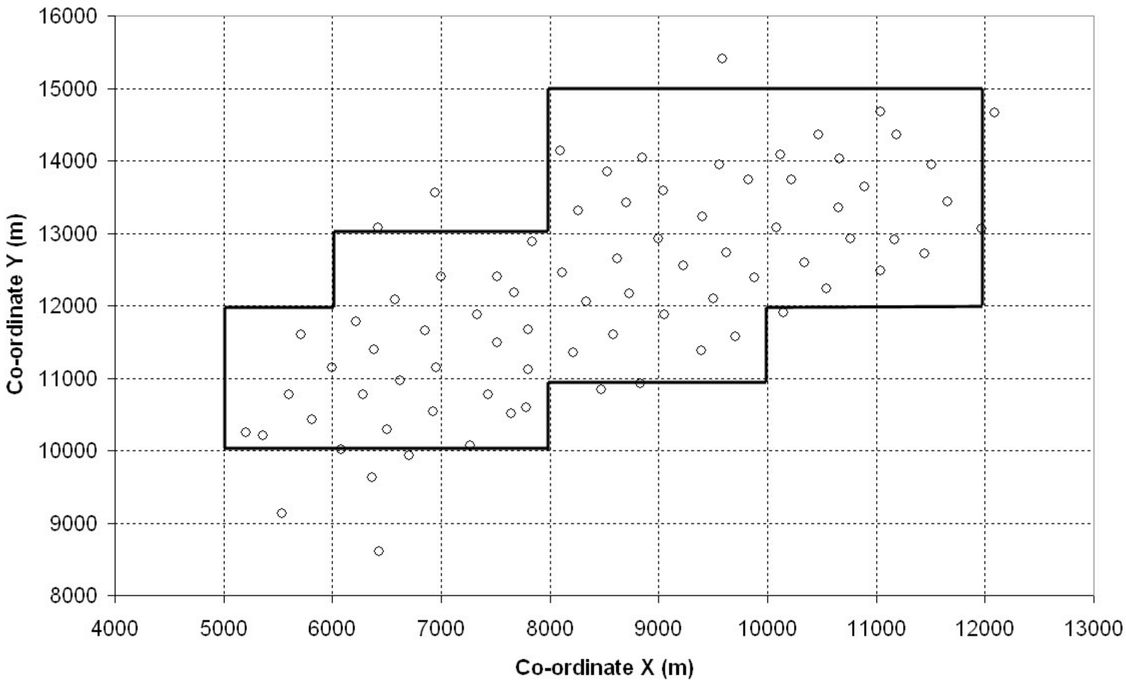


Figure 2. Location of drill holes and limits of the area of the case study.

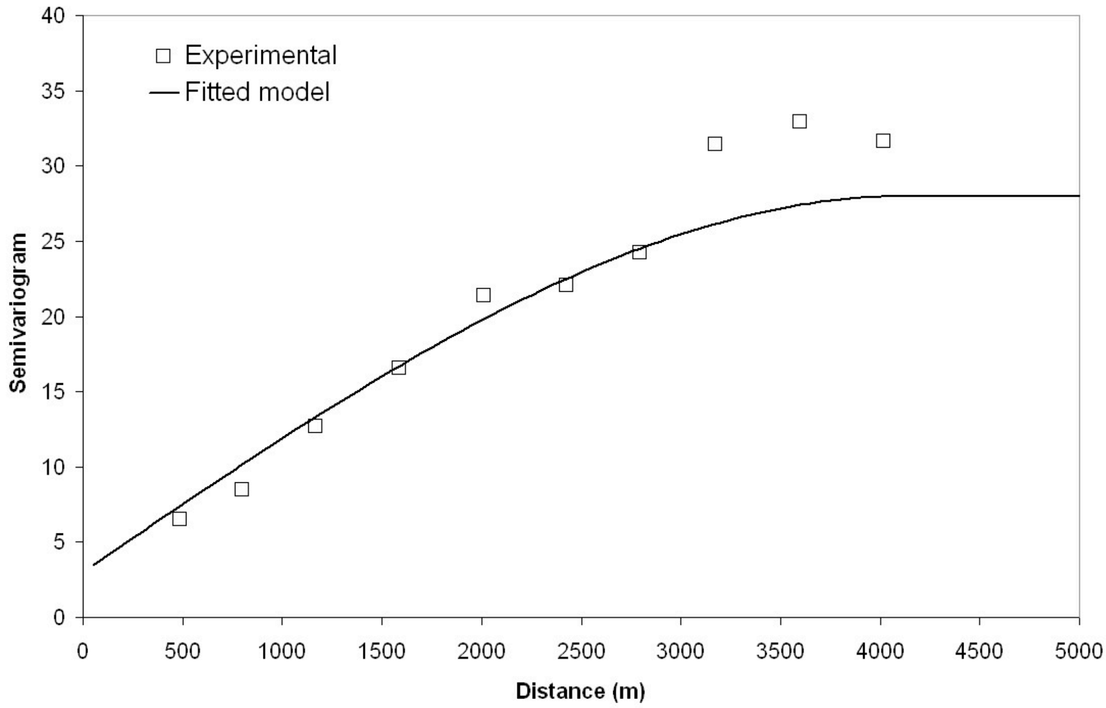


Figure 3. Experimental semi-variogram and model by fitted by eye.

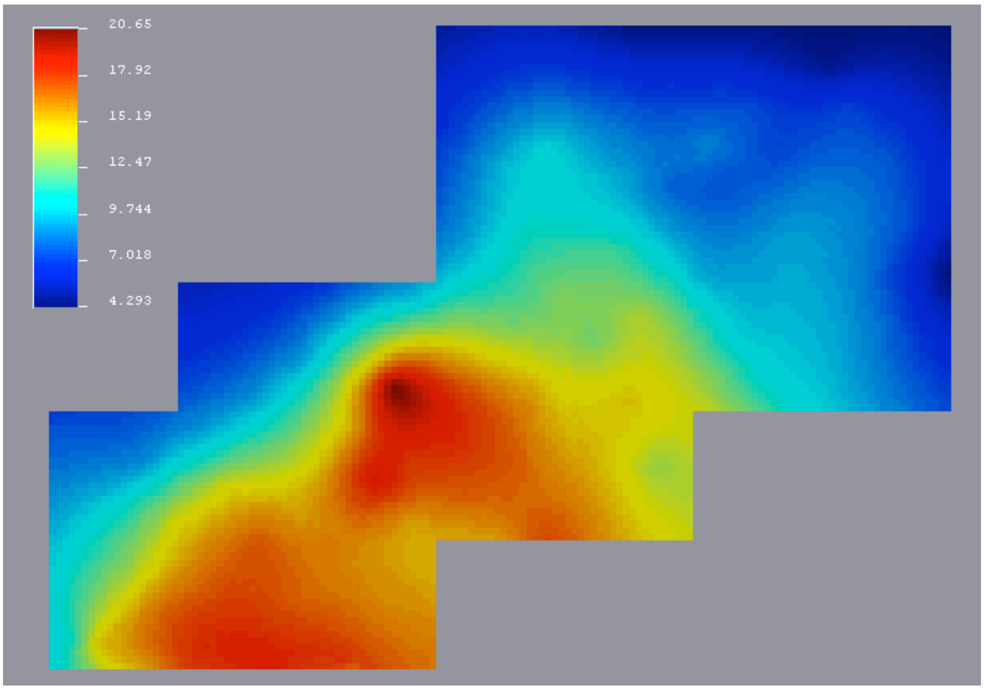


Figure 4. Kriging estimates of thickness in metres.

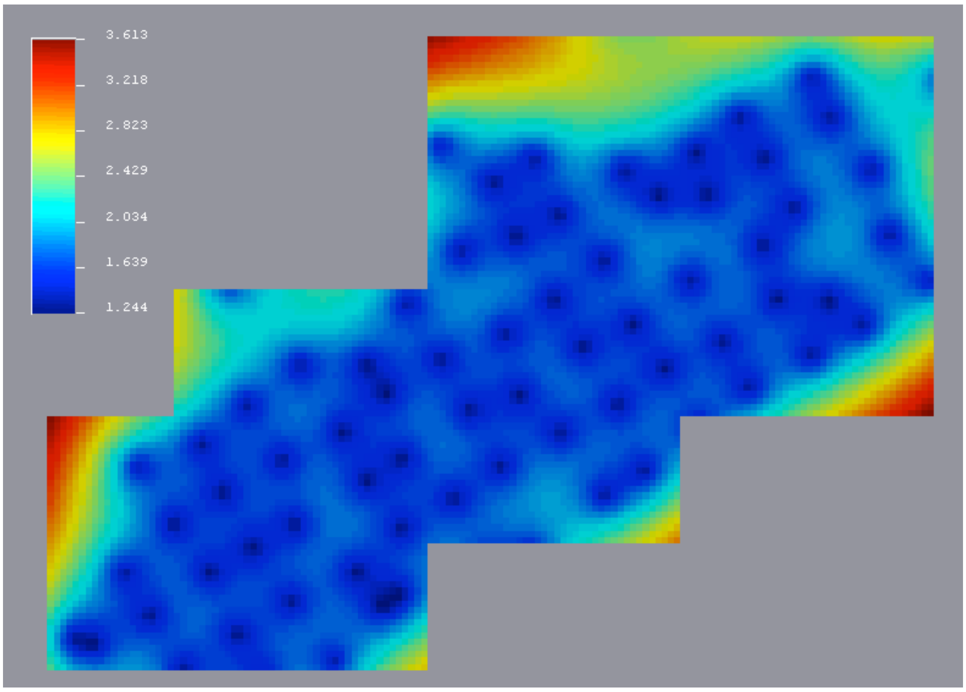


Figure 5. Kriging error (square root of the estimation variance) in metres.

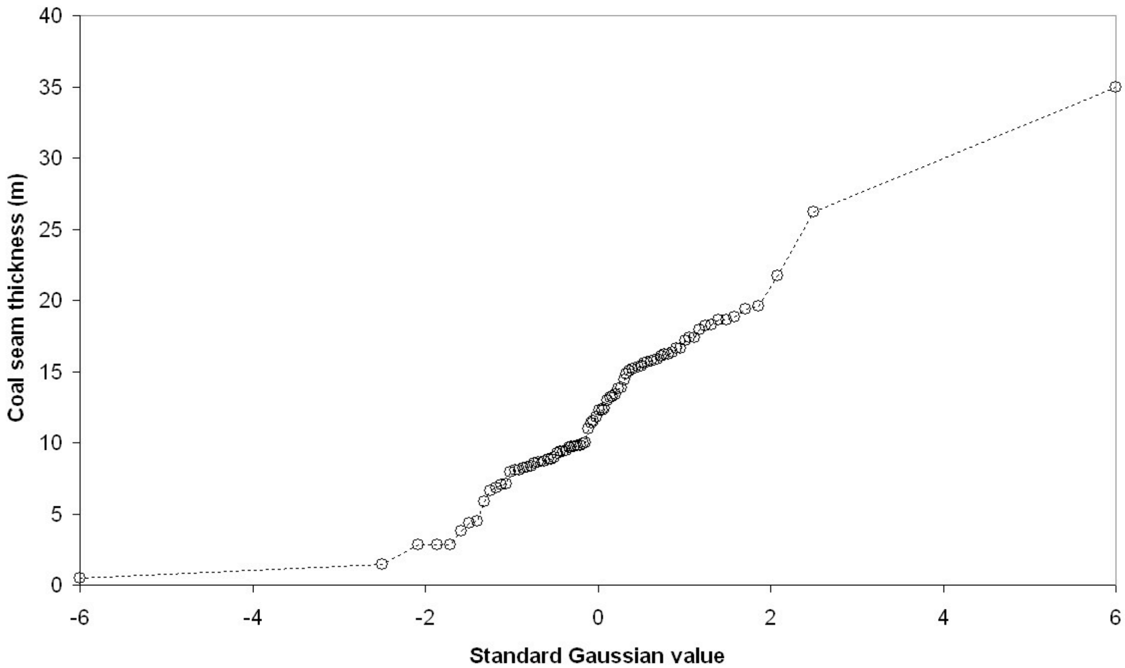


Figure 6. Normal scoring transformation.

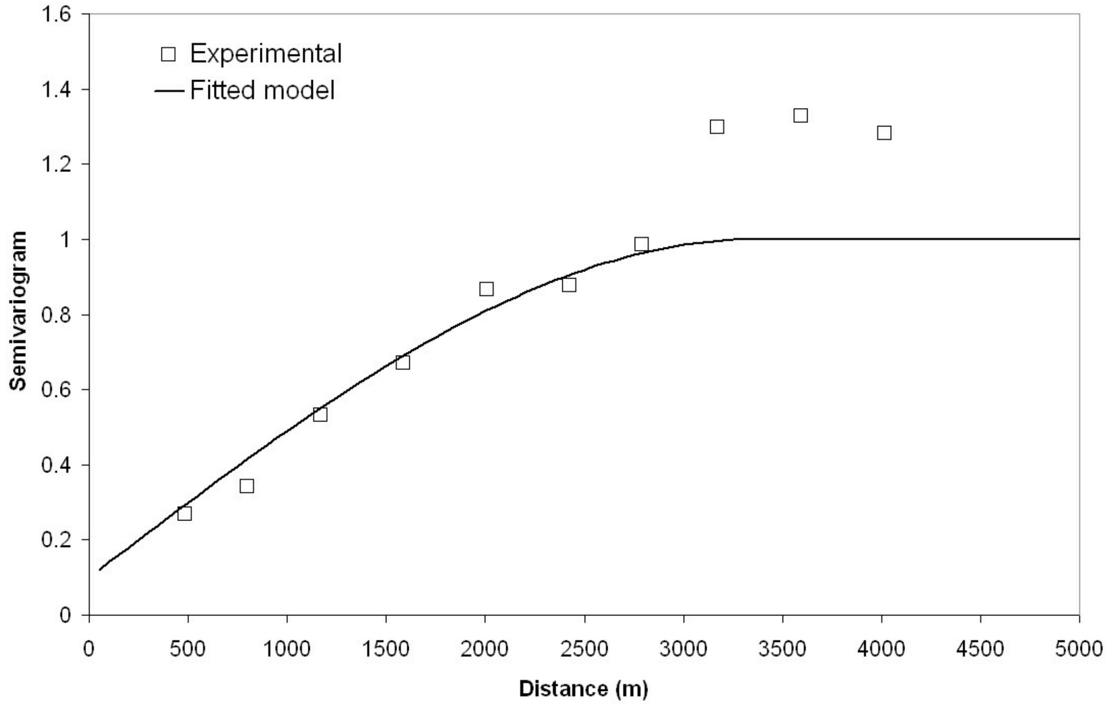


Figure 7. Semi-variogram values of the normal scores together with model fitted to them.

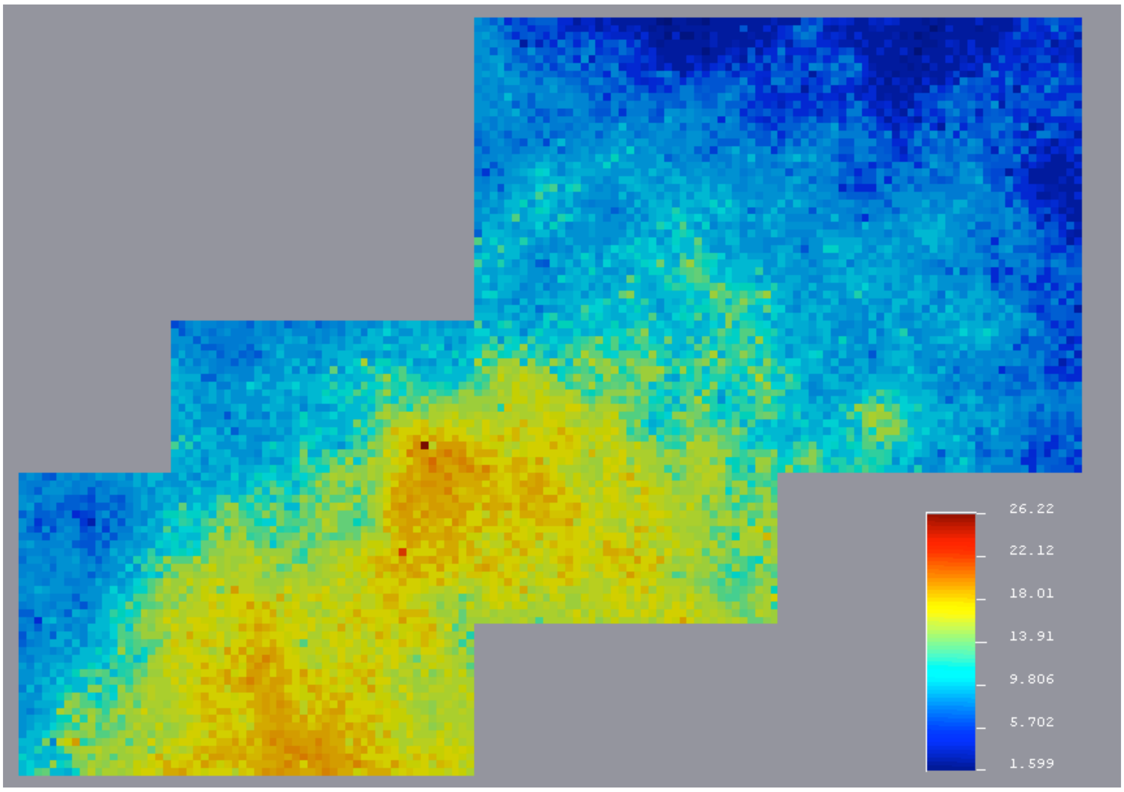


Figure 8. A realization of a conditional simulation of the thickness of the coal seam.

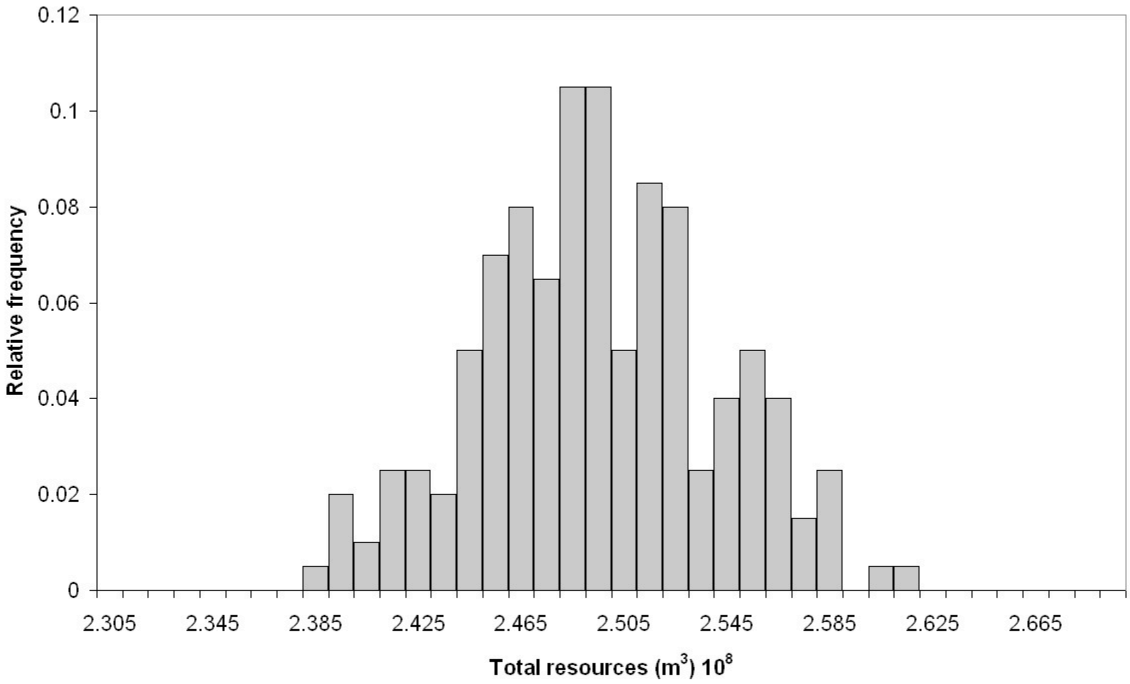
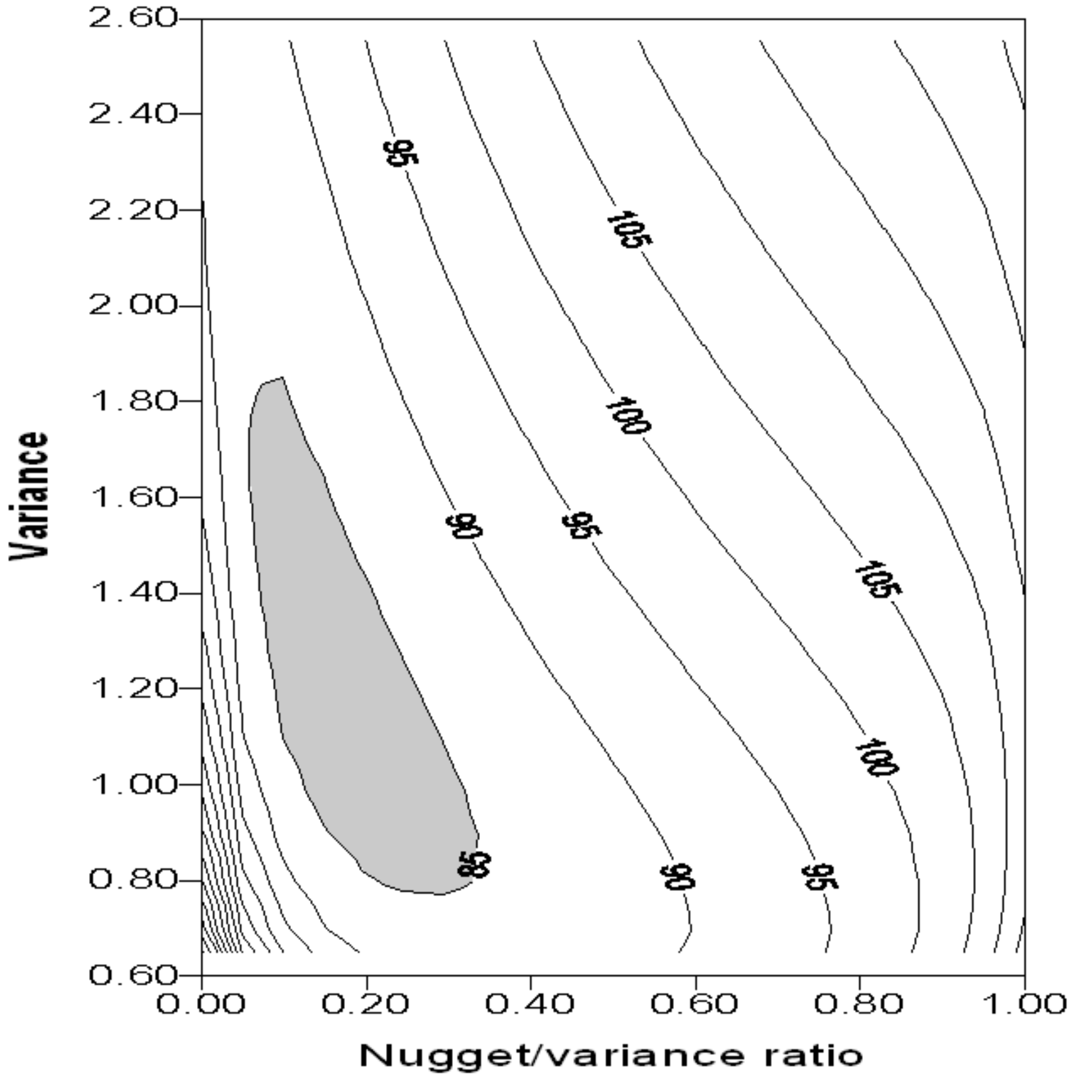
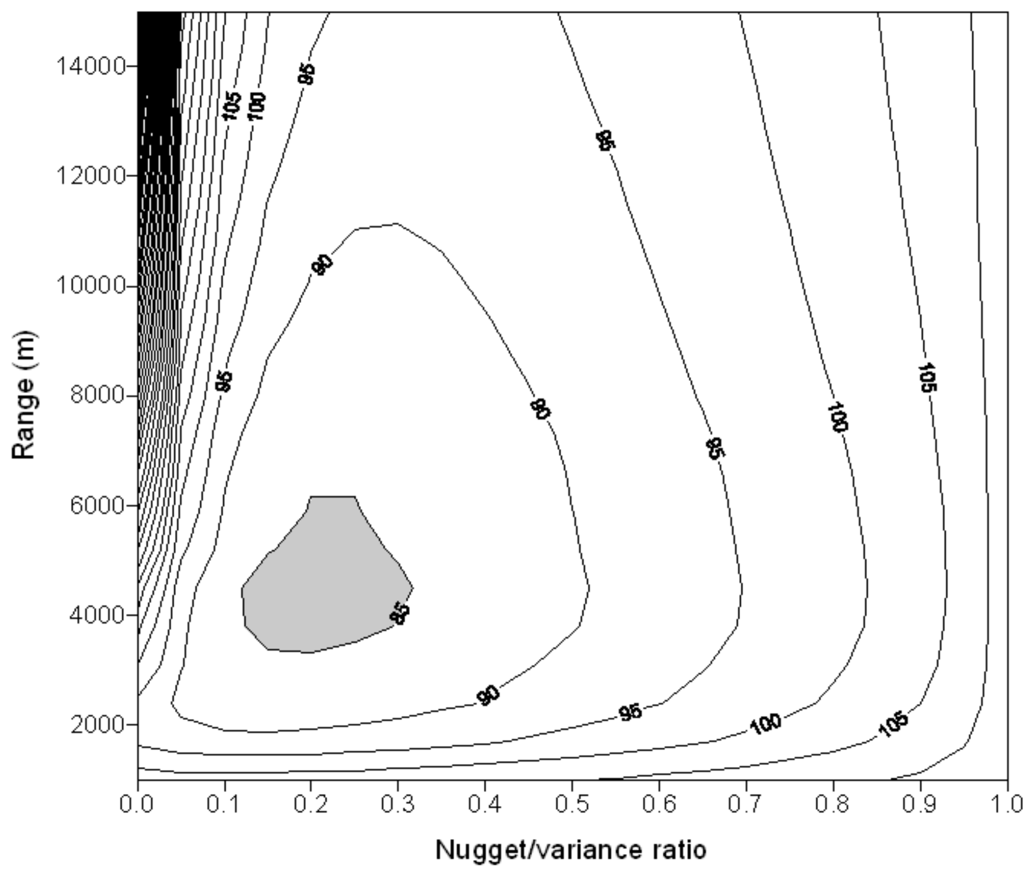


Figure 9. Histogram of total resources calculated by geostatistical simulation and assuming that the semi-variogram model parameters are known with certainty.

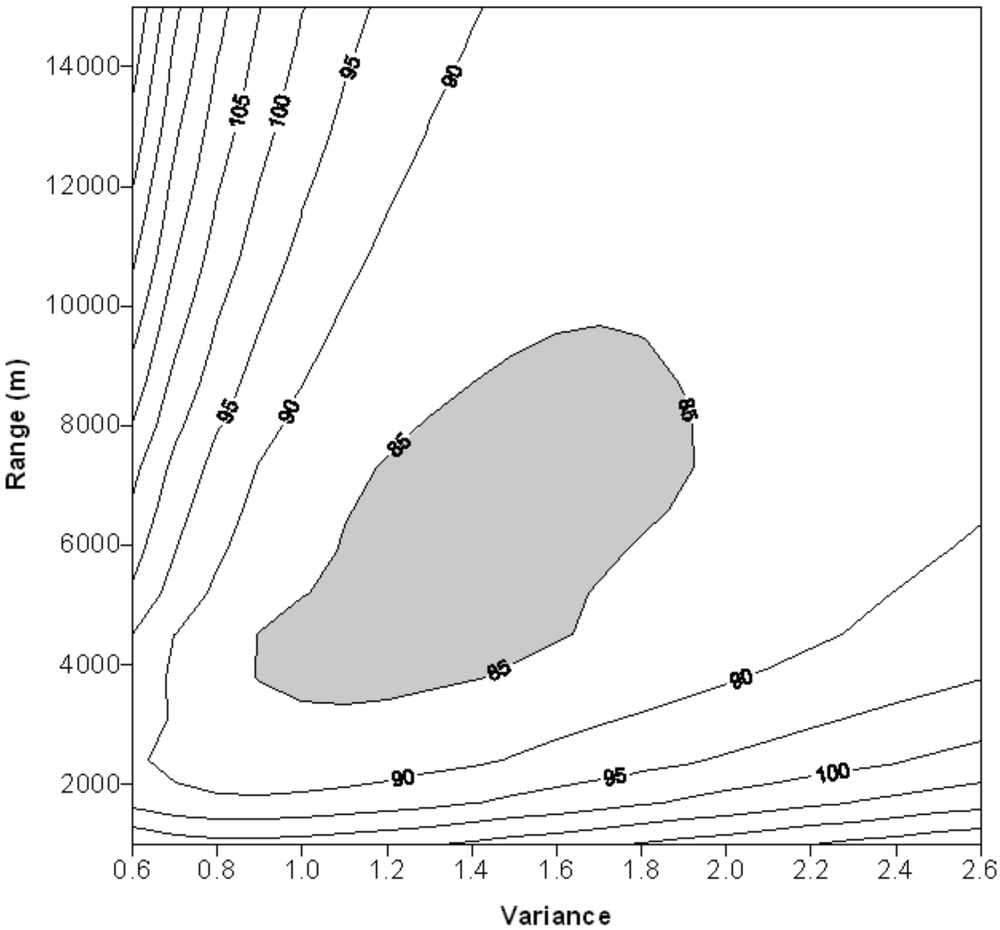

2.60
2.40
2.20
2.00
1.80
1.60
1.40
1.20
1.00
0.80
0.60
Variance
0.00
0.20
0.40
0.60
0.80
1.00
Nugget/variance ratio
85
90
95
100
105
90
95
100
105
90
95

A



Range (m)
14000
12000
10000
8000
6000
4000
2000
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
Nugget/variance ratio
85
90
95
100
105

B



C

Figure 10. Negative log-likelihood function for the parameter planes of a spherical semi-variogram model. A: nugget/variance ratio and variance parameters with the range fixed at 4500m. B: nugget/variance ratio and range with the variance fixed at 1. C: variance and range with the nugget/variance ratio fixed at 0.15. All pairs of parameters inside the grey area are in the 75% confidence region.

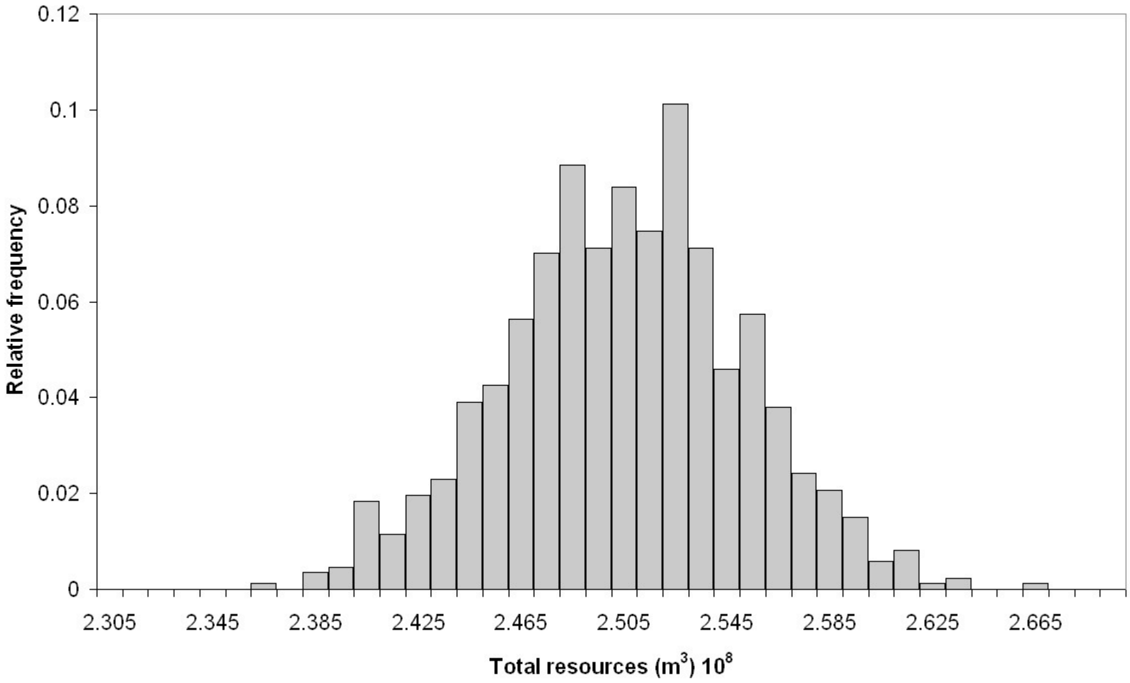


Figure 11. Histogram of total resources calculated by geostatistical simulation and including the uncertainty of the semi-variogram model parameters.