A New Approach to Direct Sequential Simulation that Accounts for the Proportional Effect: Direct Lognormal Simulation

John Manchuk, Oy Leuangthong and Clayton Deutsch

Department of Civil & Environmental Engineering
University of Alberta

Abstract

Direct kriging and simulation avoids the common Gaussian transform and permits unbiased integration of multiscale data. Currently, kriging is performed on Gaussian data since all conditional distributions are Gaussian and fully described by the kriging estimate and homoscedastic kriging variance. Application of kriging to data in original units will almost certainly lead to a variance that is incorrect since real data exhibit heteroscedastic features, that is, a proportional effect. This paper shows that the naïve form of direct sequential simulation, where the kriging variance is taken as homoscedastic, leads to poor results. A method of DSS is developed that corrects the kriging variance to account for the proportional effect. A multivariate lognormal distribution is developed since it has an analytical model of the proportional effect.

Introduction

Direct sequential simulation (DSS) [1, 2, 3] has been applied because of its ability to account for data of various support volumes and populate unstructured grids with data at different support. Kriging with the available data in original units is the essential idea of DSS. Although kriging provides a valid estimate and variance for a conditional distribution, the resulting homoscedastic variance poses a significant problem when original data units are considered; the uncertainty in low-valued areas is over stated and the uncertainty in high-valued areas is understated.

Real data often exhibit a classical heteroscedastic relationship between the local mean and variance, commonly referred to as the proportional effect [4]. With kriging as the main engine in DSS, the resulting simulated values do not reproduce a heteroscedastic feature; a method must be developed to account for the proportional effect inherent in original data units.

Simple kriging (SK) is important in DSS/simulation because of its ability to reproduce the covariance even if the conditional distributions are not Gaussian [1]. Covariance reproduction using SK can be easily demonstrated (Appendix B). Reproduction of the covariance only holds if the variance of the data is homoscedastic, but in the case of lognormal data the variance is clearly heteroscedastic.

This paper proposes a solution to the homoscedastic kriging variance problem of DSS. This is a particularly interesting case since the mathematical relationship between the lognormal and the commonly used normal distribution is well known, as are the equations that describe the proportional effect of lognormal data [5]. Knowing these relations, the kriging variance can be calibrated to honour the heteroscedasticity inherent in lognormal data. This well posed case provides valuable insight into the nature of DSS.

Simulation is commonly performed using data that has undergone a Gaussian/normal transform and simulated values are then back-transformed to original units to produce a set of realizations. In normal space, all local distributions are also normal and fully defined by the local mean and the kriging variance; however, in original space this is not the case. For direct simulation, the local distributions must be determined in original space (*Z-space*). An example of lognormal data will be used; below we will see how lognormal data provides a very good fit to real data.

Theoretical Background

A key requirement in the derivation of SGS/DSS (see Appendix B) is that the variance be independent of the conditional mean. The lognormal model is unique in that this requirement is *not* met; it is a different model.

In order to move from simulation in normal space to simulation in original space, an idea of how the two methods are linked would be useful. Many natural variables have an approximately lognormal histogram. There is an analytical relationship between normal and lognormal space providing a method to transform data between the two. Transformations involve the distributions, the data values, and the variograms. All transformations are analytical.

Normal to Lognormal Transformation

Equations exist that describe a lognormal distribution and its relation to a normal distribution. Since these equations are known, applying direct kriging on lognormal data is possible. A random variable, $Z \mid z(\mathbf{u})>0$, is lognormal with a mean m and standard deviation σ if the natural logarithm of $Z(\mathbf{u})$, $X(\mathbf{u}) = ln(Z(\mathbf{u}))$ is normally distributed with mean α and standard deviation β. Knowing the relation between $Z(\mathbf{u}) \rightarrow logN(m,\sigma)$ and $X(\mathbf{u}) \rightarrow N(\alpha,\beta)$, one can transform a Gaussian distribution, $Y(\mathbf{u}) \sim N(0,1)$, into a lognormal distribution. Equations 1 and 2 show the relation between $X(\mathbf{u})$, $Y(\mathbf{u})$, and $Z(\mathbf{u})$, where Y(u) is a standard normal distribution. Equations 3 and 4 show the relation between m and σ of the lognormal with α and β of the normal distribution.

$$X(\mathbf{u}) = \alpha + \beta \cdot Y(\mathbf{u}) \tag{1}$$

$$Z(\mathbf{u}) = e^{X(\mathbf{u})} \tag{1.1}$$

Substituting Equation *1* into Equation *1.1* yields Equation 2:

$$Z(\mathbf{u}) = e^{\alpha + \beta \cdot Y(\mathbf{u})} \tag{2}$$

$$\alpha = \ln(m) - \frac{\beta^2}{2} \tag{3}$$

$$\beta^2 = \ln\left(1 + \frac{\sigma^2}{m^2}\right) \tag{4}$$

Equations 5 and 6 describe the normal and lognormal probability distribution curves, which are quite similar in arrangement. Figure 1 shows the change in the distribution shapes as $Y(\mathbf{u})$ is converted into $X(\mathbf{u})$ and as $X(\mathbf{u})$ is transformed into $Z(\mathbf{u})$.

$$f(x) = \frac{\exp\left[-\frac{1}{2}\left(\frac{\ln(x)-\alpha}{\beta}\right)^2\right]}{\beta \cdot x\sqrt{2\pi}} \tag{5}$$

$$g(x) = \frac{\exp\left[-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2\right]}{\sigma\sqrt{2\pi}} \tag{6}$$

The remaining theoretical relationships are easier to appreciate when referenced to the model and data used for application of direct sequential simulation. For this purpose, an unconditional Gaussian model was initially produced with dimensions of 256 by 256 (65536 data points) using a spherical variogram with zero nugget effect and a range of 32. The simulated Gaussian values were then transformed using Equations 1 to 4 to give a lognormal model with arbitrarily chosen mean and standard deviation of 100 (Figure 2 shows the resulting unconditional models). From this model, 625 values were sampled and used for kriging, see Figure 2.

Variogram Transformation

If the variogram in Gaussian space is known, it can be converted to the variogram in lognormal space through the use of Equation 7. This actually relates the correlograms, but these are easily converted to the variogram as shown with Equation 7.

$$\rho(\mathbf{h}) = \frac{m^2}{\sigma^2}\left[e^{\beta^2 \cdot r(\mathbf{h})} - 1\right] \tag{7}$$

$$\rho(\mathbf{h}) = 1 - \frac{\gamma_Z}{\sigma_Z^2}\ ,\ \ r(\mathbf{h}) = 1 - \gamma_Y$$

where $r(\mathbf{h})$ is the correlation in *Y*-space and $\rho(\mathbf{h})$ is the correlation in *Z*-space.

Figure 3 shows the variogram used to create the unconditional model along with the theoretical variogram for the resulting lognormal model. The difference between the variograms becomes somewhat significant as half the range is approached.

Inference of Conditional Distributions

Our goal is to calculate a conditional distribution (conditional to some number of local data) for simulation. In a multivariate Gaussian case we transform the data, infer the parameters in Gaussian units, and then back transform the result. The transform and back transform are particularly easy when the data are lognormal. In fact, the shapes of all conditional distributions in original units are lognormal when the original global histogram is lognormal (see Appendix A).

The classic approach consists of kriging in Gaussian units; then, the distribution in original units is inferred. The key idea of DSS is to krige in original units, but we must establish the correct variance, which is heteroscedastic, that is it depends on the magnitude of the data and estimate.

The heteroscedasticity is automatically accounted for in the back transform. There is no back transform in DSS. We would have to build in some form of correction.

Homoscedastic Variance Correction

We could imagine a linear estimate that is heteroscedastic (e.g. lognormal). The kriging variance is often assumed to be homoscedastic, which is inconsistent with data that exhibit a proportional effect. With lognormal data, an equation exists for correcting the variance using the mean or estimate and it can be derived from Equation 4:

$$\beta_L^2 = \ln\left(1 + \frac{\sigma_Z^2}{m_Z^2}\right)$$

$$1 + \frac{\sigma_Z^2}{m_Z^2} = e^{\beta_L^2}$$

$$\sigma_Z^2 = m_Z^2 (e^{\beta_L^2} - 1)$$

where β_L^2 is the homoscedastic kriging variance in X units and m_Z^2 and σ_Z^2 are the estimate and variance from kriging original data.

Since m_Z^2 is the estimate from kriging it can be denoted by $z^*(\mathbf{u})$. From Equation A2 in Appendix A it is shown that the local β_L^2 value can be determined from the kriging variance in Y-space and the global β_G^2 value (the global variance in X units). Substituting these results into the equation arrived at above yields Equation 8:

$$\sigma_{Z,C}^2 = \left[z^*(\mathbf{u})\right]^2 (e^{\beta_G^2 \cdot \sigma_Y^2} - 1) \qquad (8)$$

Where $\sigma_{Z,C}^2$ is the corrected variance, σ_Y^2 is the local variance in normal space, and β_G^2 is the global variance of *ln*(*Z*).

To experimentally show this relation between Gaussian data and its lognormal transform, kriging was performed on both the normal and lognormal data and the GAM program [6] was run on the results at a specified lag (half the range was used) and the $Y(\mathbf{u}+\mathbf{h})$ values were extracted. Splitting the results into 50 quantiles and determining the mean and standard deviation of each quantile shows that the variance is homoscedastic for Gaussian data and the variance depends on the mean with lognormal data. For comparison, the analytical lines were plotted on Figure 4.

A major implication from Equation 8 is that kriging would have to be performed twice; once to get the kriging variance in Gaussian space (σ_Y^2) and again to get the estimate in lognormal space ($z^*(\mathbf{u})$). To avoid this, a relation was fit to the uncorrected Z-space kriging variance and the Y-space kriging variance. For this particular data set, the resulting kriging variance values are shown in Figure 5 and fitted using Equation 9. The fit is very good with an R-squared value of 0.998 and a standard error of estimate equal to 0.006456.

$$\sigma_Y^2 = -0.0005 + 0.7237(\sigma_Z^2) + 0.0597(\sigma_Z^2)^2 - 0.2425(\sigma_Z^2)^3 + 0.4597(\sigma_Z^2)^4 \quad (9)$$

Implementation of Direct Simulation

To provide a set of results for comparing direct kriging and simulation, the current method of simulation using SGSIM was initially applied. By setting up a simple example in Excel, it was shown that the local distributions are in fact lognormal so the same equation used to transform the normal model to a lognormal model as in Figure 2 could be used to back transform Gaussian values to lognormal values in SGSIM. This result also allows the development of equations to relate the local Gaussian distributions to the local lognormal distributions. Equations 10 and 11 show how the local Gaussian mean and variance can be transformed to the local alpha and beta values for use in Equations 12 and 13, which are used to determine the local lognormal mean and variance. See Appendix A for the kriging example in Excel and derivations of Equations 10 and 11.

$$\alpha_L = \alpha_G + \beta_G \cdot m_N \quad (10)$$

where m_N is the local normal mean, α_G is the global mean of $ln(Z)$, and α_L is the local mean of $ln(Z)$.

$$\beta_L^2 = \beta_G^2 \cdot \sigma_N^2 \quad (11)$$

where σ_N^2 is the local normal variance and β_L^2 is the local variance of $ln(Z)$.

$$m_L = e^{\left(\alpha_L + \beta_L^2/2\right)} \quad (12)$$

$$\sigma_L^2 = m_L^2\left(e^{\beta_L^2} - 1\right) \quad (13)$$

Three options of simulation were explored:

Option 1 Transform a set of lognormal samples to normal space and perform kriging and MCS, then back-transform to lognormal space. This is the standard/common approach. The limitation is that multiscale data are not easily handled.

Option 2 Perform direct kriging with the lognormal values with an adjusted variogram and do MCS without correcting the kriging variance. This is the published approach to DSS. The limitation is that heteroscedasticity/the proportional effect is not accounted for.

Option 3 Perform direct kriging on the lognormal values with an adjusted variogram and correct the kriging variance prior to MCS. This is the new approach that we are advocating in this paper. Multiscale data can be used in direct kriging and the proportional effect is explicitly accounted for.

For each option, 100 conditional realizations were produced and the conditional mean and variance at every location was determined. Figure 6 shows the simulation results for all three options. To check the validity of each simulation method, reproduction of the global statistics as well as the variogram were checked. These are shown in Figure 7.

In Figure 6, it is obvious that option 3 compares closely to the conventional simulation method (option 1); however, performing a naïve direct simulation as in option 2 results in a variance with little fluctuation through out the map (Figure 6). Option 2 shows that performing direct simulation, with no variance correction, tends to hide the proportional effect inherent in lognormal data. Regardless of this incorrect variance, all three options should theoretically reproduce the mean, variance and variogram as shown by Figure 7. It seems that with direct simulation of lognormal data, the estimated mean value is higher than that found using conventional Gaussian simulation. If the mean is higher, Equation 8 will force the variance at that location to be higher as well. These problems may lead to overestimating an area, however the differences are minimal in this case.

For additional comparison, three points were chosen from the option 1 results; one with low mean and low variance (point 1); one with high mean and low variance (point 2); and one with high mean and high variance (point 3). For each point, a local distribution was produced by extracting the simulated value from the 100 realizations. Figure 8 (along with a summary table and chart) shows the distribution for each point and for each simulation option.

From Figure 8, it is clear that the distributions for options 1 and 3 are similar; however, the variance for option 2 does not compare. Over the three locations, the variance for option 2 remains relatively constant. This indicates that the proportional effect has been removed and the variance is homoscedastic as would be expected with Gaussian data. To check how the proportional effect was honored for all three options, the kriged mean and variance was extracted at all locations and plots of the mean versus the standard deviation were produced and are shown in Figure 9.

Conclusion

The proportional effect is a common characteristic for many data sets and cannot be reproduced with kriging alone since the resulting variance is homoscedastic and must be corrected to reproduce the proportional effect. The lognormal distribution is closely related to the Gaussian/normal distribution, but it has an analytically defined proportional effect.

The results of conventional simulation and direct sequential simulation compare well with minor differences in the overall mean and variance between the realizations. Also, the local distributions at various locations closely resembled one another. These findings provide insight into a possible solution to DSS when dealing with the proportional effect and lognormal data. It is apparent that the kriging variance must be corrected such that the proportional effect is reproduced with direct simulation.

By imposing a correction to the kriging variance prior to simulation, it is possible to perform direct sequential simulation of lognormal data with correct/reasonable results. Correcting the proportional effect in this manner imparts a dependency between the estimate and the variance that is in direct contradiction to the simple kriging principle, which requires independence between the estimate and the variance. The lognormal model is a truly different approach to direct simulation.

References

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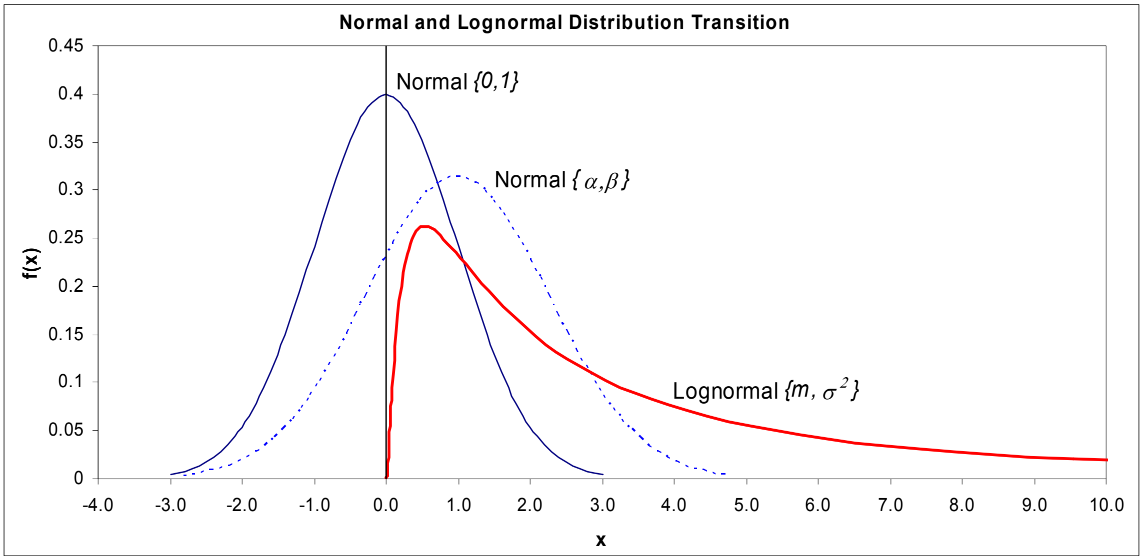


Figure 1: Normal and corresponding lognormal distributions. The lognormal distribution was calculated from the Gaussian distribution by using the transformation equations 1 to 4 above. The lognormal distribution has a mean of 6 and a standard deviation of 3.

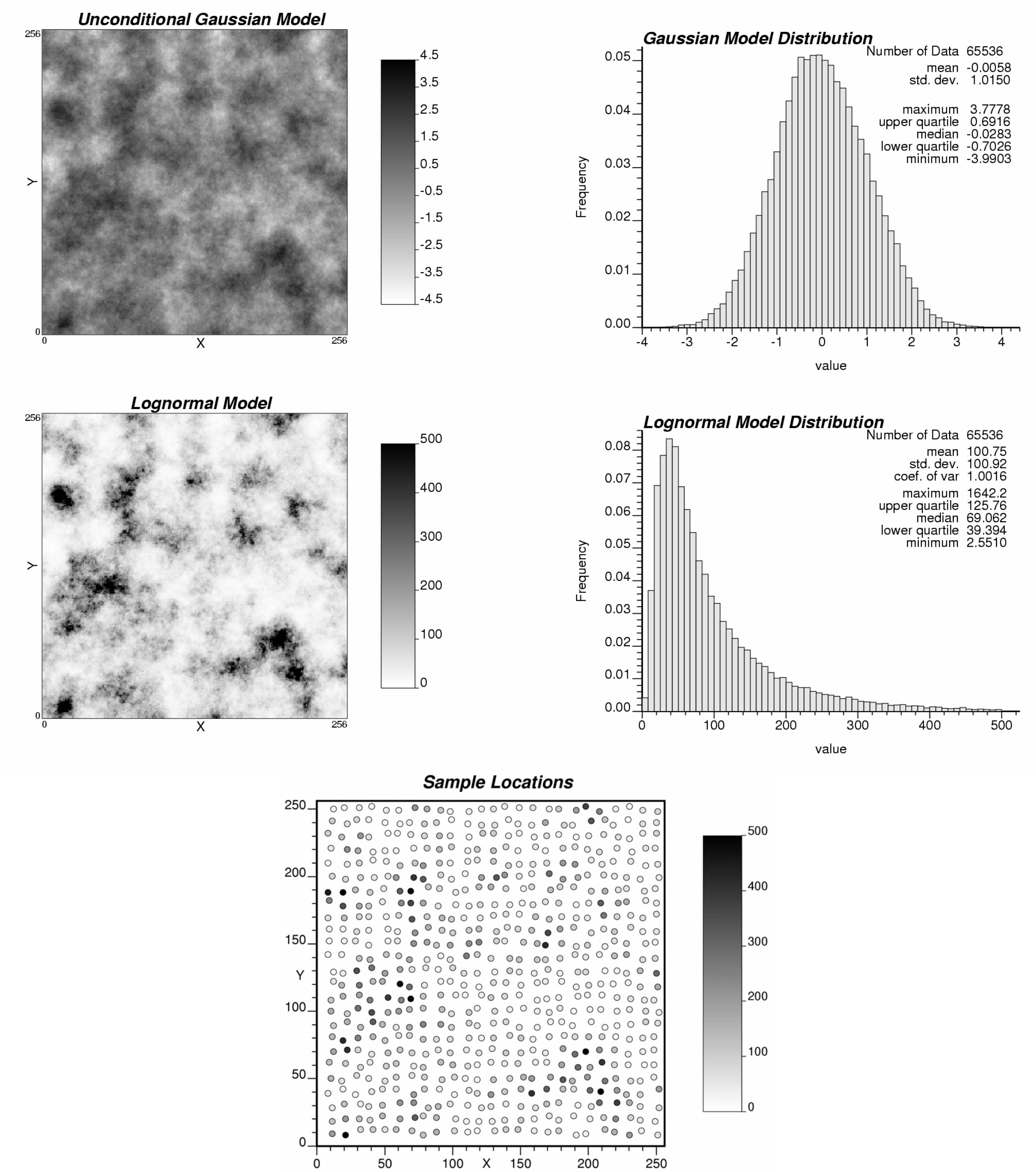


Figure 2: Gaussian model and corresponding lognormal model along with their distributions. The set of 625 samples is also shown (bottom).

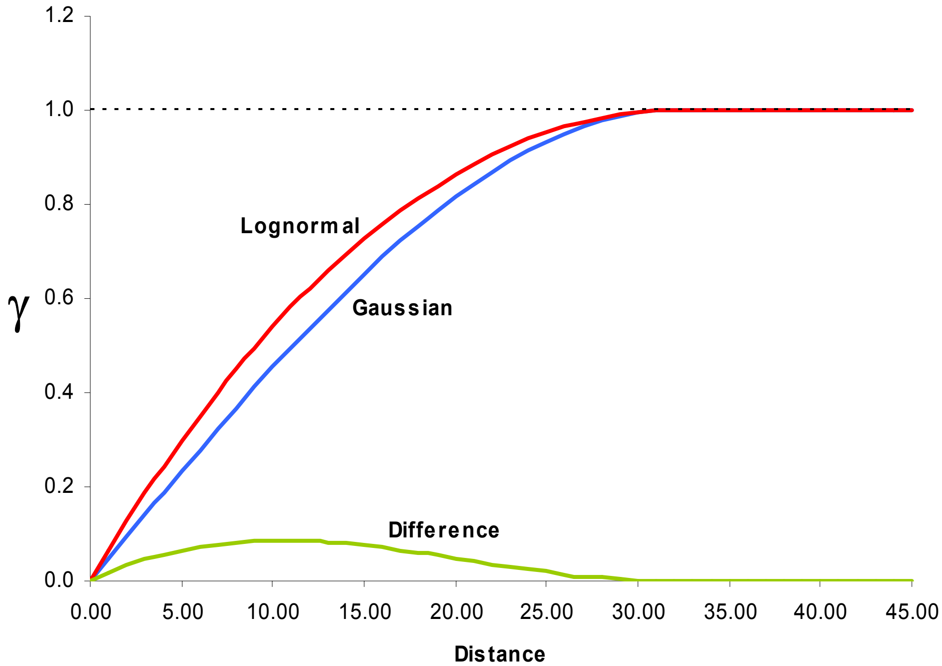


Figure 3: Variogram model used to generate the unconditional model. The Gaussian model is spherical with no nugget effect and a range of 32. The corresponding variogram of the lognormal variable is shown with the difference between the two functions.

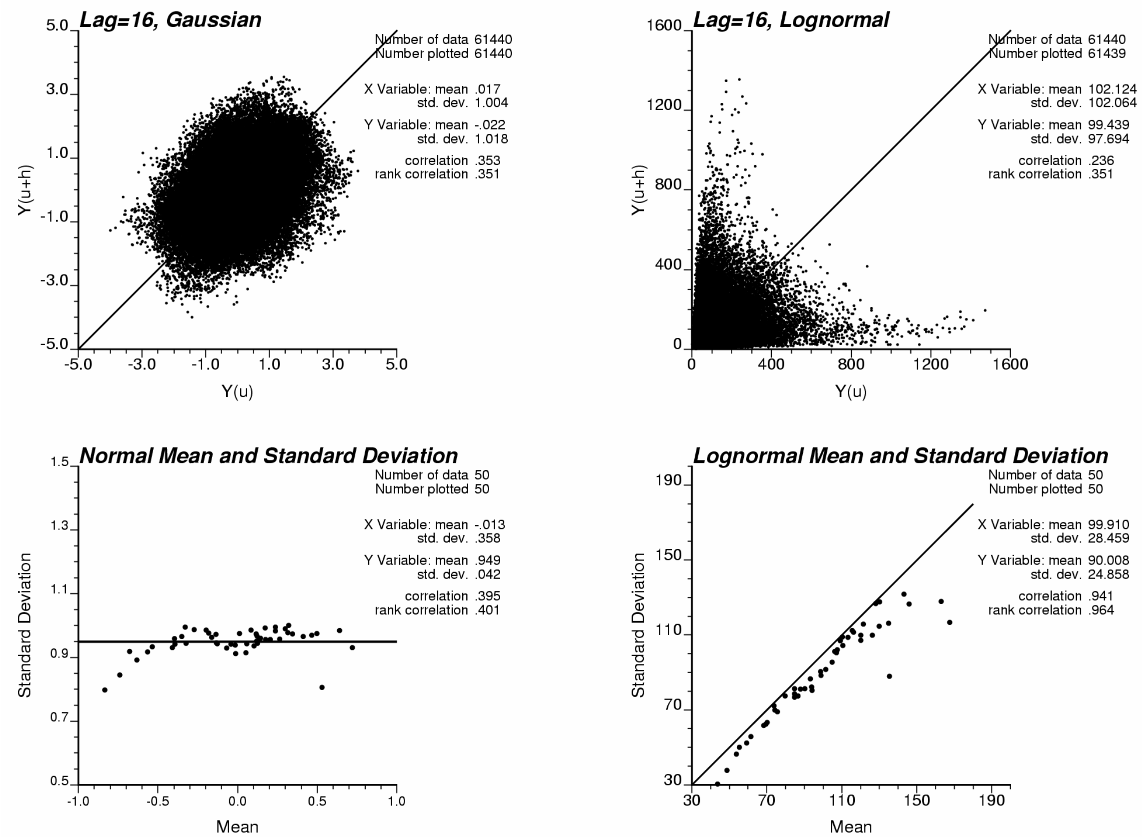


Figure 4: Scatterplots of $Y(\mathbf{u})$ versus $Y(\mathbf{u+h})$ for Gaussian (upper left) and lognormal (upper right) data. Gaussian data showing the variance is homoscedastic (lower left) and Lognormal data displaying the proportional effect (lower right). The analytical line in the lower right plot was determined using Equation 8. Because the global variance in *Y*-space is 1 and β_G^2 is equal to *ln(2)* (see Equation 4) in normal$\{\alpha,\beta\}$ space, the slope of the theoretical line on the lower right graph is one.

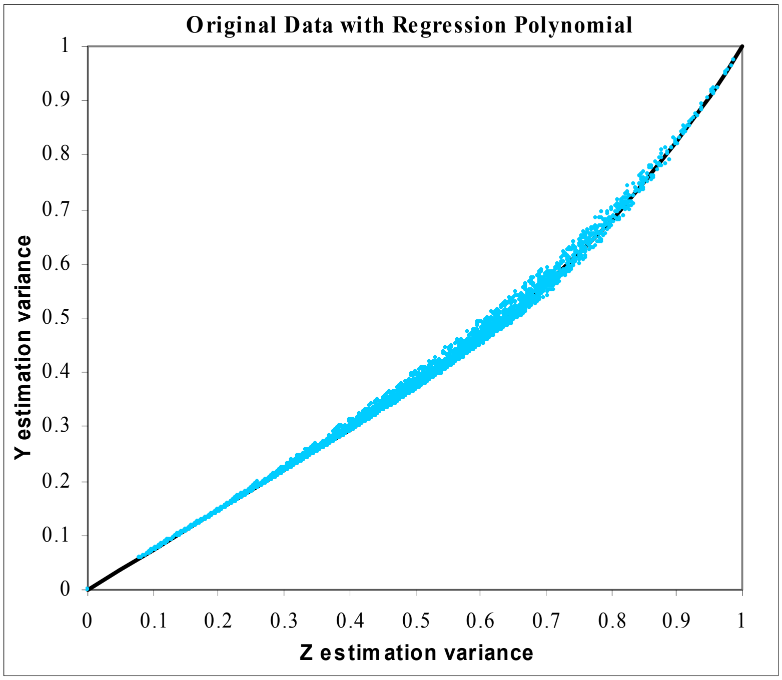


Figure 5: A fit of the estimation variance in Z-space versus the estimation variance in Y-space prior to correcting the lognormal kriging variance. Bullets represent data and the black curve displays Equation 9.

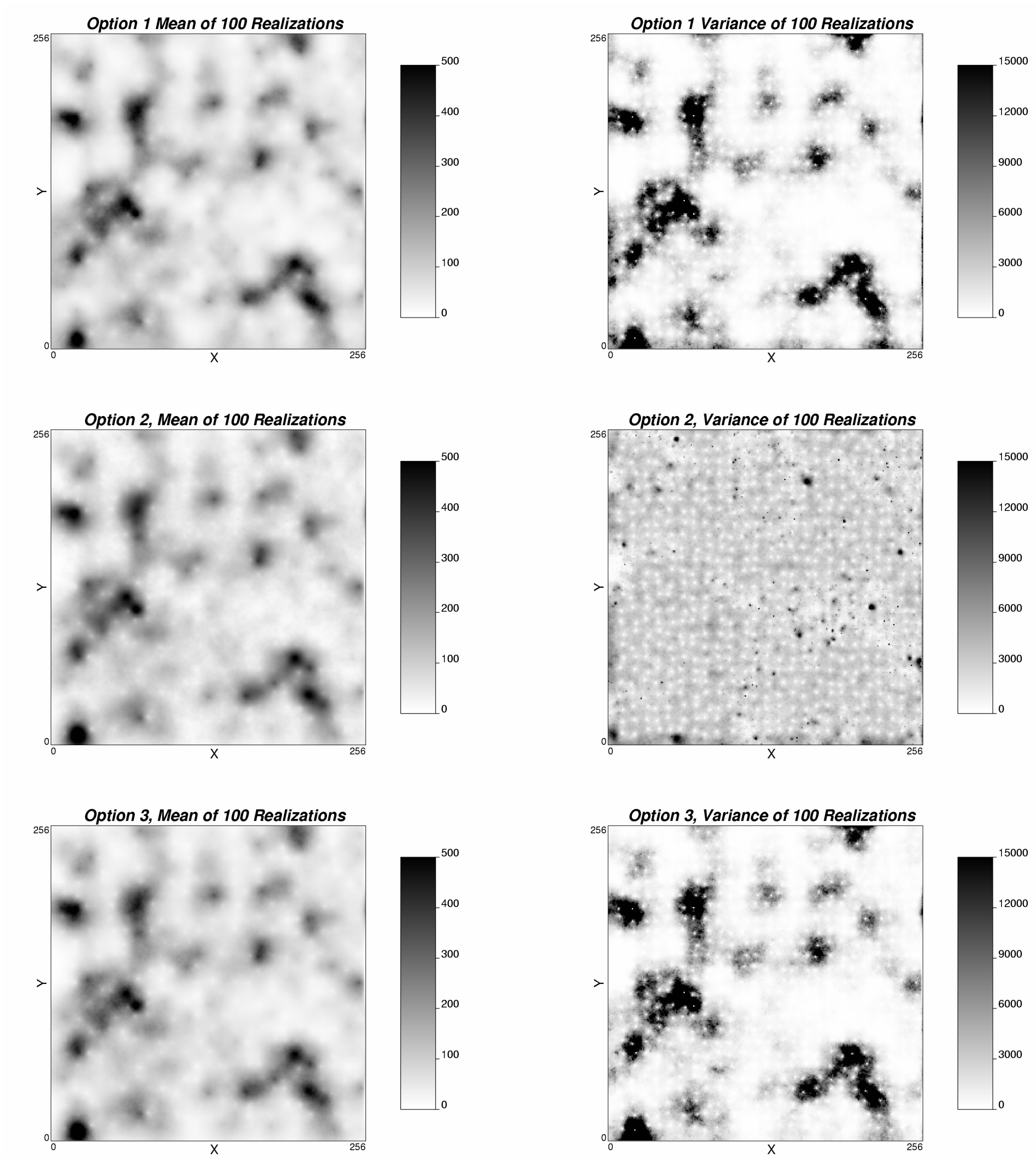


Figure 6: The mean and variance taken over 100 realizations for all three simulation approaches. Top – option 1; traditional method of data transformation prior to kriging and simulation, then back transformation to get lognormal results. Middle – Option 2; naïve direct simulation with no variance correction. Bottom – Option 3; direct simulation of lognormal data with a variance correction to account for the proportional effect.

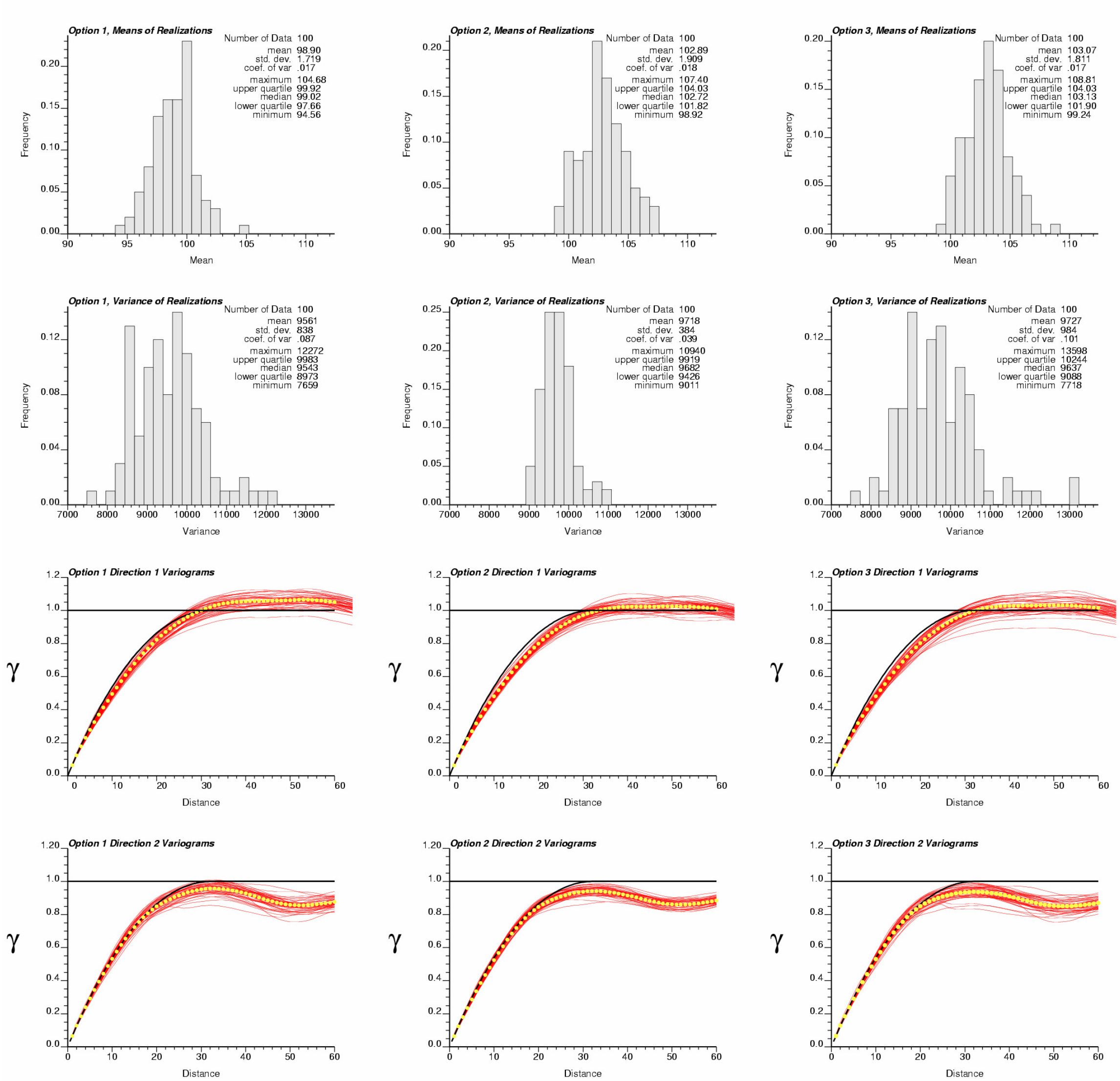
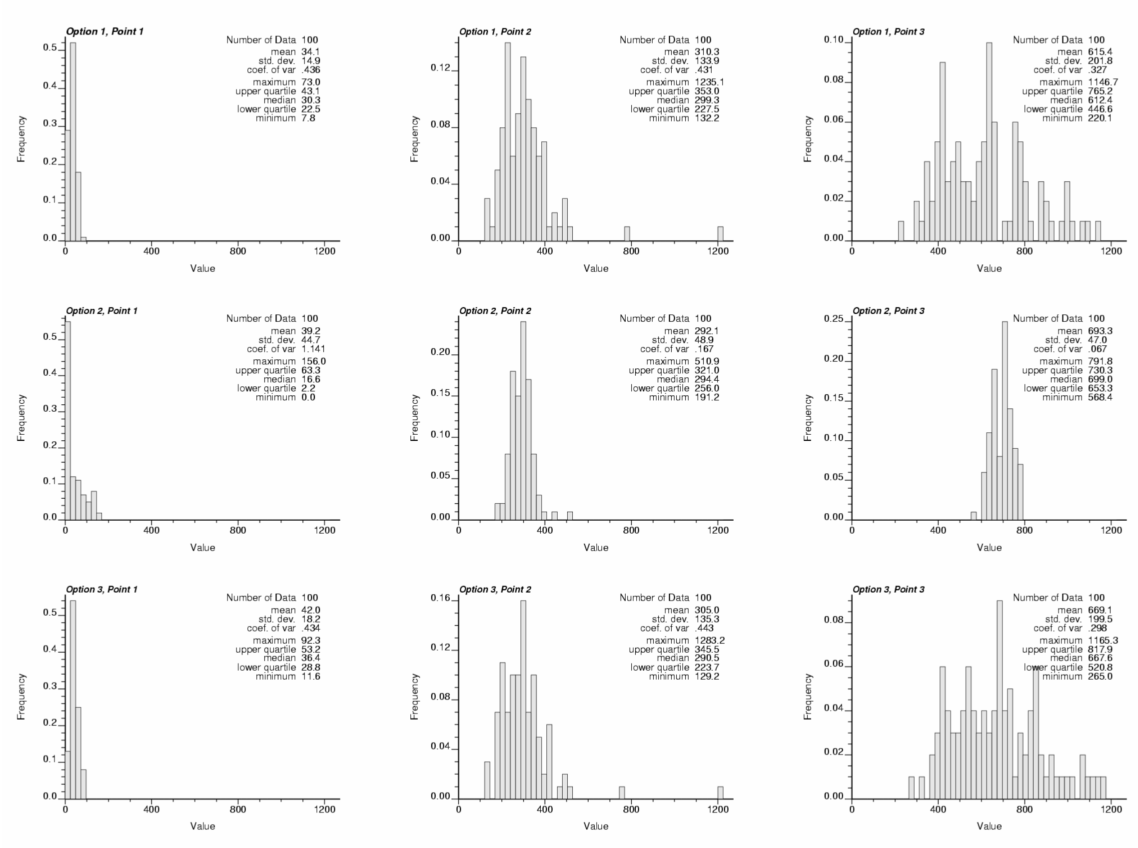


Figure 7: A check for mean, variance and variogram reproduction for the 100 realizations. Top – mean reproduction; both options 2 and 3 result in a slightly higher mean than option 1. Middle – variance reproduction; the three option compare well. Bottom – variogram reproduction (two directions shown); all options are close to following the analytical variogram model (solid line). Bullets represent the average of the 100 variograms.



		Options		
Points		1	2	3
1	mean	34.13	39.22	42.05
	st dev	14.90	44.77	18.27
2	mean	310.33	292.15	305.03
	st dev	133.94	48.99	135.31
3	mean	615.45	693.38	669.16
	st dev	201.81	47.01	199.60

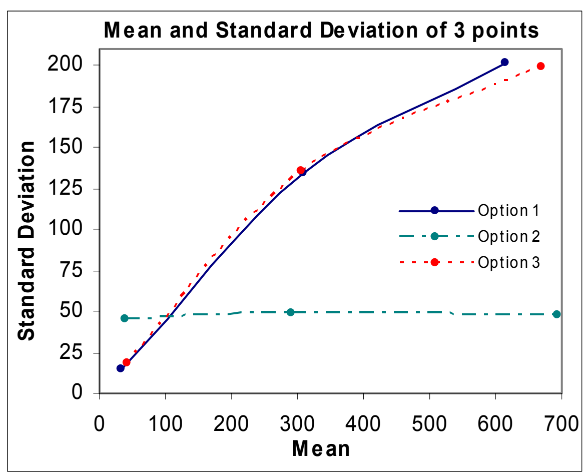


Figure 8: Distributions of three points for simulation options. Left – point 1; low grade, low variance. Centre – point 2; high grade, low variance. Right – point 3; high grade, high variance. A summary table (lower left) and associated graph (lower right) of the mean and standard deviation at each location are also provide.

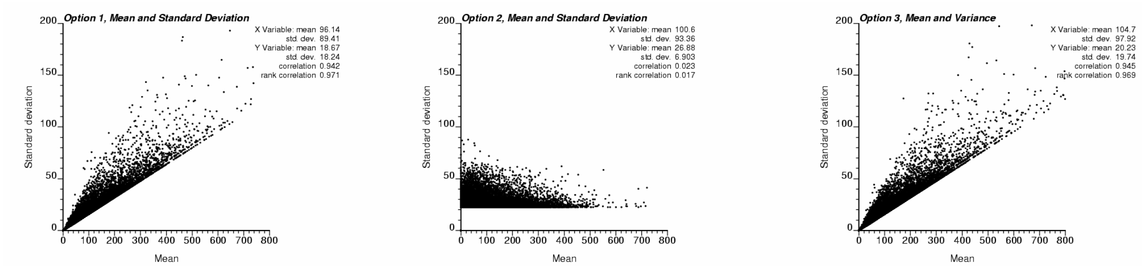
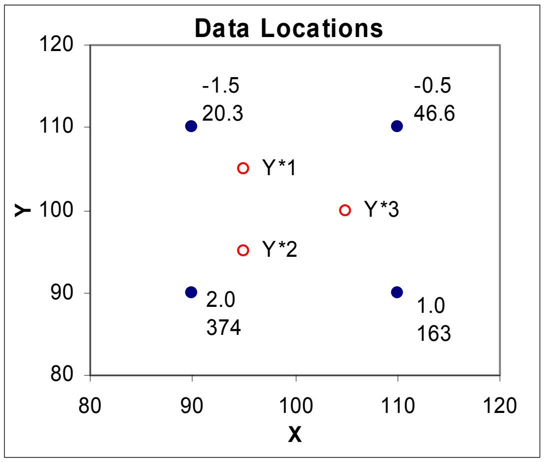


Figure 9: Local mean versus standard deviation at every estimated location for options 1 (left), 2 (middle), and 3 (right). Options 1 and 3 show the proportional effect and compare nicely. Option 2 shows a homoscedastic variance since no correction was applied.

Appendix A

Kriging of Gaussian Data and Determination of Local Distributions

To check if the local distributions at each location being estimated are lognormal, a simple kriging example was set up in Excel with 4 known data and 3 locations to be sequentially estimated, see Figure A1.



Location	m_N	σ_N^2
Y*1	-0.546	0.462
Y*2	1.073	0.396
Y*3	0.267	0.444

Figure A1: Data configuration for kriging (top) and kriging results prior to transformation to lognormal space (bottom). Solid bullets are known data and circles are the points to be estimated. The data values are also shown, both Gaussian (above) and lognormal (below).

To generate the local distributions corresponding to the global lognormal data with a mean and standard deviation of 100, a set of 199 quantiles was chosen ranging from 0.005 to 0.995 and the value corresponding to each for the local normal distributions was found. Using

$$Z(\mathbf{u}) = e^{\alpha + \beta \cdot Y(\mathbf{u})}$$

to transform the values to Z-space and plotting the results revealed that the local distributions are lognormal. To check if equations A1 and A2 (below) are correct, they were used to find the local alpha and beta values and then the LOGINV function in MS Excel was used to determine the corresponding value for each quantile. Both methods gave equal results, see Figure A2.

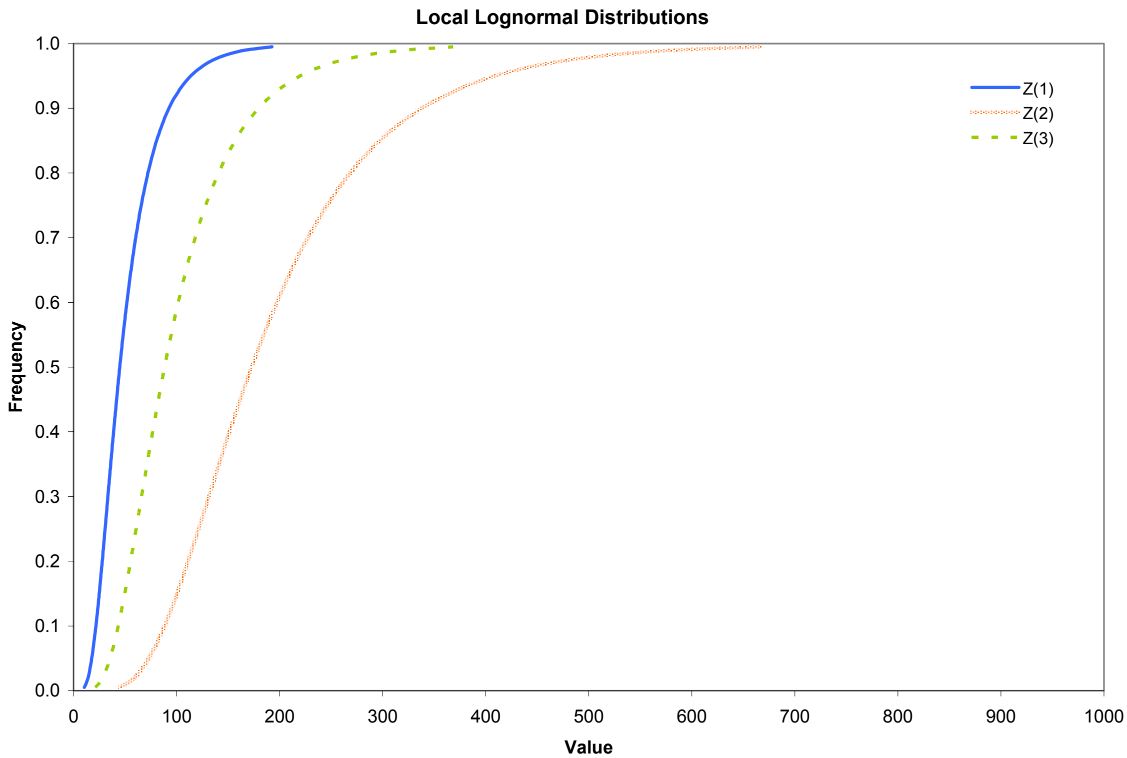


Figure A2: Local Lognormal Distributions at each estimated location. Using both a transformation method with tables as well as an analytical method gave equal results.

Derivation of Equations A1 and A2

Starting with the equation for transforming Gaussian data, Y(u) ~ $N(0,1)$, to normal X-space data, $X(\mathbf{u}) \rightarrow N(\alpha,\beta)$:

$$X(u) = \alpha_G + \beta_G \cdot Y(u)$$

Replacing Y(u) with the kriged mean and X(u) with the local mean of $ln(Z)$, we get Equation A1, which relates the local mean in X-space to that in Gaussian space.

$$\alpha_L = \alpha_G + \beta_G \cdot m_N \qquad \text{(A1)}$$

Where α_L is the local mean in X-space, α_G is the global mean of X(u), β_G is the global variance of X(u), and m_N is the kriged mean in Gaussian space.

To derive Equation A2, the Equation for transforming Y-space values to X-space along with the equation defining the variance of a data set was used. The local normal kriging variance can be defined by the following equation:

$$\sigma_N^2 = \frac{1}{n}\sum_{i=1}^{n}(u_i - m_n)^2$$

Where σ_N^2 is the variance in Gaussian space, u_i is the value at location i, and m_N is the mean of all u_i, $i=1 \ldots n$.

To determine the local variance of *ln(Z)* we need to know the values of u_{iX} and m_X that correspond to u_i and m_N in Gaussian space. Equation A1 can be used to perform this transformation:

$$u_{iX} = \alpha_G + \beta_G \cdot u_i$$

$$m_X = \alpha_G + \beta_G \cdot m_N$$

Substituting these into the equation for the variance in normal space (X-space), the local variance of *ln*(*Z*) can be solved for:

$$\beta_L^2 = \frac{1}{n}\sum_{i=1}^{n}(u_{iX} - m_X)^2$$

$$\beta_L^2 = \frac{1}{n}\sum_{i=1}^{n}((\alpha_G + \beta_G u_i) - (\alpha_G + \beta_G m_N)^2$$

$$\beta_L^2 = \frac{1}{n}\sum_{i=1}^{n}\left[\beta_G(u_i - m_N)\right]^2$$

$$\beta_L^2 = \frac{\beta_G^2}{n}\sum_{i=1}^{n}(u_i - m_N)^2$$

$$\beta_L^2 = \beta_G^2 \cdot \sigma_N^2 \qquad \text{(A2)}$$

Where β_L^2 is the local variance of *ln*(*Z*), β_G^2 is the global variance of *ln*(*Z*), and σ_N^2 is the local normal variance in Y-space.

Appendix B

The Simple Kriging Principle

Simple kriging is the key to direct sequential simulation due to the property of covariance reproduction even if the conditional probability distributions are not Gaussian. Reproducing the covariance only holds if the conditional variance is independent of the data values (homoscedastic). A proof of the covariance reproduction is provided with the following assumptions: the data stationary variable z has a mean and variance of 0 and 1, respectively. The conditional distributions are fully described by the kriging mean and variance. Equations B1, B2, and B3 describe the kriging mean and variance along with the simple kriging system considering N previous data:

$$z^*(\mathbf{u}) = \sum_{\alpha=1}^{N} \lambda_\alpha z(\mathbf{u}_\alpha) \qquad \text{(B1)}$$

$$\sigma_{SK}^2(\mathbf{u}) = 1 - \sum_{\alpha=1}^{N} \lambda_\alpha \rho(\mathbf{u} - \mathbf{u}_\alpha) \qquad \text{(B2)}$$

$$\sum_{\beta=1}^{N} \lambda_\alpha \rho(\mathbf{u}_\beta - \mathbf{u}_\alpha) = \rho(\mathbf{u} - \mathbf{u}_\alpha), \quad \alpha = 1,\dots,N \qquad \text{(B3)}$$

Where $z^*(\mathbf{u})$ is the simple kriging mean, $\sigma_{SK}^2(\mathbf{u})$ is the simple kriging variance, and λ_α, $\alpha=1,\dots,N$ are the kriging weights.

A random value $R_S(\mathbf{u})$ can be drawn from a distribution described by a mean of zero and a variance equal to the kriging variance $\sigma_{SK}^2(\mathbf{u})$. The kriged mean and $R_S(\mathbf{u})$ are added together to get the simulated value for the location, $Z_S(\mathbf{u})$. An important aspect of $R_S(\mathbf{u})$ is that its value is chosen independent of the mean $Z^*(\mathbf{u})$.

$$Z_S(\mathbf{u}) = Z^*(\mathbf{u}) + R_S(\mathbf{u}) \qquad \text{(B4)}$$

Now that one location has been simulated, there are $N+1$ data values for simulation of the next node which will be denoted $\mathbf{u}'=\mathbf{u}_{N+1}$. The simple kriging mean and variance at $\mathbf{u}'$ are given by Equations B5 and B6 along with the kriging system shown in Equations B7 and B8:

$$Z^*(\mathbf{u}') = \sum_{\alpha=1}^{N} \lambda_\alpha z(\mathbf{u}_\alpha) + \lambda_{N+1} Z_s(\mathbf{u}) \qquad \text{(B5)}$$

$$\sigma_{SK}^2(\mathbf{u}') = 1 - \sum_{\alpha=1}^{N} \lambda_\alpha \rho(\mathbf{u}' - \mathbf{u}_\alpha) - \lambda_{N+1} \rho(\mathbf{u}' - \mathbf{u}) \qquad \text{(B6)}$$

$$\sum_{\beta=1}^{N} \lambda_\beta \rho(\mathbf{u}_\beta - \mathbf{u}_\alpha) + \lambda_{N+1} \rho(\mathbf{u} - \mathbf{u}_\alpha) = \rho(\mathbf{u}' - \mathbf{u}_\alpha), \quad \alpha = 1,\dots,N \qquad \text{(B7)}$$

$$\sum_{\beta=1}^{N}\lambda_\beta \rho(\mathbf{u}_\beta - \mathbf{u}) + \lambda_{N+1} = \rho(\mathbf{u}' - \mathbf{u}) \quad \text{(B8)}$$

Where $Z^*(\mathbf{u}')$ and $\sigma_{SK}^2(\mathbf{u}')$ are the simple kriging mean and variance at location $\mathbf{u}'$ respectively. Note that the weights λ_α, $\alpha=1,\ldots,N+1$ are *not* the same as the weights λ_α, $\alpha=1,\ldots,N$ in Equation B1 to B3.

Once $Z^*(\mathbf{u}')$ and $\sigma_{SK}^2(\mathbf{u}')$ are known, a random value $R_S(\mathbf{u}')$ can be drawn from a distribution with a mean of zero and a variance equal to $\sigma_{SK}^2(\mathbf{u}')$. The simulated value at $\mathbf{u}'$ is calculated as follows:

$$Z_S(\mathbf{u}') = Z^*(\mathbf{u}') + R_S(\mathbf{u}') \quad \text{(B9)}$$

Let's calculate the covariance between the two simulated values:

$$\begin{aligned} E\{Z_S(\mathbf{u}) \cdot Z_S(\mathbf{u}')\} &= E\{Z^*(\mathbf{u}) \cdot Z^*(\mathbf{u}')\} + E\{Z^*(\mathbf{u}) \cdot R_S(\mathbf{u}')\} + \\ &\quad E\{Z^*(\mathbf{u}') \cdot R_S(\mathbf{u})\} + E\{R_S(\mathbf{u}) \cdot R_S(\mathbf{u}')\} \end{aligned} \quad \text{(B10)}$$

Where $E\{Z^*(\mathbf{u}) \cdot R_S(\mathbf{u}')\}$ and $E\{R_S(\mathbf{u}) \cdot R_S(\mathbf{u}')\}$ are zero since $Z^*(\mathbf{u})$ and $R_S(\mathbf{u}')$ are independent of each other and $R_S(\mathbf{u})$ and $R_S(\mathbf{u}')$ are also independent. The remaining portions of the right hand side are non zero since the kriged means depend on one another and also because the kriged mean at the second location depends on the randomly drawn value at the first location.

$$E\{Z_S(\mathbf{u}) \cdot Z_S(\mathbf{u}')\} = E\{Z^*(\mathbf{u}) \cdot Z^*(\mathbf{u}')\} + E\{Z^*(\mathbf{u}') \cdot R_S(\mathbf{u})\} \quad \text{(B11)}$$

Expanding and simplifying the first term from the right hand side of Equation B11:

$$\begin{aligned} E\{Z^*(\mathbf{u}') \cdot Z^*(\mathbf{u})\} &= \sum_{\beta=1}^{N}\lambda_\beta\left[\sum_{\alpha=1}^{N}\lambda_\alpha \rho(\mathbf{u}_\beta - \mathbf{u}_\alpha)\right] \\ &\quad + \lambda_{N+1}\sum_{\alpha=1}^{N}\lambda_\alpha E\{Z_S(\mathbf{u})Z(\mathbf{u}_\alpha)\} \end{aligned} \quad \text{(B12)}$$

Now, expanding the first term of Equation B12 and recalling Equation B3:

$$\sum_{\beta=1}^{N}\lambda_\beta\left[\sum_{\alpha=1}^{N}\lambda_\alpha \rho(\mathbf{u}_\beta - \mathbf{u}_\alpha)\right] = \sum_{\beta=1}^{N}\lambda_\beta \rho(\mathbf{u}_\beta - \mathbf{u}) \quad \text{(B13)}$$

Expanding the second term of Equation B12:

$$E\{Z_S(\mathbf{u})Z(\mathbf{u}_\alpha)\} = E\{Z^*(\mathbf{u})Z(\mathbf{u}_\alpha)\} + E\{R_S(\mathbf{u})Z(\mathbf{u}_\alpha)\} \quad \text{(B14)}$$

Knowing that $E\{R_S(\mathbf{u})Z(\mathbf{u}_\alpha)\} = 0$ and $E\{Z^*(\mathbf{u})Z(\mathbf{u}_\alpha)\} = \rho(\mathbf{u}-\mathbf{u}_\alpha)$:

$$\sum_{\alpha=1}^{N} \lambda_\alpha E\{Z_S(\mathbf{u})Z(\mathbf{u}_\alpha)\} = \sum_{\alpha=1}^{N} \lambda_\alpha \rho(\mathbf{u}-\mathbf{u}_\alpha) = 1-\sigma_{SK}^2(\mathbf{u}) \qquad \text{(B15)}$$

Substituting B13 and B15 back into B12:

$$E\{Z^*(\mathbf{u}')\cdot Z^*(\mathbf{u})\} = \sum_{\beta=1}^{N} \lambda_\beta \rho(\mathbf{u}_\beta-\mathbf{u}) + \lambda_{N+1}\left[1-\sigma_{SK}^2(\mathbf{u})\right] \qquad \text{(B16)}$$

Now, let's go back to Equation B11 and expand and simplify the second term of the right hand side:

$$E\{Z^*(\mathbf{u}')\cdot R_S(\mathbf{u})\} = \sum_{\alpha=1}^{N} \lambda_\alpha E\{Z(\mathbf{u}_\alpha)R_S(\mathbf{u})\} + \lambda_{N+1}E\{Z_S(\mathbf{u})R_S(\mathbf{u})\} \qquad \text{(B17)}$$

The $\sum_{\alpha=1}^{N} \lambda_\alpha E\{Z(\mathbf{u}_\alpha)R_S(\mathbf{u})\}$ term is zero since $Z(\mathbf{u}_\alpha)$ and $R_S(\mathbf{u})$ are independent.

By expanding the $E\{Z_S(\mathbf{u})R_S(\mathbf{u})\}$ portion of the second term in Equation B17, it can be shown that it is equivalent to the simple kriging variance:

$$E\{Z_S(\mathbf{u})R_S(\mathbf{u})\} = E\{Z^*(\mathbf{u})R_s(\mathbf{u})\} + E\{R_S^2(\mathbf{u})\} \qquad \text{(B18)}$$

Since $E\{Z^*(\mathbf{u})R_s(\mathbf{u})\}$ is zero (the variance is homoscedastic. If the variance was heteroscedastic, $E\{Z^*(\mathbf{u})R_s(\mathbf{u})\} \neq 0$ and the covariance would not be reproduced):

$$E\{Z_S(\mathbf{u})R_S(\mathbf{u})\} = E\{R_S^2(\mathbf{u})\} = \sigma_{SK}^2(\mathbf{u}) \qquad \text{(B19)}$$

Substituting B19 back into Equation B17:

$$E\{Z^*(\mathbf{u}')\cdot R_S(\mathbf{u})\} = \lambda_{N+1}\sigma_{SK}^2(\mathbf{u}) \qquad \text{(B20)}$$

Substituting B16 and B20 into B11 and simplifying:

$$E\{Z_S(\mathbf{u})\cdot Z_S(\mathbf{u}')\} = \sum_{\beta=1}^{N} \lambda_\beta \rho(\mathbf{u}_\beta-\mathbf{u}) + \lambda_{N+1}\left[1-\sigma_{SK}^2(\mathbf{u})\right] + \lambda_{N+1}\sigma_{SK}^2(\mathbf{u})$$

$$E\{Z_S(\mathbf{u})\cdot Z_S(\mathbf{u}')\} = \sum_{\beta=1}^{N} \lambda_\beta \rho(\mathbf{u}_\beta-\mathbf{u}) + \lambda_{N+1}$$

$$\boxed{E\{Z_S(\mathbf{u})\cdot Z_S(\mathbf{u}')\} = \rho(\mathbf{u}'-\mathbf{u})} \qquad \text{(B21)}$$

By working through from Equation B11 to Equation B21, the covariance is correct. The marginal covariance is reproduced.