A Stochastic Trend Approach to Calculate Uncertainty in the Mean

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Geostatistics techniques often lead to less uncertainty for larger domains even if the number of data stays the same. An alternative to evaluate uncertainty in these domains could be to use a trend equation and define the mean dependent on the location within the domain. The trend model could be used to predict the value at unsampled locations. A global mean is evaluated with the set of coefficients evaluated at all locations within the domain. The stochastic trend approach proposes to randomize these coefficients considering the correlation of the original fitted coefficients. Different coefficients provide different mean values that are combined to a distribution of uncertainty in the mean.

1. Introduction

Estimates are made under uncertainty because few data are present in the evaluations and many input parameters are required in the estimates. The uncertainty in the input parameters must be transferred into the estimates to provide a more realistic assessment of uncertainty. Decision making often considers the uncertainty. The chance of success/failure, potential gain and potential loss are some considerations in risk analyses. These considerations rely on the estimates and their uncertainty (Rose, 2001). We are motivated to accurately evaluate the uncertainty of our estimates.

The conditional finite domain requires the setting of many parameters that affect the distribution of uncertainty in a non-intuitive and non-transparent manner. Relatively minor changes in geostatistical parameters could have a large effect on probabilistic estimates (Deutsch, Leuangthong, & Ortiz C., 2006). Sensitivity analysis shows that an increase in the nugget effect, a reduction of the range of correlation or an increase in the size of the domain leads to less uncertainty in large scale averages. This makes statistical sense because random variations in the variable average out.

A domain is an area or volume where samples follow a known distribution (e.g., normal or lognormal distribution). The domain includes samples that are not often uniformly spaced; preferential sampling is common in places of high grade. Geostatistics techniques often lead to less uncertainty for larger domains even if the number of data stays the same. An alternative to evaluate uncertainty in these domains could be to relax the assumption of stationarity. Stationarity permits calculation of the mean, covariance and semi variogram by pooling the data within the chosen domain (Goovaerts, 1997). The use of a trend equation relaxes this assumption of stationarity and defines the mean dependent on the sample location within the domain, see Equation (1). L symbolizes the number of drift or trend terms, a_l represents the unknown coefficients and the f_l ($\mathbf{u}$) terms are functionals that represent the shape of the trend. The functional may be linear, quadratic, sine/cosine, drawn by hand or specified arbitrarily.

$$m(\mathbf{u}) = \sum_{l=0}^{L} a_l f_l(\mathbf{u}) \tag{1}$$

Although the linear and the quadratic equations are considered in the implementation here, different equations could be used if required. A FORTRAN code called *uncregcoef.for,* which is a modification of the *correlate* program, was developed to implement the stochastic trend technique. The trend model could be used to predict the value at unsampled locations, that is, nodes or locations in the domain are evaluated with a polynomial with coefficients computed by least square method. A global mean is then evaluated with the set of coefficients evaluated at all locations within the domain. The stochastic trend (ST) approach developed below proposes to randomize these coefficients taking account the correlation of the original fitted coefficients. Many sets of coefficients provide different mean values. Then, the uncertainty in the input parameter is calculated from the distribution of these means.

2. Methodology

The coefficients of the trend are calculated based on the well-known linear regression theory. The sum of the squared difference between the estimates and the available data are as small as possible. This difference is not zero because the estimated value fluctuates about its expected value, that is, the method of least square selects the regression coefficients with the criteria of minimizing the sum square of these fluctuations (Carl Friedrich Gauss, 1794), (Johnson & Wichern, 2007)

The coefficients of the trend and their individual variances are calculated by the theory of multiple regression models. The linear regression model is defined by the equation matrix (2). The dependent variable is denoted as **Z** and the independent variables **X**. The dependent variable in ST is the data values and the independent variables are the coordinates of the data. The model could be written in matrix notation as:

$$\mathbf{Z} = \mathbf{X}\mathbf{a} + \boldsymbol{\varepsilon} \tag{2}$$

The dependent variable **Z** represents the ($n \times 1$) vector of the data, where n is the number of data available. **X** is the ($n \times L$) matrix of the levels of the independent variables, where L is the number of parameters, explanatory variables or regressor predictor that define the fitted equation of the model equation. For instance, if the data have coordinates at East, North and Elevation, the (n , 2), (n , 3) and (n , 4) of matrix **X** may correspond to the coordinate data. Then, (n , 5 - L) columns are interaction of the coordinates to better define the shape of the trend with more parameters. **a** corresponds to the ($L \times 1$) vector of the coefficients or vector of regression parameters. The last element **ε** regards to an error ($n \times 1$) vector, this error vector is assumed as a random part of the model equation that has a distribution of mean zero and unknown variance s^2. The next equation shows the explained variables:

$$\begin{bmatrix} z_1 \\ z_2 \\ \vdots \\ z_n \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & x_{12} & \cdots & x_{1L} \\ 1 & x_{21} & x_{22} & \cdots & x_{2L} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n1} & x_{n2} & \cdots & x_{nL} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ \vdots \\ a_L \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_n \end{bmatrix} \tag{3}$$

$$\mathbf{Z} \quad = \quad \mathbf{X} \qquad\qquad \mathbf{a} \quad \boldsymbol{\varepsilon}$$

The location of the available data is translated to the **X** matrix based on the specified functional polynomials or trend model. The method of least squares is commonly used to estimate the regression coefficients in a multiple linear regression models, the term *linear* because the model is a linear function of the unknown parameters a_0, a_1,...,a_L. The model describes a hyper-plane in L-dimensional space of the regressor variables $\{x_l\}$ (Montgomery, 2000). The coefficients selected by the least square are called least squared estimates of the regression parameter **a**. They are denoted by **â** because they are estimates of **a**.

$$\hat{\mathbf{a}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Z} \tag{4}$$

Then, the fitted regression equation is given in matrix notation. This fitted model predicts the value at unsampled locations as a function of its coordinates:

$$\hat{\mathbf{Z}} = \mathbf{X}\hat{\mathbf{a}} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Z} \tag{5}$$

The residual describes the error in the fitting of the trend model to the n samples z_i, i = 1,...,n. The vector of residuals is the difference between the original value samples and the ones calculated by the fitted equation at known sample locations. The variance of the residuals (7) is the sum of the squared residuals divided by the (n - (L+1)) degree of freedom, where (L+1) is the number of parameters or coefficients. Notice that the number of data must be greater than number of coefficients.

$$\hat{\boldsymbol{\varepsilon}} = \mathbf{Z} - \hat{\mathbf{Z}} \tag{6}$$

$$s^2 = \frac{\hat{\boldsymbol{\varepsilon}}^T\hat{\boldsymbol{\varepsilon}}}{n-(L+1)} \tag{7}$$

$$E\{s^2\} = \sigma^2 \tag{8}$$

The method of least squares produces an unbiased estimator of the parameters **a** in the multivariate linear regression model. Properties of the **â** estimators are defined below:

$$E\{\hat{\mathbf{a}}\} = \mathbf{a} \tag{9}$$

$$Cov(\hat{\mathbf{a}}) = \sigma^2 (\mathbf{X}^T \mathbf{X})^{-1} \tag{10}$$

The next matrix shows the covariance between the regression coefficients. Then, the variances of the coefficients are acquired from the diagonal of the symmetric matrix because $C(a_l, a_l) = \sigma^2_{al}$

$$Cov(\hat{\mathbf{a}}) = \begin{bmatrix} c_{a_{00}} & c_{a_{01}} & \cdots & c_{a_{0L}} \\ c_{a_{10}} & c_{a_{11}} & \cdots & c_{a_{1L}} \\ \vdots & \vdots & \ddots & \vdots \\ c_{a_{L0}} & c_{a_{L1}} & \cdots & c_{a_{LL}} \end{bmatrix} = \begin{bmatrix} \sigma^2_{a_{00}} & c_{a_{01}} & \cdots & c_{a_{0L}} \\ c_{a_{10}} & \sigma^2_{a_{11}} & \cdots & c_{a_{1L}} \\ \vdots & \vdots & \ddots & \vdots \\ c_{a_{L0}} & c_{a_{L1}} & \cdots & \sigma^2_{a_{LL}} \end{bmatrix}$$

Now each term of the covariance is divided by their respective combined standard deviations to obtain the correlation matrix between the coefficients.

$$\rho(\hat{\mathbf{a}}) = \begin{bmatrix} 1/\sigma_{a_{00}} & 0 & 0 & 0 \\ 0 & 1/\sigma_{a_{11}} & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & 1/\sigma_{a_{LL}} \end{bmatrix} \times \begin{bmatrix} \sigma^2_{a_{00}} & c_{a_{01}} & \cdots & c_{a_{0L}} \\ c_{a_{10}} & \sigma^2_{a_{11}} & \cdots & c_{a_{1L}} \\ \vdots & \vdots & \ddots & \vdots \\ c_{a_{L0}} & c_{a_{L1}} & \cdots & \sigma^2_{a_{LL}} \end{bmatrix} \times \begin{bmatrix} 1/\sigma_{a_{00}} & 0 & 0 & 0 \\ 0 & 1/\sigma_{a_{11}} & 0 & 0 \\ 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & 1/\sigma_{a_{LL}} \end{bmatrix}$$

$$\rho(\hat{\mathbf{a}}) = \begin{bmatrix} 1 & \rho_{a_{01}} & \cdots & \rho_{a_{0L}} \\ \rho_{a_{10}} & 1 & \cdots & \rho_{a_{1L}} \\ \vdots & \vdots & \ddots & \vdots \\ \rho_{a_{L0}} & \rho_{a_{L1}} & \cdots & 1 \end{bmatrix} \tag{11}$$

Many sets of coefficients could be generated by Monte Carlo simulation to evaluate uncertainty in the fitted trend. The correlation between the regression coefficients will be preserved. Each coefficient $\hat{a}_l$, l = 0, 1,...,L has a distribution defined by its mean and its variance. Then, many sets of coefficients are drawn from their distributions. Those sets take account the correlation of the original regression coefficients. Otherwise, different techniques like spatial bootstrap use the covariance matrix of the sample locations ($\mathbf{C}_{11}$) to conditional the sampling and evaluate uncertainty. Both matrices are symmetric and positive definite. The steps of the proposed stochastic trend (ST) approach are as follows:

- Define the number of parameters or terms L for the trend equation, the model could be linear or quadratic.
- Compute the regression coefficients of the trend by least square method $\hat{a}_l$, l = 0, 1,...,L where the best fit minimizes the sum of squared residuals.
- Define the covariance matrix and deduce the variance of the coefficients σ_{al}, l = 0, 1,...,L.
- Define the correlation matrix for the regression coefficients.
- Perform Cholesky decomposition of the correlation matrix $\boldsymbol{\rho}$ = **LU**
- Sample independent normal Gaussian score values $w = G^{-1}(p)$ and correlate them by the use of the lower decomposed correlation matrix **L**, **Y** = **L w**.
- Non-standardize these **Y** values by the use of their respective fitted regression coefficient a_l and their respective standard deviation σ_{al}.

$$a_l^k = \hat{a}_l + \sigma_{a_l} \times y_l^k, \quad l = 0,\ 1,...,L \tag{12}$$

- Use the set of coefficients in the polynomial to evaluate the fitted mean Z(**u**) at all locations within the domain. The mean of the values at these locations is the mean of the first realization m_k, k = 1,...,K (where K is the number of times the workflow is repeated)

The distribution of m_k means can be assembled to model the uncertainty in the mean.

3. Criteria in the Implementation

All techniques to calculate the uncertainty in the mean require implementation choices. The stochastic trend approach does not require as many input parameters as most techniques. This approach only requires the form of the trend model. One should choose the polynomial representation that appears reasonable given the data. The uncertainty in the mean will be sensitive to the number of terms.

The uncertainty in the mean using the stochastic trend approach does not require a variogram; the variogram is required for other techniques like the spatial bootstrap and the conditional finite domain.

The fitted regression equation or trend model is used to predict the mean at all locations. The linear relationship may not be necessarily valid for extrapolation purposes (Montgomery & Runger, 2006). Uncertainty in the regression model is used specifically to calculate the uncertainty in the mean. The generation of the stochastic trends is explained with a simple example. A synthetic data set of 11 values is located in one dimension. The mean of the values is 2.409 and the variance 0.695.

$$\begin{bmatrix} 2.0 \\ 1.8 \\ 1.4 \\ 1.2 \\ 1.8 \\ 2.4 \\ 2.6 \\ 2.8 \\ 3.0 \\ 3.5 \\ 4.0 \end{bmatrix} = \begin{bmatrix} 1 & 5 \\ 1 & 10 \\ 1 & 16 \\ 1 & 22 \\ 1 & 32 \\ 1 & 45 \\ 1 & 60 \\ 1 & 70 \\ 1 & 80 \\ 1 & 85 \\ 1 & 95 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} + \begin{bmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \vdots \\ \varepsilon_{11} \end{bmatrix}$$

$$\mathbf{Z} \quad = \quad \mathbf{X} \quad \mathbf{a} \quad \boldsymbol{\varepsilon}$$

The trend of the data is model with a linear trend that considers only two coefficients a_0 and a_1. The location of the data is transferred to matrix **X**(11 × 2) according the linear trend model, where the East coordinate of the data correspond to the column two. The vector **Z** with dimension (11 , 1) represent the values of the data set. The least squares method gives the estimates $\hat{a}_0$ and $\hat{a}_1$ of the parameters a_0 and a_1 through the simplified operations of matrices. Then, the first coefficient is 1.2403 and second coefficient is 0.0247.

$$\hat{\mathbf{a}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Z} = \begin{bmatrix} 1.2403 \\ 0.0247 \end{bmatrix}$$

The trend model is defined by the equation that evaluates $Z(\mathbf{u})$ as a function of location in one dimension.

$$Z(\mathbf{u}) = 1.2403 + 0.0247x$$

The data location is replaced in the regression line to calculate the **ε** residual or deviation of the data from the estimated regression model. Then, the variance of the residuals σ^2 is as follow:

$$\sigma^2 = \frac{\hat{\boldsymbol{\varepsilon}}^T\hat{\boldsymbol{\varepsilon}}}{n-p} = \frac{1.21}{11-2} = 0.134$$

The covariance of the coefficients is defined and the variance of the regression coefficients are extracted from the diagonal of this $Cov(\hat{\mathbf{a}})$.

$$Cov(\hat{\mathbf{a}}) = \sigma^2(\mathbf{X}\mathbf{X}^T)^{-1} = \begin{bmatrix} 4.19E-02 & -6.22E-04 \\ -6.22E-04 & 1.32E-05 \end{bmatrix}$$

Then, each term of the covariance matrix is divided by their respective standard deviations to obtain the correlation matrix.

$$\rho = \begin{bmatrix} \dfrac{C_{a_{00}}}{\sigma_{a_0}\sigma_{a_0}} & \dfrac{C_{a_{01}}}{\sigma_{a_0}\sigma_{a_1}} \\ \dfrac{C_{a_{10}}}{\sigma_{a_1}\sigma_{a_0}} & \dfrac{C_{a_{11}}}{\sigma_{a_1}\sigma_{a_1}} \end{bmatrix} = \begin{bmatrix} \rho_{a_{00}} & \rho_{a_{01}} \\ \rho_{a_{10}} & \rho_{a_{11}} \end{bmatrix} = \begin{bmatrix} 1 & -0.837 \\ -0.837 & 1 \end{bmatrix}$$

The correlation matrix is symmetric and is positive-definite, then, the Cholesky decomposition is possible. The lower triangular matrix helps to correlate the independent normal values w_0 and w_1.

$$\begin{bmatrix} y_0^k \\ y_1^k \end{bmatrix} = \underbrace{\begin{bmatrix} \rho_{a_{00}} & 0 \\ \rho_{a_{10}} & \sqrt{1-\rho_{a_{10}}^2} \end{bmatrix}}_{\text{Lower matrix}} \begin{bmatrix} w_0 \\ w_1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ -0.837 & \sqrt{1-(-0.837)^2} \end{bmatrix} \begin{bmatrix} 0.772 \\ 0.279 \end{bmatrix}$$

The k realization of y_0^k and y_1^k coefficients are in Gaussian units. These are non-standardized to get a_0^k and a_1^k in original units.

$$a_0^k = a_0 + \sigma_{a_0} y_0^k = 1.2403 + 0.2048 \times 0.772$$
$$a_1^k = a_1 + \sigma_{a_1} y_1^k = 0.0247 + 0.0036 \times (-0.493)$$

The values of the first realization k = 1 correspond to the set of coefficients a_0^1 = 1.398 and a_1^1 = 0.023. Then, one hundred times k = 1,…,100 are sampled from the distribution of regression coefficients with mean $\hat{a}_0$ and $\hat{a}_1$ and standard deviation σ_{a0} and σ_{a1}. The original correlation of the coefficients is -0.837, and then the correlation between the two coefficients after one hundred realizations is preserved. The scatter plot of the first stochastic trend coefficients is illustrated in a red dot and the next ones are illustrated in black small dots see Figure 1.

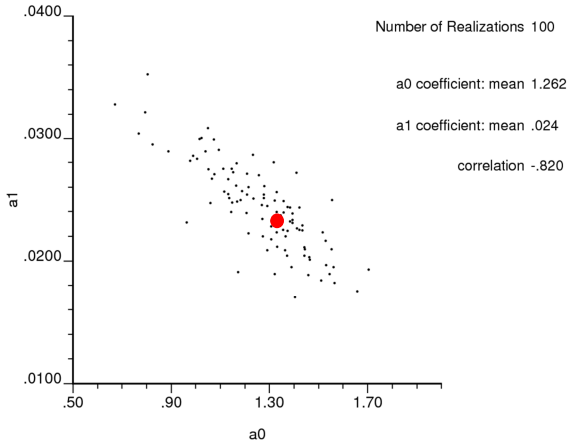

Figure 1: Verification whether the correlation of the 100 realizations of â0 and â1 reproduce the input correlation -0.837 between the regression coefficients, the red dot correspond to the first realization developed before.

One hundred sets of coefficients are used in the trend model. Then, one hundred stochastic trends are defined. A trend model is used to evaluate the value at all locations and the corresponding global mean. The fluctuations of the trend provide one hundred means. The fluctuations of the trend are illustrated in Figure 2.

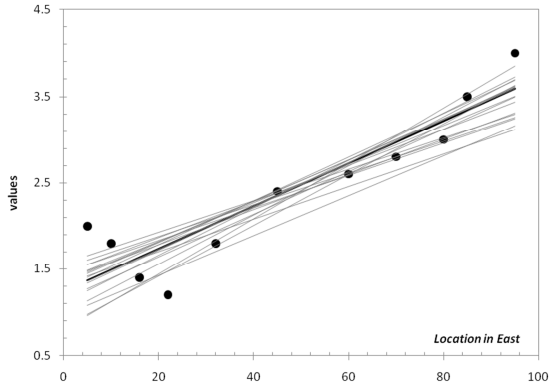

Figure 2: Stochastic trend model, where the black points are the data; the solid black line is the linear trend model with two parameters; and the grey lines are the realizations.

One hundred stochastic trend models provide an uncertainty of 0.114. This value represent 45 % of the uncertainty assuming independence of the data σ/√n = 0.251.

4. Application and Challenges

The stochastic trend is applied to a 3-D data set. Also, the influence of variable domains on the uncertainty and the complexity of the model in the uncertainty are evaluated. The gold values are located in a domain of 200 meters by 200 meters in the horizontal direction and 20 meters in the vertical direction. The mean of the gold values is 1.10 g/t and the standard deviation is 1.4. The evaluations consider three different domains:

- Pessimistic criteria, the domain which limits are less than half distance between samples.
- Normal criteria, the reasonable domain which limits are around the half of the median distance between samples.
- Optimistic criteria, the domain which limits are excessively far from the sample, it means almost twice or more than the median distance between samples.

The uncertainty of the gold values is calculated by a quadratic trend of 10 coefficients and a linear trend of 4 coefficients.

$$Z(\mathbf{u}) = a_0 + a_1 x + a_2 y + a_3 z + a_4 x^2 + a_5 y^2 + a_6 z^2 + a_7 xy + a_8 xz + a_9 yz$$
$$Z(\mathbf{u}) = a_0 + a_1 x + a_2 y + a_3 z$$

The variables *x*, *y* and *z* are the coordinates East, North and Elevation of the vector location **u**. These values are transferred to the matrix **X** to obtain the regression coefficients, $\hat{\mathbf{a}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{Z}$. The vector **Z** contains the 49 gold values. The regression coefficients are computed for both trend models.

$$Z(\mathbf{u}) = 8.554 - 0.0029x + 0.0685y - 0.7056z + 0.0001x^2 + 0.0003y^2 + 0.0092z^2 - 0.0008xy + 0.0024xz - 0.0017yz$$
$$Z(\mathbf{u}) = 5.403 - 0.0008x + 0.004y - 0.153z$$

Each trend model requires a covariance matrix and a correlation matrix of the regression coefficients. One hundred realizations of the coefficients are simulated with the LU methodology described above. Sets of the coefficients $\hat{\mathbf{a}}$ are replaced in their trend models to estimate the gold value at each node of the domain. The uncertainty with the quadratic trend results greater than the linear trend for the three domains.

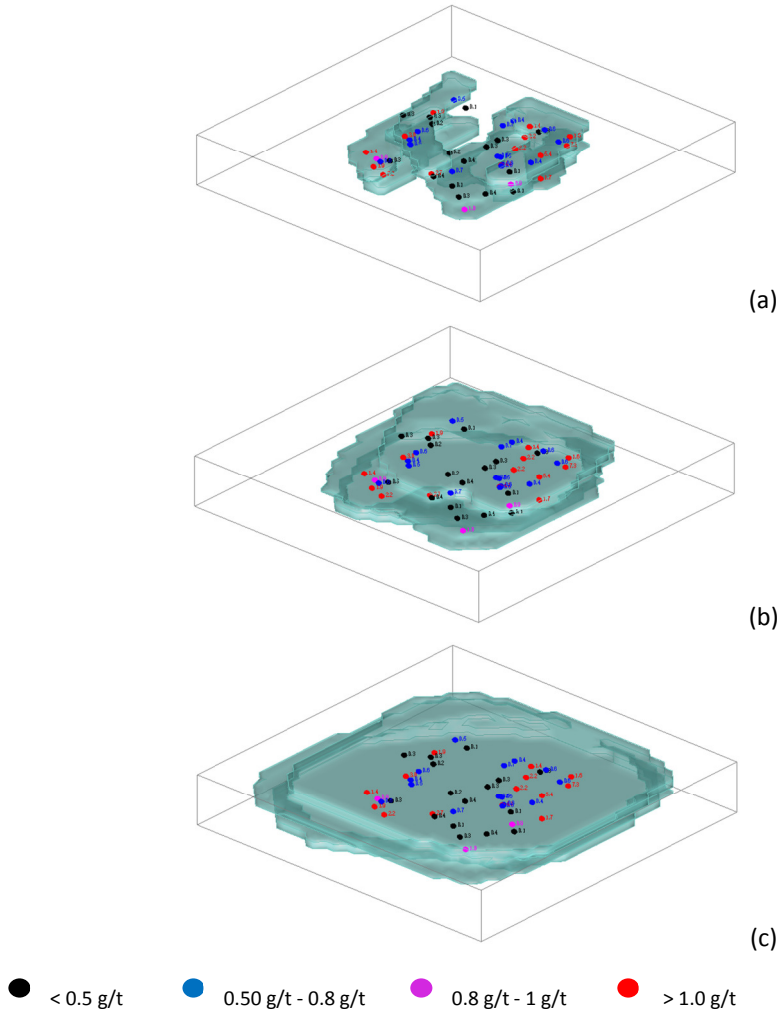

Figure 3: The data are illustrated with points, the first graphic (a) shows the pessimistic criteria used to model the domain, the second graphic (b) shows the reasonable criteria and the third graphic (c) shows the optimistic criteria.

Forty-nine data of gold values located in a pessimistic domain give an uncertainty of 0.227 (std) using a linear trend and 0.515 (std) using a quadratic trend. Those values are greater than $1.4/\sqrt{49} = 0.20$ (std) with CB that assumes independence. As expected, the uncertainty increases as the domain increases. The optimistic (large) domain provides an uncertainty of 0.234 using linear trend and 0.721 using quadratic trend. The sudden increase of uncertainty as the domain increases without support of data is an advantage of the ST approach because traditional geostatistics techniques struggle with less uncertainty in this scenario.

The technique is simple to apply because it does not require a covariance model of the data and does not need to be set many parameters during the implementation. This technique considers the size of the domain and assume that the mean dependent of the location data; however, the specific form of the trend is an important choice. Moreover, the model parameters are assumed to be multivariate Gaussian.

5. Conclusions

Geostatistics techniques often lead to less uncertainty for larger domains even if the number of data stays the same. An alternative to evaluate uncertainty in these domains could be to use a trend equation and define the mean dependent on the location within the domain. The trend model could be used to predict the value at unsampled locations. A global mean is evaluated with the set of coefficients evaluated at all locations within the

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