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Stepwise Conditional Transformation for Simulation of Multiple Variables[1]

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Most geostatistical studies consider multiple-related variables. These relationships often show complex features such as nonlinearity, heteroscedasticity, and mineralogical or other constraints. These features are not handled by the well-established Gaussian simulation techniques. Earth science variables are rarely Gaussian. Transformation or anamorphosis techniques make each variable univariate Gaussian, but do not enforce bivariate or higher order Gaussianity. The stepwise conditional transformation technique is proposed to transform multiple variables to be univariate Gaussian and multivariate Gaussian with no cross correlation. This makes it remarkably easy to simulate multiple variables with arbitrarily complex relationships: (1) transform the multiple variables, (2) perform independent Gaussian simulation on the transformed variables, and (3) back transform to the original variables. The back transformation enforces reproduction of the original complex features. The methodology and underlying assumptions are explained. Several petroleum and mining examples are used to show features of the transformation and implementation details.

KEY WORDS: multivariate transformation, multivariate geostatistics, model of coregionalization.

INTRODUCTION

The increasing demand for realistic geologic models has brought greater attention to the field of geostatistics. For their simplicity, Gaussian techniques are most commonly applied to create numerical models of continuous variables. Implicit to these techniques is the requirement for multivariate Gaussianity; however, geologic data rarely conform to such well-behaved Gaussian distributions.

Large scale lithofacies or rock-type modeling is typically followed by smaller scale modeling of continuous petrophysical properties or metal concentrations. Different simulation methods can be used to build numerical models of geologic heterogeneity for uncertainty assessment. These include sequential indicator simulation (Gómez-Hernández and Srivastava, 1990), *p*-field simulation (Froidevaux,

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1993), simulated annealing (Deutsch, 1992), and the more commonly used Gaussian simulation.

The use of Gaussian techniques, such as sequential Gaussian simulation (Isaaks, 1990) or turning bands simulation (journel, 1974), to simulate regionalized variables is dependent on the characteristics of a Gaussian variable. In the presence of two or more variables, the conventional procedure is to transform each variable to a Gaussian distribution one at a time. This ensures that each variable is univariate Gaussian; however, the multivariate distributions (of two or more variables at a time) are not explicitly transformed to be multivariate Gaussian. An important assumption inherent in these techniques is that the multivariate distribution is also Gaussian, thus it must follow a very particular functional form:

$$f(X) = \frac{1}{(2\pi)^{n/2}|\Sigma|^{1/2}} \cdot \exp[-(X-\mu)'\Sigma^{-1}(X-\mu)/2] \tag{1}$$

where X is a random vector of n random variables $[X_1, \ldots, X_n]'$, Σ is the $n \times n$ covariance matrix, and μ is a $1 \times n$ matrix of the means of each random variable X_i (Johnson and Wichern, 1998). Important characteristics of the multivariate Gaussian distribution are homoscedasticity and linearity. Real multivariate distributions show nonlinearity, heteroscedasticity, and mineralogical constraints. Figure 1 shows a schematic illustration of these common non-Gaussian behaviors.

Other transformation techniques could be used, including ACE (Brieman and Friedman, 1985a,b), hermite polynomials, or power law transformations. However, these techniques do not necessarily produce univariate Gaussian variables and must often be applied in conjunction with a normal scores transform to ensure univariate Gaussianity. Consequently, similar departures from multivariate Gaussianity (as those shown in Fig. 1) may arise with the transformed multivariate distribution.

Common practice is to transform each variable to a univariate Gaussian distribution and assume that higher order distributions are all multivariate Gaussian.

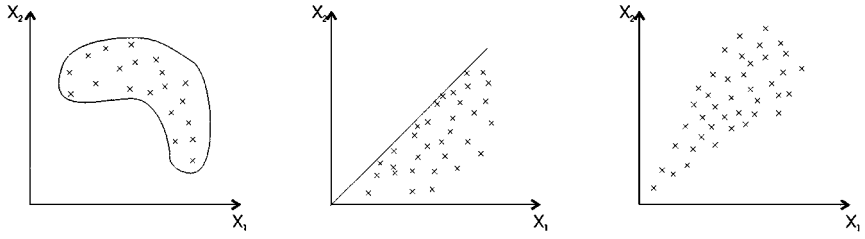

Figure 1. Examples of problematic bivariate distributions for geostatistical simulation: nonlinear relations (left), mineralogical constraints (centre), and heteroscedasticity (right).

Under this assumption of multivariate Gaussianity, the only statistics needed to quantify the relationship between multiple variables are the correlation coefficients. These correlation coefficients are derived from a model of coregionalization. The variogram and cross variograms are modeled with the linear model of coregionalization (LMC) (Journel and Huijbregts, 1978) or a Markov model of coregionalization (Xu and others, 1992). This common practice is limiting and does not address the case when the multi-Gaussian assumption is violated.

The stepwise conditional transformation ensures that the transformed variables, taken together, are multivariate Gaussian with zero correlation. Thus, conventional Gaussian simulation techniques can be applied with no requirement for cokriging or to fit a model of coregionalization. The correlation between the variables is accounted for in the transformation and back transformation. There is an implicit model of coregionalization in the transformation/back transformation that is explored in this paper. Several mining and petroleum related examples are shown to compare the results to conventional normal transformation.

METHODOLOGY

The stepwise conditional transformation technique was first introduced by Rosenblatt (1952). The technique is identical to the normal score transform in the univariate case. For bivariate problems, the normal scores transformation of the second variable is conditional to the probability class of the first variable. Correspondingly, for n-variate problems, the nth variable is conditionally transformed on the basis of the first $n-1$ variables, that is,

$$\begin{aligned} Y_1' &= G^{-1}[F_1(z_1)] \\ Y_2' &= G^{-1}[F_{2|1}(z_2 \mid z_1)] \\ &\vdots \\ Y_n' &= G^{-1}[F_{n|1,\ldots,n-1}(z_n|z_1, \ldots, z_{n-1})] \end{aligned}$$

where Y_i', $i = 1, \ldots, n$ are multivariate Gaussian variables that are independent at lag distance of zero, that is,

$$C_{ij}'(0) = C(Y_i'(\mathbf{u}), Y_j'(\mathbf{u})) = 0, \quad i \neq j, \ i = 1, \ldots, n, \ j = 1, \ldots, n$$

Moreover, all multivariate distributions are Gaussian in shape at distance lag $\mathbf{h} = \mathbf{0}$. The covariance at $\mathbf{h} > 0$ may not be zero. There are two possible options for fitting

the cross covariance $C'_{ij}(\mathbf{h})$, $\mathbf{h} > 0$ at large scale:

1. Assume independence for all lag distances,

$$C'_{ij}(\mathbf{h}) = 0, \qquad i \neq j, \forall \mathbf{h}$$

2. Model $C'_{ij}(\mathbf{h})$ consistent with a valid LMC.

The first option is simplest. Calculation of $C'_{ij}(\mathbf{h})$, $i \neq j$ will identify if further modeling is required due to significant departures from independence.

As mentioned above, the significant advantage of this method is that complex multivariate distributions are transformed to the well-behaved Gaussian distribution. For example, nonlinear, heteroscedastic and constraint features (see Fig. 1) are automatically built into the transformation and model of coregionalization. Other features of the method are explored below; the Appendix investigates the model of coregionalization implicit to the stepwise conditional transformation and the assumption that all covariances at all spatial scales are zero, $C'_{ij}(\mathbf{h}) = 0$, $i \neq j, \forall \mathbf{h}$.

IMPLEMENTATION

This technique applies a quantile transformation of observed univariate conditional distributions to standard Gaussian distributions. The input multivariate distribution can be of any arbitrary form. The original multivariate distribution is honoured by back-transformation via a reverse quantile transform.

Figure 2 shows two mining examples for oil sands data and nickel laterite data. For each sample data set, cross plots are shown for the original data, conventional normal score transformation, and stepwise conditional transformation. For the oil sands data, the cross plot of the normal scores shows an almost linear bivariate distribution with negative correlation. Application of the stepwise conditional transform yields a bivariate Gaussian distribution with almost no correlation. Conventional normal scores transformation of the nickel laterite data shows a positively correlated bivariate distribution that appears slightly heteroscedastic; while the stepwise conditional scores show a bivariate Gaussian distribution with essentially zero correlation.

Figure 3 shows two petroleum-related examples which are referred to as the “two-well” data and the “East Texas core” data. The bivariate distributions after a direct normal scores transform are clearly more problematic than those obtained using the mining data. The normal scores cross plot on the left is heteroscedastic, while the cross plot on the right is nonlinear and constrained in some fashion. After applying the stepwise conditional transformation, the bivariate

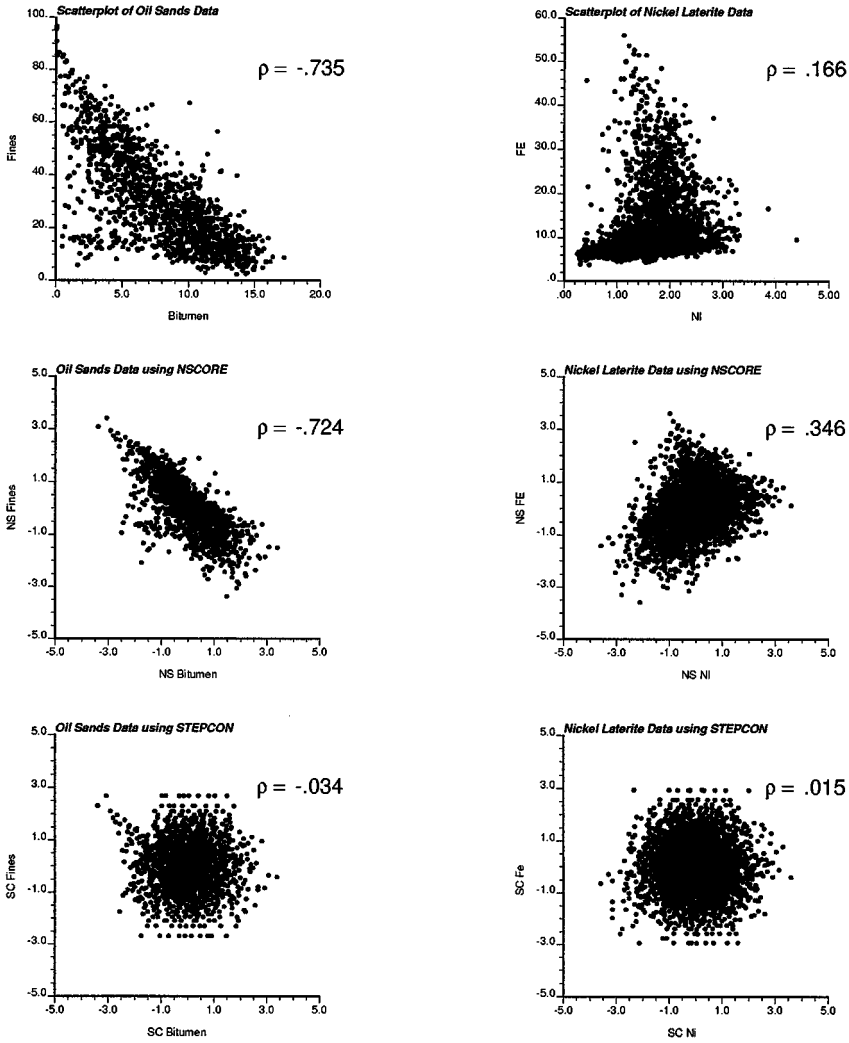

Figure 2. Comparative illustration of cross plots of the original data, normally transformed data, and the stepwise conditionally transformed data for Oil Sands data (left side) and Nickel Laterite data (right side).

distributions again exhibit a bivariate Gaussian distribution with essentially zero correlation.

In practice, the following three issues are important: (1) cross covariance for $\mathbf{h} > 0$, (2) effect of ordering on covariance models, and (3) inference of multivariate distributions in presence of sparse data.

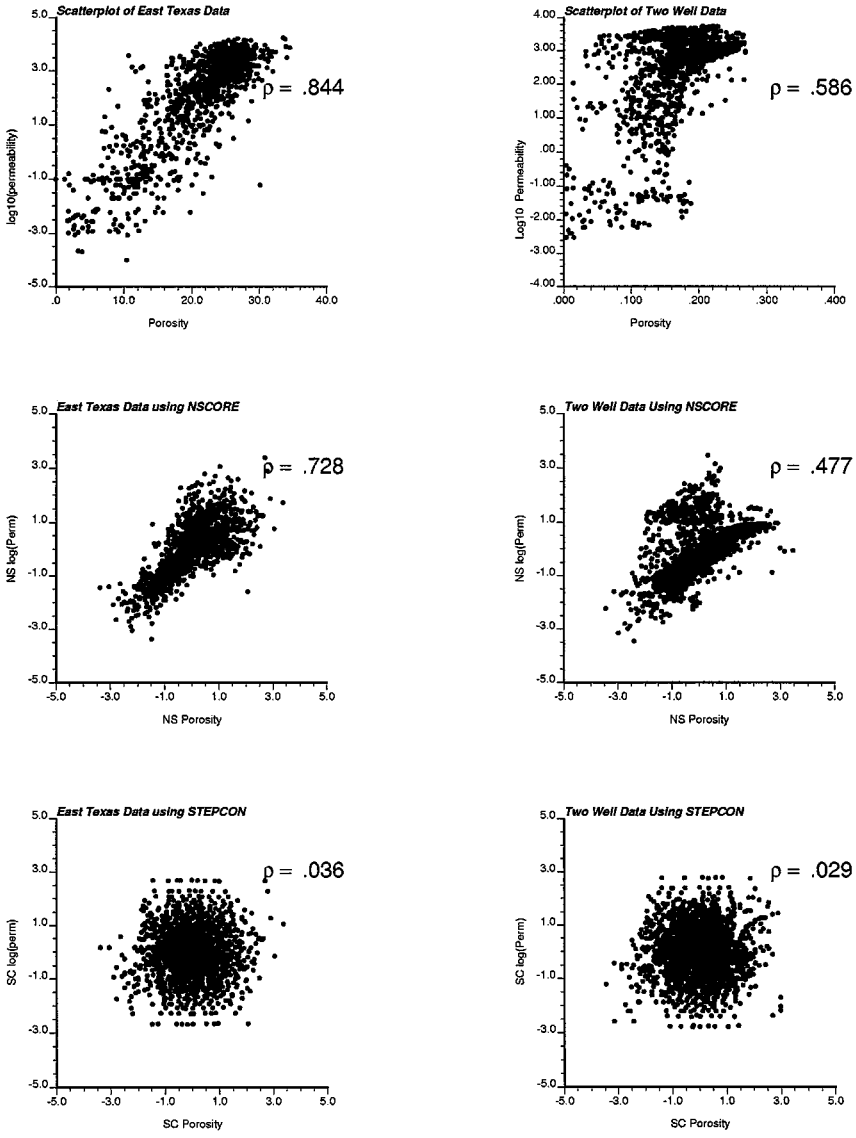

Figure 3. Illustration of cross plots of the original data, normally transformed data, and the stepwise conditionally transformed data for porosity and log(permeability) for East Texas core data (left side) and the Two Well data set (right side).

Covariance Structure for h > 0

The result of applying this transformation is independence of the transformed variables at $\mathbf{h} = 0$, since each class of Y_2 data is independently transformed to a standard normal distribution. There is no guarantee of independence for distance lags greater than zero ($\mathbf{h} > 0$). The new model of coregionalization is complex. The assumption of $C'_{ij}(\mathbf{h}) = 0, \forall \mathbf{h}, i \neq j$ holds only for the case of an intrinsic coregionalization (Appendix A). To validate this theoretical result, a numerical exercise was performed involving two multi-Gaussian variables, Y_1 and Y_2, with the same direct isotropic variogram:

$$\gamma(\mathbf{h}) = 0.5\text{Sph}_{\alpha=3}(\mathbf{h}) + 0.5\text{Sph}_{\alpha=15}(\mathbf{h})$$

The correlation between Y_1 and Y_2 was chosen to be 0.70. Three different cross variograms were considered: "short-range," "intrinsic," and "long-range." The "short-range" case gives maximum variance contribution to the short range structure; while the "long-range" case gives maximum variance contribution to the long-range structure. Note that *maximum variance contribution* refers to the maximum contribution allowable under the linear model of coregionalization. The cross semivariogram models are given below and illustrated in Figure 4.

$$\textit{short-range} : \gamma(\mathbf{h}) = 0.50\text{Sph}_{\alpha=3}(\mathbf{h}) + 0.20\text{Sph}_{\alpha=15}(\mathbf{h})$$
$$\textit{intrinsic} : \gamma(\mathbf{h}) = 0.35\text{Sph}_{\alpha=3}(\mathbf{h}) + 0.35\text{Sph}_{\alpha=15}(\mathbf{h})$$
$$\textit{long-ange} : \gamma(\mathbf{h}) = 0.20\text{Sph}_{\alpha=3}(\mathbf{h}) + 0.50\text{Sph}_{\alpha=15}(\mathbf{h})$$

For each case, stepwise conditional transformation was applied, direct and cross variograms were calculated and modeled, sequential Gaussian simulation

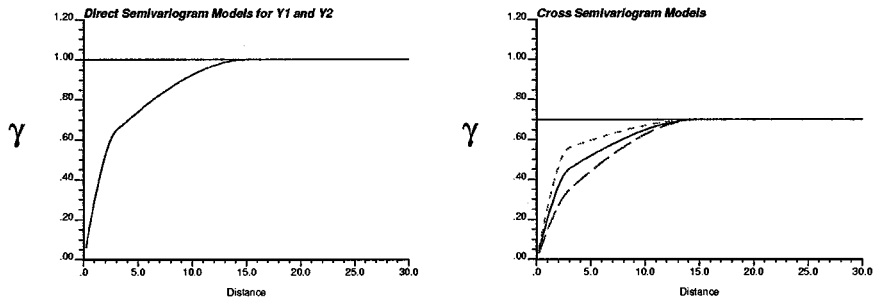

Figure 4. Direct semivariogram of Y_1 and Y_2 (left), and the three different cross semivariogram models (right) : short-range (top left, short dash), intrinsic (middle, solid), and long-range (lower right, long dash).

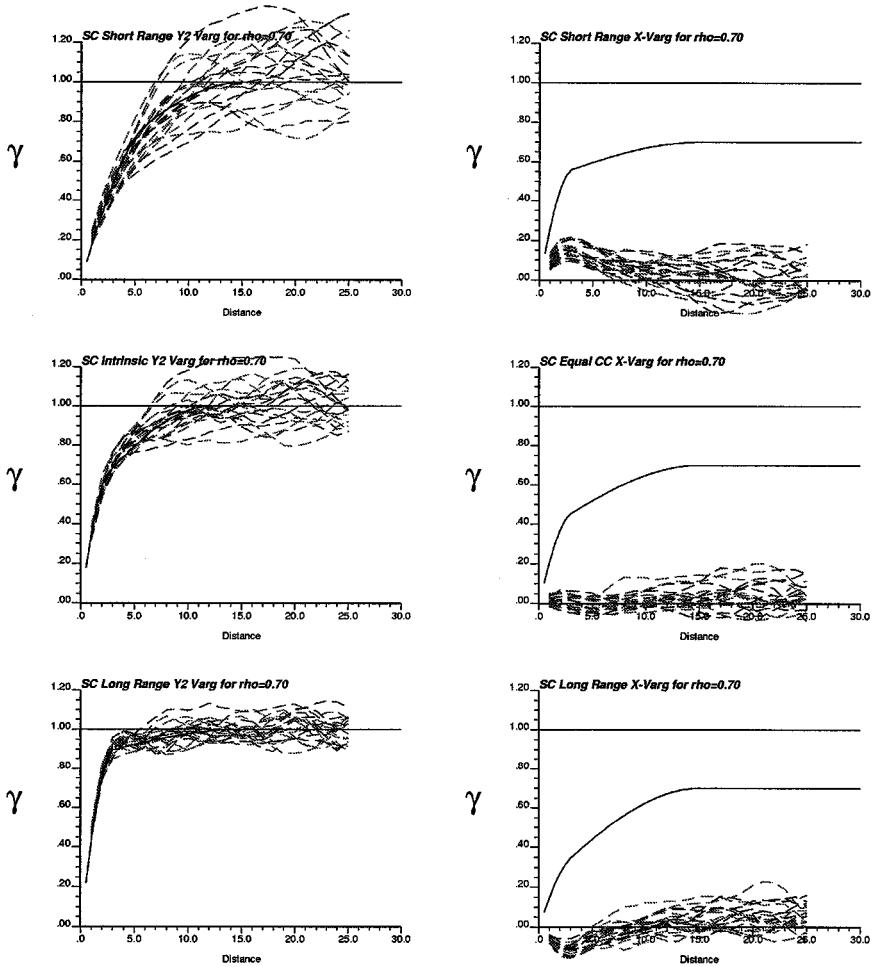

Figure 5. Direct semivariogram of Y_2' (left) and cross semivariogram of Y_1' and Y_2' (right), after stepwise conditional transformation. The solid black line on the cross semivariograms represent the cross semivariogram model used to create the unconditioned simulation prior to transformation.

was performed, simulated values were back transformed, and the resulting simulated direct and cross variograms were examined. Figure 5 shows the direct variograms for $Y_{2|1}$ and the cross variogram of Y_1 and $Y_{2|1}$, following application of the stepwise transform.

In the short-range scenario, the cross variogram is slightly higher than zero over small lag distances and then returns to zero. Conversely, the long-range scenario shows that the cross variogram is negative over the short-range. Unlike the

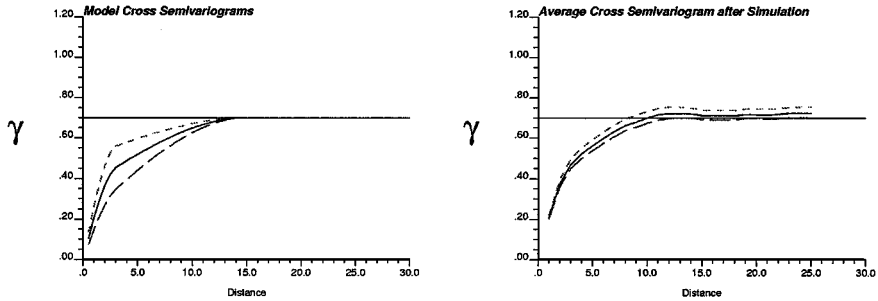

Figure 6. Input model of cross variogram of Y_1 and Y_2 (left), and the average cross variogram obtained after simulating with stepwise transformed variables Y_1' and Y_2' (right). In both cases, the variograms follow the same line code: short-range (top left, short dash), intrinsic (middle, solid), and long-range (bottom right, long dash).

two extreme cases, the intrinsic case shows independence of the transformed pairs, with no deviation from zero over all lags. As predicted by theory, independence at $\mathbf{h} > 0$ is satisfied for the intrinsic case.

Following simulation, the values were back transformed and the cross variogram was checked for each scenario. Figure 6 shows the model cross variograms of the original variables and the average cross variogram obtained after simulation of the conditionally transformed variables. The range of correlation is approximately preserved, i.e., the short-range model produces an average cross variogram with the shortest range of the three simulated scenarios. In all three cases, the range of correlation following simulation shows that the stepwise conditional transform reduces the overall range of correlation of the variables. As well, the variogram structure of the extreme cases (short- and long-range cross variograms) appear to be shifted toward the intrinsic model.

Effect of Ordering

Consider two variables, Z_1 and Z_2. Two possible scenarios exist for transformation: (1) choose Z_1 as primary variable and normal score transform to get Y_1, and then transform Z_2 to get $Y_{2|1}$; and (2) choose Z_2 as the primary variable to get Y_2, and then Z_1 is transformed to produce $Y_{1|2}$. In case (1), the simulation results for Y_1 would be identical to those obtained by conventional simulation using the normal scores of Z_1, and the same can be said for Y_2 in the second scenario.

Simulation of the secondary variables does not produce the same results as conventional simulation. The variogram of the secondary variable is a combination of the spatial structure of both original variables and the cross correlation of the two.

For both ordering sequences, the semivariogram is calculated for both the primary and secondary variable. Sequential Gaussian simulation is independently

performed for the transformed variables. Back transformation of the simulated values returns the original units. We determine the normal scores semivariogram of the simulated values. The resulting semivariogram of the primary variable is that obtained from sequential Gaussian simulation. A comparison of the semivariograms for the same variable, when it is taken as (1) the primary variable and (2) the secondary variable, will show the effect of ordering.

This methodology was applied to the "two-well" and "East Texas core" data. Porosity and permeability were the two variables of interest. The first transformation order takes porosity as the primary variable, and the second takes permeability as the primary variable.

Figure 7 shows the comparison of the semivariograms for both ordering sequences of the "two-well" data set. The semivariograms for porosity show that when porosity is chosen as the primary variable, the postsimulation semivariograms closely follow the input normal scores semivariogram—as they should. Conversely, the semivariograms corresponding to the scenario in which porosity is the secondary variable shows greater variability and a shorter range. Differences in the permeability variograms as a result of transformation ordering sequence are not so obvious; however, the secondary semivariograms for permeability have longer range.

Figure 8 shows the comparison of the semivariograms for the East Texas data. Similar to the previous example, each scenario of ordering clearly shows departure of the secondary variable semivariograms from the direct semivariograms using the traditional normal scores. Unlike the Two Well example, the permeability semivariograms differ considerably after stepwise transformation. Further investigation showed that the stepwise transformation produced a secondary variable with higher nugget effect and longer range of correlation.

Overall, numerical examples show variogram mismatch is minimized when the more continuous variable is chosen as the primary variable.

Transformation in Presence of Sparse Data

There must be sufficient data to identify all conditional distributions in the stepwise transformation. Sparse data leads to erratic and nonrepresentative conditional distributions. There is no general rule, however, 10^N to 20^N data, where N is the number of variables, would permit each distribution to be discretized into 10–20 classes with 10–20 data each. Sparse data could be supplemented by a smoothing algorithm to "fill-in" gaps in the raw-data multivariate distribution.

Smoothing using kernel densities is robust and flexible (Scott, 1992):

$$\hat{f}(x) = \frac{1}{nh} \sum_{i=1}^{n} K\left(\frac{x - x_i}{h}\right) \tag{2}$$

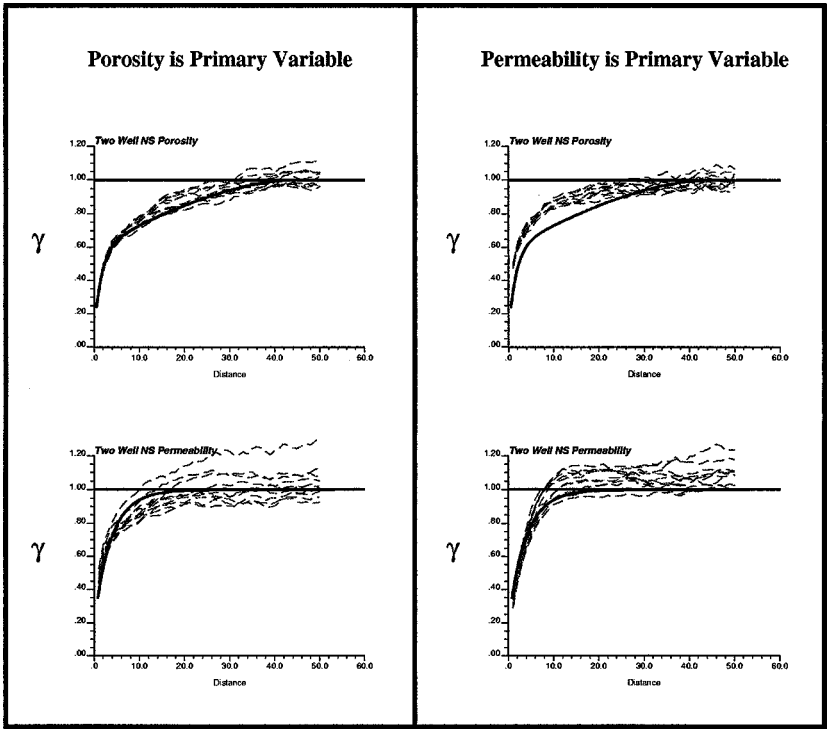

Figure 7. Effect of ordering using Two Well Data: normal scores semivariogram using simulated data for porosity (top) and permeability (bottom). In first scenario, porosity is taken as primary variable (left), and in the second scenario, permeability is chosen as the primary variable (right). In all cases, the thick solid line is the normal scores semivariogram model, the dashed lines correspond to the variogram of the simulated variable. Porosity is more continuous than permeability, and the greatest mismatch occurs when porosity is taken as the secondary variable.

where n is the number of data, h is the bin width obtained by partitioning the range of the data (i.e. between the minimum and maximum observed values) (Izenman, 1991), $K(\cdot)$ is a kernel function associated to some specified density function. Since we are primarily concerned with discretizing the bivariate distribution, the kernel density is chosen to be a nonstandard bivariate Gaussian density distribution with specified correlation:

$$f_{xy} = \frac{1}{2\pi\sigma_x\sigma_y\sqrt{1-\rho^2}} \cdot \exp\left[\frac{-1}{2(1-\rho^2)} \cdot \left(\frac{(x-m_x)^2}{\sigma_x^2} - \frac{2\rho(x-m_x)(y-m_y)}{\sigma_x\sigma_y} + \frac{(y-m_y)^2}{\sigma_y^2}\right)\right]$$

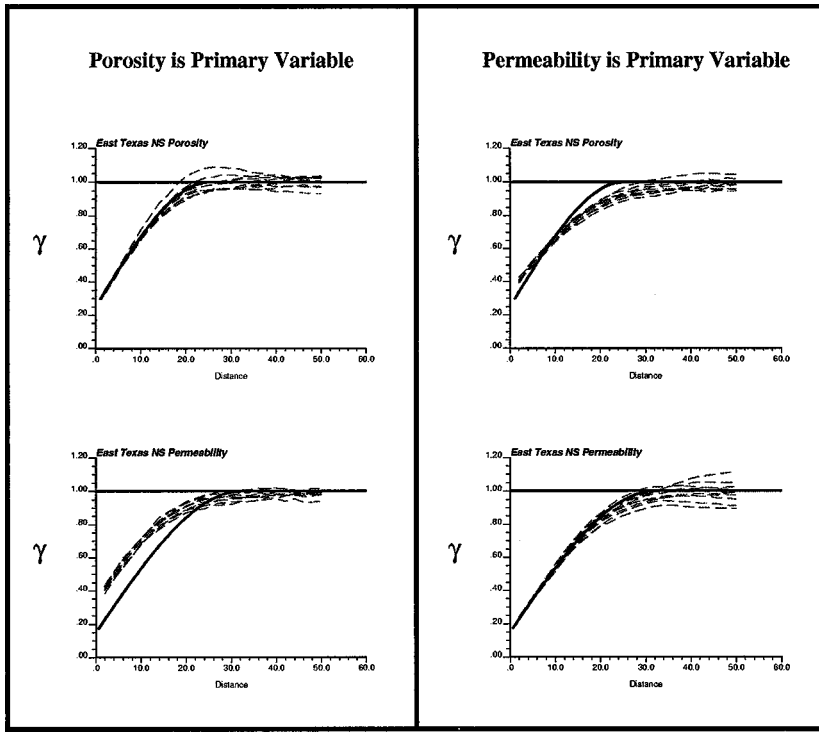

Figure 8. Effect of ordering using East Texas core data: normal scores semivariogram using simulated data for porosity (top) and permeability (bottom). In first scenario, porosity is taken as primary variable (left), and in the second scenario, permeability is chosen as the primary variable (right). In all cases, the thick solid line is the normal scores semivariogram model, the dashed lines correspond to the variogram of the simulated variable. Permeability is more continuous than porosity, and the most significant mismatch in the semivariogram models occur when it is taken as the secondary variable.

where m_x and m_y are assigned the paired data values, σ_x^2 and σ_y^2 are user-specified variances associated to the two variables, and ρ is the correlation coefficient. Note that the above density function is the bivariate representation of Eq. (1).

The general approach is to generate a bivariate density distribution centered about each data pair. The calculated frequencies are then averaged to obtain density estimates for that particular pair. The result is a "cloud" of values centered about the data. The size of this "cloud" is based on the variance specified by the user; for practical purposes, the variance can be determined empirically (typically 0.05–0.15). Further, the correlation coefficient of the kernel densities is typically set to the global correlation. Discretizing the bivariate distribution for the stepwise conditional transformation will then be accomplished using the smoothed bivariate

distribution. The basic steps in smoothing using a kernel estimator are (with user specified correlation coefficient, ρ, and variance for each variable, σ_1 and σ_2):

1. Using the scatterplot limits for both variables, discretize the scatterplot to create a regular grid of X and Y values.
2. Go to each data pair:
   - Set $m_x = x$ and $m_y = y$.
   - Visit each node in the new scatterplot grid and calculate the bivariate frequency using the nonstandard Gaussian density function.
3. Average all the calculated frequencies at each node.

The data should first be transformed into normal scores. Using the normal score values of the multivariate data, we smooth the bivariate distribution of the normal scores, then perform the stepwise conditional transformation on the original data and the smoothed distribution. Independent simulation of the model variables can now proceed in Gaussian space. Back transformation of the simulated values is implemented by calling on the univariate and the bivariate transformation tables.

This methodology was applied to a small petroleum-related data set consisting of only 27 data pairs of porosity and log(permeability). Figure 9 shows several comparative cross plots. The two cross plots of the stepwise conditionally transformed variables resulting from (1) only the data, and (2) the smoothed distribution have similar correlation magnitudes, but with opposite signs. Simulation and back transformation of the transformed variables according to the smoothed distribution shows good reproduction of the bivariate distribution. The banding effect that is visible in this crossplot is a consequence of back transforming values within a sparsely defined class—smoothing in this instance does not fully compensate for defining a class with only two data points. The choice of a larger kernel would be required with the inevitable tradeoff of too much smoothing.

The challenge of sparse data is not a limitation of the stepwise conditional transformation; all multivariate techniques require data. The limitation of working with isotopic sampling, however, could preclude use of this transformation procedure.

NONISOTOPIC SAMPLING

We have implicitly assumed that we have all data variables at all data locations; a situation called *isotopic* sampling. Consider the situation where there are j data for variable Z_1 and i data for variable Z_2, where $i < j$. If Z_2 is chosen as the primary variable, then the transformation of Z_1 depends on prior transformation of Z_2; therefore, the $j - i$ data cannot be transformed. The stepwise approach cannot be easily applied.

One solution is to transform and simulate the first variable at all locations (e.g. Z_1 in the above situation). Then, the simulated first variable can be used for

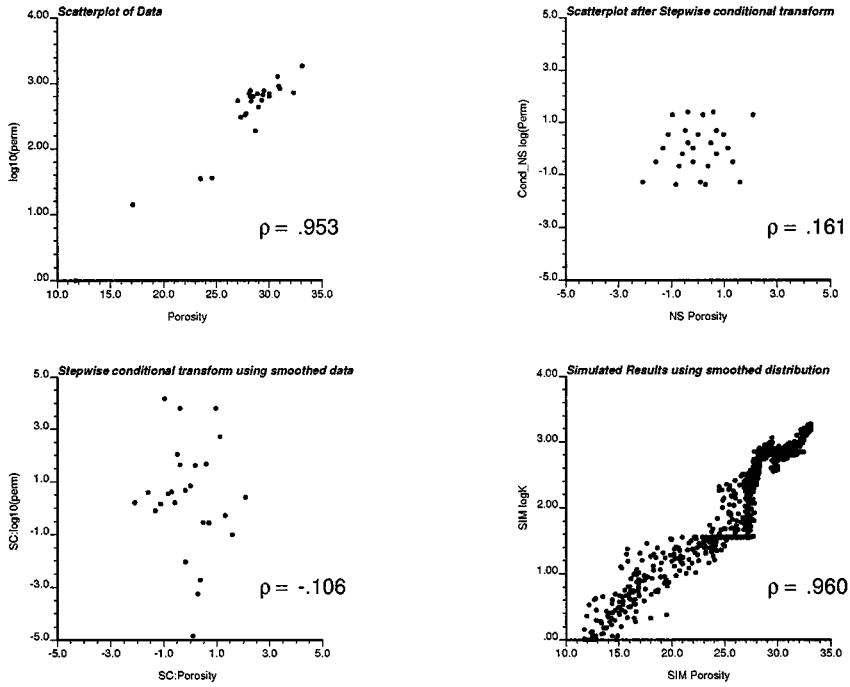

Figure 9. Small petroleum data set consisting of only 27 samples. Cross plot of the original data (top left), cross plot of the stepwise conditionally transformed data using only the original 27 data values (top right), cross plot of stepwise conditionally transformed data using the smoothed distribution (bottom left), and a cross plot of the simulated values after back transformation (bottom right).

later variables. Of course, there is no unique transformed value for secondary data at locations of nonisotopic sampling. This makes data analysis and inference of the variogram of secondary data difficult.

DISCUSSION

Conditional transformation of the data results in transformed secondary variables that are combinations of multiple "real" variables. Consequently, the associated covariance structure of the secondary transformed variables implicitly incorporates the direct and the cross covariance structure of the original variables. Thus, a new model of coregionalization is implicitly invoked in the covariance structure of all transformed secondary variables.

Several "features" of this technique are important:

- No assumption is made on the shape of the input distributions of the multivariate data. The transform removes all structure in the input multivariate

distribution, making it particularly robust in handling problematic characteristics of multivariate distributions such as heteroscedasticity, nonlinearity, and mineralogical-type constraints. Restoration of the input structure is achieved in back transformation.

- The resulting variables are independent at lag distance $h = 0$ because all conditional distributions are transformed to standard normal distributions.
- Cosimulation may not be required. Independent simulation of the transformed variables can proceed after verification that $C'_{ij}(\mathbf{h}) \simeq 0, i \neq j$, $\mathbf{h} > 0$. Back transformation restores the multivariate dependence between the original variables (Fig. 10).
- The covariance structure of the original variables is embedded in the covariance structure of the conditionally transformed variables. This results from the transformed secondary variables being a combination of the original variables.
- The order of the transformation matters since the nth variable is a function of the first $n - 1$ variables. Choosing the most continuous variables first appears to work the best in practice.
- In presence of insufficient data for reliable inference of all conditional distributions. A smoothing algorithm could be used to "fill in" the multivariate distribution so that reliable conditional distributions can be identified.

CONCLUSION

The application of Gaussian simulation techniques requires that model variables be multivariate Gaussian. Conventional practice involves independently transforming each variable, modeling the variograms and the cross variograms, and performing cosimulation. This implicitly assumes that the multivariate distribution of all variables is Gaussian (homoscedastic, linear, and characterized by elliptical probability contours—no mineralogical constraints).

The stepwise conditional tranformation removes all correlation features between the variables producing independent model variables at $\mathbf{h} = 0$. Cosimulation can proceed in one of two ways: (1) assume that $C'_{ij}(\mathbf{h}) \simeq 0, i \neq j$ for $\mathbf{h} > 0$, or (2) model the multiple variograms consistent with LMC. The former case simplifies the cumbersome cosimulation process to independent simulation of the transformed variables. The correlation between the variables is injected during back transformation. This is a big advantage of transforming multiple variables in a stepwise conditional fashion. The latter case mitigates any adverse effects of simulating nonmultivariate Gaussian variables, by ensuring that the multivariate distributions are truly Gaussian.

The covariance structure of the conditionally transformed secondary variables is a function of the direct and cross covariance model between the original

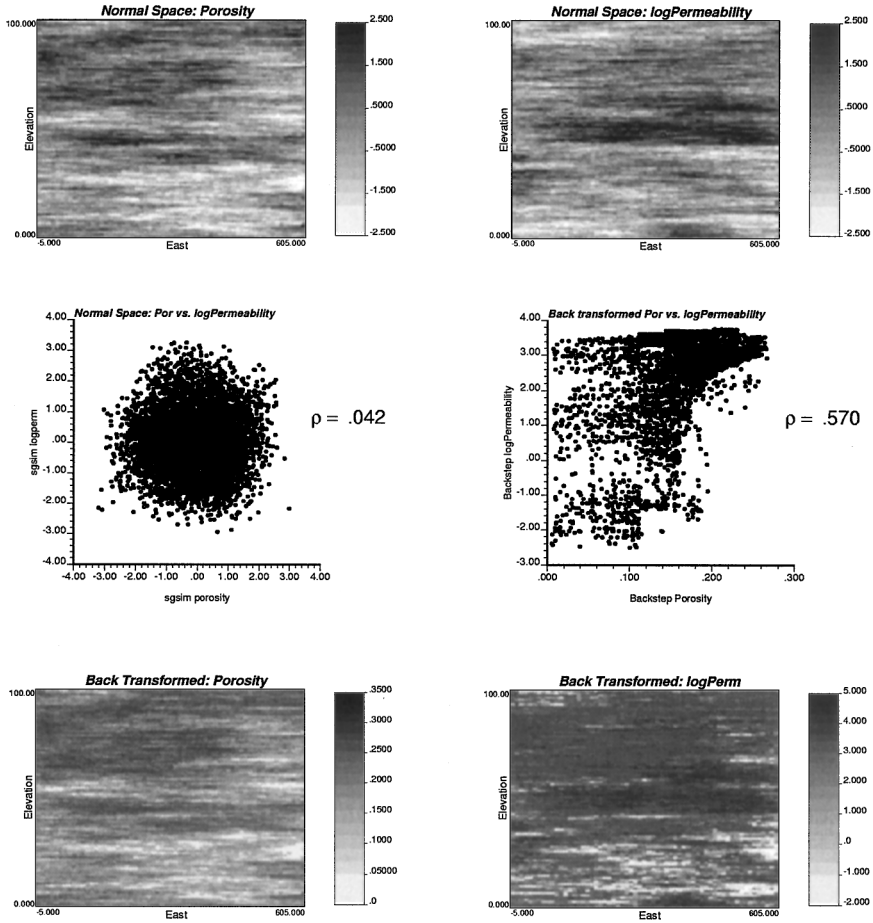

Figure 10. Example of independent simulation and back transformation of porosity and log permeability for Two Well Data: A cross section of one realization for porosity (left) and log permeability (right) in normal space (top row), crossplot of simulated values in normal space (middle left) and in original space after back transformation (middle right), and corresponding cross section of simulated porosity and log permeability in original space (bottom row). Cross plot reproduction can be compared to top right crossplot in Figure 3.

variables. The effect of transformation ordering is observable in the departure of the semivariogram of the transformed variable from the original variable. This departure can be minimised by choosing the most continuous variable as the primary variable for stepwise transformation. In the presence of sparse data, a smoothing algorithm can be applied to model the conditional distributions based on the available data so that stepwise conditional transformation can be effectively applied.

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APPENDIX

Transformation by the stepwise conditional procedure leads to an implicit model of coregionalization. The model of coregionalization is embedded within the transformation and back transformation. The model of coregionalization can always be understood numerically via simulation and calculation. This may be important for complex situations; however, we can look at the model for the simplified case of two homoscedastic, multi-Gaussian variables Y_1 and Y_2 where the covariance structure of the variables is defined analytically by a valid LMC.

The stepwise conditional transformation of the primary variable is identical to its normal score transform (denoted by the index 1). As a result, the covariance structure of the primary variable is the same as the covariance calculated from the conventional normal scores, that is, $C'_{11}(\mathbf{h}) = C_{11}(\mathbf{h})$.

Stepwise conditional transformation of the secondary variable results in

$$Y'_2(\mathbf{u}) = \frac{Y_2(\mathbf{u}) - \mu_{2|1}(\mathbf{u})}{\sigma_{2|1}} \tag{A1}$$

The covariance model of the transformed secondary variable, Y'_2, is,

$$C'_{22}(\mathbf{h}) = E\left\{\left(\frac{Y_2(\mathbf{u}) - \mu_{2|1}(\mathbf{u})}{\sigma_{2|1}}\right) \cdot \left(\frac{Y_2(\mathbf{u}+\mathbf{h}) - \mu_{\mathbf{2}|1}(\mathbf{u}+\mathbf{h})}{\sigma_{2|1}}\right)\right\} \tag{A2}$$

where $\mu_{2|1}$ and $\sigma_{2|1}$ are the mean and standard deviation of the conditional distribution. These parameters are calculated by solving the kriging system of equations. For example, in the simple case of conditioning to two primary data, the conditional mean and variance are given by

$$\mu_{2|1}(\mathbf{u}) = \lambda_1(\mathbf{u}) \cdot Y_1(\mathbf{u}) + \lambda_1(\mathbf{u}+\mathbf{h}) \cdot Y_1(\mathbf{u}+\mathbf{h})$$
$$\sigma^2_{2|1}(\mathbf{u}) = 1 - \{\lambda_1(\mathbf{u}) \cdot C_{12}(\mathbf{0}) + \lambda_1(\mathbf{u}+\mathbf{h}) \cdot C_{12}(\mathbf{h})\}$$

Solving for the weights yields

$$\lambda_1(\mathbf{u}) = \left(\frac{\rho - C_{12}(\mathbf{h}) \cdot C_{11}(\mathbf{h})}{1 - C^2_{11}(\mathbf{h})}\right)$$
$$\lambda_1(\mathbf{u}+\mathbf{h}) = \left(\frac{C_{12}(\mathbf{h}) - \rho \cdot C_{11}(\mathbf{h})}{1 - C^2_{11}(\mathbf{h})}\right)$$

and $\mu_{2|1}$ and $\sigma_{2|1}$ become

$$\mu_{2|1}(\mathbf{u}) = \left(\frac{\rho - C_{12}(\mathbf{h}) \cdot C_{11}(\mathbf{h})}{1 - C^2 11(\mathbf{h})}\right) Y_1(\mathbf{u}) + \left(\frac{C_{12}(\mathbf{h}) - \rho \cdot C_{11}(\mathbf{h})}{1 - C^2 11(\mathbf{h})}\right) Y_1(\mathbf{u}+\mathbf{h})$$

$$\sigma^2_{2|1}(\mathbf{u}) = 1 - \left\{\left(\frac{\rho - C_{12}(\mathbf{h}) \cdot C_{11}(\mathbf{h})}{1 - C^2_{11}(\mathbf{h})}\right) C_{12}(0) + \left(\frac{C_{12}(\mathbf{h}) - \rho \cdot C_{11}(\mathbf{h})}{1 - C^2_{11}(\mathbf{h})}\right) C_{12}(\mathbf{h})\right\}$$

The mean and standard deviation of the conditional distribution, $\mu_{2|1}$ and $\sigma_{2|1}$, are known in the case of multi-Gaussian variables. In fact, all conditional distributions are Gaussian with known mean and standard deviation. We only need the mean and variance for the purposes of calculating the covariance structure.

Substitution of $\mu_{2|1}$ and $\sigma_{2|1}$ into Eq. (A2) shows that the covariance structure of the conditionally transformed variable, $Y_{2|1}$, implicitly incorporates the direct and cross-covariance structure of the original variables, Y_1 and Y_2. The new model of coregionalization implicitly invoked via the stepwise conditional transform is a function of the original variable covariance structures, that is,

$$C'_{11}(\mathbf{h}) = C_{11}(\mathbf{h})$$
$$C'_{12}(\mathbf{h}) = g(C_{11}(\mathbf{h}), C_{12}(\mathbf{h}), C_{22}(\mathbf{h}))$$
$$C'_{22}(\mathbf{h}) = f(C_{11}(\mathbf{h}), C_{12}(\mathbf{h}), C_{22}(\mathbf{h}))$$

where f and g are different functions of the direct and cross covariance structure of the original variables. $C'_{12}(\mathbf{h})$ can be assumed to be zero, after numerical verification.

For the special case of an intrinsic coregionalization, that is when $C_{22}(\mathbf{h}) = C_{11}(\mathbf{h})$ and $C_{12}(\mathbf{h}) = \rho_{12}(0) \cdot C_1(\mathbf{h})$, the cross covariance of the transformed variables, $C'_{12}(\mathbf{h})$, is zero. The mean and variance of the conditional distribution reduce to

$$\mu_{2|1}(\mathbf{u}) = \rho \cdot Y_1(\mathbf{u}) \tag{A3}$$
$$\sigma^2_{2|1}(\mathbf{u}) = 1 - \rho^2 \tag{A4}$$

and the covariance model of the transformed variable in Eq. (A2) simplifies to:

$$C'_{22}(\mathbf{h}) = C_{11}(\mathbf{h}) \tag{A5}$$

This is derived by taking the product in Eq. (A2) and substituting $C_{22}(\mathbf{h}) = C_{11}(\mathbf{h})$, $C_{12}(\mathbf{h}) = \rho_{12}(0) \cdot C_1(\mathbf{h})$, and the mean and variance given in Eqs. (A3) and (A4). The result is then simplified to the result in Eq. (A5). The cross covariance for the intrinsic coregionalization case, $C'_{22}(\mathbf{h})$, is zero for all distances. This theoretical result is validated in the body of the paper.

The direct and cross covarainces of the transformed variables is a function of the direct and cross covariances at all *lower* levels. This is a useful property.