Spatial correlation of permeability in cross-stratified sediment with hierarchical architecture

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[1] Cross-stratified deposits can give rise to a hierarchy of permeability modes, across scales, corresponding to a hierarchy of sedimentary unit types. The shape of the sample semivariogram for permeability can be largely controlled by the shape of the cross-transition probabilities of unit types having the greatest contrast in permeability. The shape of those cross-transition probabilities can be, in turn, largely determined by the variance of the lengths of those unit types. A sufficient condition for an exponential-like semivariogram is the repeated occurrence of unit types having both a contrast in permeability and a large length variance. These relationships are shown through writing the identities for spatial correlation of permeability in a hierarchical and multimodal form and as a function of the transition probabilities for the sedimentary unit types. These relationships are also illustrated through analyzing data representing cross-stratified sediments within a point bar deposit. INDEX TERMS: 1829 Hydrology: Groundwater hydrology; 1869 Hydrology: Stochastic processes; 1832 Hydrology: Groundwater transport; KEYWORDS: hierarchical architecture, permeability, spatial correlation


1. Introduction

[2] In this paper we examine the architecture of cross-stratified sedimentary deposits and relate it to the spatial correlation of permeability. The focus is on what controls the shape of the spatial correlation structure as expressed through either the centered or noncentered covariance or the semivariogram.

[3] We are motivated to understand correlation structure in detail because it is used in the Lagrangian formulation of stochastic models for groundwater flow and solute transport (macrodispersivity models). These models relate the spatial variability of permeability to that of the velocity field and, ultimately, the variation in fluid-particle location within a spreading plume [e.g., Dagan, 1989; Gelhar, 1993; Neuman, 1997; Rubin, 1995; Zhang, 2002; Dai et al., 2004]. Early theory assumed that the permeability field could be characterized by its two-point bivariate statistics such as the centered spatial covariance or semivariogram. Furthermore, it was assumed that these statistics could be modeled with one of a set of functions conventionally used in geostatistics such as the Gaussian, the spherical, or the exponential functions.

[4] Exponential functions were used to model the spatial correlation of permeability exhibited in field data from the Borden [Woodbury and Sudicky, 1991] and the Cape Cod [Hess et al., 1992] sites. The macrodispersion theory based on the exponential correlation model explained the observed solute spreading reasonably well. However, we do not know what attributes of the sediment give rise to the exponential-like shape of the spatial correlation that was observed. The sediments at these sites contain cross stratification [LeBlanc et al., 1991, Figure 3; Burt et al., 2002]. How does cross-stratification contribute to an exponential-like shape in the correlation structure?

[5] It is known that certain correlation models (e.g., linear, spherical, or exponential) represent nondifferentiable (in space) permeability series [see Kitanidis, 1997, p. 57], whereas other models (e.g., Gaussian) represent smoother, differentiable series (see Davis et al. [1997] for field examples). Furthermore, it is known that permeability series can be nondifferentiable when sampled across strata [e.g., Jensen et al., 1996], and strata often exist across a range of scales within a hierarchical framework. If so, which scales and what attributes of the stratal units defined at those scales control the shape of the global permeability structure? Will the shape be limited to those of linear, spherical or exponential-like structures?

[6] In addressing these questions, we make a close link between the geologic framework and stochastic models. The need for such a link was articulated well by Davis et al. [1997]. Other recent studies have strengthened this link, including those by Scheibe and Freyberg [1995], Barrash and Clemo [2002], and Gaud et al. [2004]. These papers have discussed the hierarchical organization of sedimentary units and have shown how units defined at different hierarchical levels give rise to permeability or porosity modes. We further discuss those studies in relation to our work through the following sections of this paper. Further-
more, Rubin [1995], Barrash and Clemo [2002], Lu and Zhang [2002], Ritzi et al. [2002], and Neuman [2003] have written the statistical identities for the covariance and the semivariogram in multimodal, hierarchical forms. We show the relationship among the forms in which the identities have been previously written and we expand these forms to span more than two hierarchical levels. Such identities are an important tool in our analysis.

[7] In the next section we review the aspects of sedimentary architecture relevant to our discussion. We then study how these affect the spatial correlation of permeability by using a multimodal, hierarchical identity. We show a relationship between variability in the geometry of the units defined at lower hierarchical levels of a cross-stratified deposit and the shape of the correlation structure defined at higher hierarchical levels. We then illustrate this relationship in the study of data representing an exhaustively sampled, cross-stratified deposit.

2. Relevant Aspects of the Hierarchical Architecture of Cross-Stratified Deposits

[8] The hydrogeologic literature [e.g., Scheibe and Freyberg, 1995] contains discussions and applications of the hierarchical framework used by sedimentologists to describe deposits [e.g., Allen, 1983; Miall, 1985, 1988]. Here we briefly summarize the points relevant to our analysis, largely following Scheibe and Freyberg [1995]. In doing so, we refer to the point bar deposit in Figure 1 as an example.

2.1. Microforms

[9] At the base of the hierarchical organization (first level) are occurrences of beds (>1 cm thick) or laminae (<1 cm), the smallest regions that have some degree of uniformity within and some difference with adjacent regions. The uniformity within these units is created during deposition by hydrodynamic sorting of grains, primarily by size, but also by shape and density. A variety of processes cause this sorting and give rise to a variety of bed or laminae (strata) types. Figure 2 depicts the creation of two of these. One type of cross strata is created by intermittent avalanching of grains down the slopes of subaqueous dunes, ripples, or bars. Repeated avalanches create a single unit of the avalanche bed microform [Scheibe and Freyberg, 1995]. Single units of the interbed microform are created when small fluctuations in flow velocity cause increased deposition of suspended sediment. Although both contain cross strata, the interbed microform differs from the avalanche bed microform in having a smaller median grain size. Thus the different microform types can have different modes of both median grain size and permeability [Basumallick, 1966; Robertson and Caudle, 1971; Weber et al., 1972; Beard and Weyl, 1973; Blatt et al., 1980; Chandler et al., 1989; Jensen et al., 1996].

[10] Other types of microforms may give rise to other permeability modes. For example, cross strata are usually organized into sets, created by the migration of individual bed forms, and cosets, created by the vertical stacking of two or more similar sets during single depositional episodes. The boundaries between sets and cosets are created by erosion in the troughs of bed forms. Deposition directly above these boundaries is typically finer grained than in adjacent cross strata. If this type of deposition occurs it forms boundary bed microforms. Scheibe and Freyberg [1995] describe the origin of additional types of microforms. Permeability modes for microform types are depicted in Figures 3a and 3b.

2.2. Mesoforms and Macroforms

[11] Accumulations of microforms with similar lithology and geometry are grouped as mesoforms. Thus mesoforms exist at the second level in the hierarchy. One mesoform type depicted in Figure 1 is the scroll bar, with some microforms dipping shoreward. Another is the trough set mesoform, with microform types having different shapes and dipping downstream.

[12] Mesoforms are grouped together as macroforms, which represent a third hierarchical level. The point bar macroform in Figure 1 is made up of scroll bar, trough set, and mud drape mesoforms. A sequence of those mesoforms could represent deposition from flood stage through recession. There could be different grain size distributions among
the mesoforms and corresponding differences in permeability modes. Additional hierarchical levels could be added at larger scales. The next level might include the assemblage of point bar, channel fill, and overbank fines macroforms within a channel belt.

[13] Both Davis et al. [1997] and Barrash and Clemo [2002] pointed out that the depositional environments represented in sedimentary deposits usually are more varied as the scale of the sampled domain increases. This is represented in Figure 3 which shows a greater difference in the mean and a larger variance for permeability modes defined at hierarchical level N as compared to modes defined at level N-1. Jensen et al. [1996] and Ritzi et al. [2002] gave examples of permeability data with this type of scaled modality.

[14] When sampling across such deposits, unit types with different modes will occur in the samples, and the resulting data series (median grain size or permeability) can be nondifferentiable across the unit boundaries. This is shown in Figure 4 with Basumallick’s [1966] measurements of median grain size within individual strata. The series in 4b has numerous nondifferentiable alternations between higher and lower values from one stratum to the next.

[15] Note that not every sedimentary deposit is cross-stratified, has multimodal permeability, has modes that change with hierarchical levels, or gives rise to nondifferentiable permeability series (see Davis et al. [1997], site SS4). In this paper we focus on cross-stratified deposits that do have these attributes. Another issue is that, for a given cross-stratified deposit, there is not a unique hierarchical organization. For example, the channel fill and point bar macroforms in Figure 1 might be combined as one macroform on the basis of similar permeability modes that differ greatly from the overbank fines macroform. As will become apparent below, our general method of analysis can be applied to any alternate organizational scheme (i.e., subdivision of space) imposed on a given deposit.

3. Identity for Correlation in Hierarchical Multimodal Deposits

[16] Let \( Y(x) \) be a continuous space function for permeability in domain \( \mathbb{R} \). The literature contains various forms of

![Figure 3. Conceptual framework for scaling of permeability modes in a point bar deposit. Scales increase from Figure 3a to Figure 3d.](image)

![Figure 4. Figures from Basumallick [1966] showing variation in median grain size in series sampled across bed boundaries. (a) Beds and (b) associated series. Here 5* is the average of 5 and 6, 15* is the average of 15 and 16, 18* is the average of 18a and 18b, and 19* is the average of 19, 19a and 19b. Reprinted with permission of Blackwell Publishing.](image)
a global statistical identity for spatial bivariate moments on \([Y(x), Y(x')]\), written as a function of statistical identities defined within and across units at lower hierarchical levels [Rubin, 1995; Barrash and Clemo, 2002; Lu and Zhang, 2002; Ritzi et al., 2002; Neuman, 2003]. Here the focus is on an interpretive study using such expressions, not deriving them, so we present a general derivation that includes all of these forms in Appendix A.

[17] Consider \(\mathbb{R}\) to be filled with mutually exclusive units defined across the three hierarchical levels discussed above in relation to Figure 1, with macroforms numbering \(n_x\), mesoforms numbering \(n_m\), and microforms numbering \(n_k\). Let \(t_{rok}(x)\) be an indicator space function that takes on the value of 1 if \(x\) is within microform \(k\), mesoform \(\alpha\), and macroform \(r\) (region \(rok\) hereinafter), and 0 otherwise. Let \(Y_{rok}(x)\) be a continuous function for permeability or natural-log permeability, defined only within the region \(rok\). Let \(h\) be a lag vector, having tail at location \(x\) in region \(rok\) and head at location \(x'\) in region \(spm\), with \(r, s, t = 1, 2, \ldots n_r, \alpha, p = 1, 2, \ldots n_\alpha\), and \(k, m = 1, 2, \ldots n_k\).

[18] A general identity relating the global spatial correlation to correlation within and among units defined at the three lower hierarchical levels is:

\[
\xi_s(h) = \left\{ \sum_t \sum_s \sum_y \sum_x \sum_p \sum_m \xi_{Y_{rokm}}(h) \xi_{Y_{rokm}}(\hat{h}) \right\} - \mu_s(h) \mu_s(\hat{h}),
\]

Here \(\xi_s(h)\) can be, at the global scale, any one of the common measures of two-point spatial correlation including the noncentered covariance, \(K(h)\), the centered covariance, \(C(h)\), and the semivariogram, \(\gamma(h)\), as given in Table 1. \(\xi_{Y_{rokm}}(h)\) represents one of the measures of the correlation between regions \(rok\) and \(spm\) (a measure of autocorrelation if \(rok = spm\) in a function corresponding to that used for \(\xi_s(h)\)). Note that \(\mu\) is defined in Table 1 and is nonzero only if \(\xi_{Y_{rokm}}(h)\) is used, in which case it represents mean permeability. \(\xi_{Y_{rokm}}(h)\) represents any one of the forms of the indicator correlation in Table 1, which can be chosen independently of which form is used for \(\xi_{Y_{rokm}}(h)\).

[19] In the application below we will use one specific form of the identity and apply it deterministically to an exhaustively sampled, finite domain. We use the form of the sample semivariogram, \(\hat{\gamma}_s(h)\), rather than the centered or noncentered covariance to allow for direct comparisons with results from Scheibe [1993]. We use it in a moving frame of reference that encompasses any two adjacent levels (N and N-1) in the hierarchical organization, so we here switch to generic subscripts \(i, j = 1, 2, \ldots n_m\), to represent the \(n_m\) units existing at whichever is the N-1 level being considered. Thus:

\[
\hat{\gamma}_s(h) = \frac{1}{2N_p(h)} \sum_{i=1}^{N_p(h)} (Y_i(x) - Y_i(x + h))^2
\]

\[
= \sum_{i=1}^{n_m} \sum_{j=1}^{n_m} \hat{\gamma}_{ij}(h) \hat{P}_i(h) \hat{P}_j(h)
\]

The middle expression is the classical identity for the sample semivariogram. In this expression, \(N_p(h)\) is the number of sample pairs defined globally (without regard to starting or ending in specific units) by the lag vector \(h\). In the far RHS expression, \(\hat{\gamma}_{ij}(h)\) is the sample transition probability from unit \(i\) to \(j\) [e.g., Carle and Fogg, 1996; Ritzi, 2000] and \(\hat{P}_i(h)\) is the proportion of facies \(i\) among the tails. When written in this form, we see that \(\hat{P}_i(h) \hat{P}_j(h)\) represents the proportion of transitions \((x \rightarrow x')\) with tail in facies \(i\) and head in facies \(j\), which weights the \(\hat{\gamma}_{ij}(h)\). (Please see note on \(\hat{\gamma}_{ij}(h)\) following equation (A22) in Appendix A.])

[20] With this form, we can let \(i, j\) represent microforms and study how attributes of the microforms determine the mesoform-scale sample semivariogram. We can then let \(i, j\) represent mesoforms and study how attributes of the mesoform determine the macroform-scale sample semivariogram, and so on.

4. Role of the Transition Probabilities in Determining the Shape of the Global Spatial Correlation

[21] Before embarking on the application, we first consider an oversimplified, hypothetical example to illustrate relevant aspects of equation (2). Figure 5 shows a set of two microforms, labeled \(\alpha\) and \(\beta\). Consider the extremely rhythmic case where permeability is uniform within \(\alpha\) units with the value \(Y_\alpha\), and within \(\beta\) units with the value \(Y_\beta\), and \(Y_\alpha \neq Y_\beta\). In this case the microform-scale autosemivariograms are zero, the gicroform cross-semivariograms are a constant \(\frac{1}{2} (Y_\alpha - Y_\beta)^2\), and from equation (2) the semivariogram for the entire set has exactly the same shape as the cross-transition probability. Because the transition probabilities can dictate the shape of the semivariogram, it is important to discuss what dictates the shape of the transition probabilities.

[22] The shape of transition probabilities is largely dictated by the variance in the length of repeated units, as shown by Ritzi [2000]. To briefly review, consider sampling across the \(\alpha\) and \(\beta\) units in Figure 5 (assuming here and only

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**Table 1.** Common Forms That Can Be Assumed by the General Model, as Derived in Appendix A

<table>
<thead>
<tr>
<th>(\xi_s)</th>
<th>(\xi_{Y_{rokm}})</th>
<th>(\xi_{Y_{rokm}})</th>
<th>(\gamma_{Y_{rokm}})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Noncentered covariance</td>
<td>(K_s)</td>
<td>(K_{Y_{rokm}})</td>
<td>(K_{Y_{rokm}})</td>
</tr>
<tr>
<td>Centered covariance</td>
<td>(C_s)</td>
<td>(C_{Y_{rokm}} + m_{Y_{rokm}} \gamma_{Y_{rokm}})</td>
<td>(C_{Y_{rokm}} + P_A \gamma_{Y_{rokm}})</td>
</tr>
<tr>
<td>Semivariogram</td>
<td>(\gamma_s)</td>
<td>(\gamma_{Y_{rokm}})</td>
<td>(\gamma_{Y_{rokm}})</td>
</tr>
<tr>
<td>Transition probability</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>
here an unbounded domain). If there is no variability in the length of the units, the transition probabilities are piecewise linear and periodic as in curve a in Figures 6a and 6b. Variability can be represented by the coefficient of variation, $cv$, which is the ratio of the standard deviation to the mean. As $cv$ for lengths is progressively increased for both unit types, the transition probabilities evolve in shape as shown in curves b through e in Figures 6a and 6b. As $cv$ increases, periodicity is reduced, the transition probabilities take on a sill, and the effective range increases. With a $cv$ of 0.75 (curve c, Figures 6a and 6b) the transition probability is initially similar to a spherical function, shown for comparison. However, the spherical model does not represent the slight periodicity in the transition probability. As $cv$ approaches and then exceeds unity (curves d and e, respectively, Figures 6a and 6b) the transition probability approaches a sill in the asymptotic manner of an exponential function and becomes largely aperiodic, despite the repeating pattern of the units. Thus transition probabilities vary through a continuum of shapes from piecewise linear and periodic to exponential-like and aperiodic, depending on $cv$.

[23] There are other factors that affect the shape of the cross-transition probabilities. Some of these factors are differing $cv$ among unit types, unit types occurring in different numbers within a finite and bounded domain, and the degree of order in the occurrence of more than two unit types. Accordingly, we cannot, in general, link shape to exact $cv$ values but can link differences in shape to relative differences in $cv$.

[24] The overly simplified representation of a set of two microforms in Figure 5 contains no variation in microform length when sampled in directions $u_1$ or $u_2$. In this case the sample cross-transition probabilities have a piecewise linear and periodic structure with longer period in the direction in which lengths are longer. So, too, does the semivariogram (see Figure 5). The shape of the structure and the period of oscillation are defined by the cross-transition probabilities. The amplitude of the oscillation is defined by the permeability contrast across unit types, with the semivariogram oscillating between zero and $Y_a/C_0 Y_b/C_0/C_1$ around a variance of $1/2 (Y_a - Y_b)^2$ as given by equation (A20).

[25] Figure 7 illustrates ways that the lengths of microforms can vary within sets, across sets, and at set boundaries. When these kinds of variations occur, the $cv$ for the length of each microform type will be larger and the cross-transition probabilities and the mesoscale semivariogram will be less periodic and more exponential-like in shape. We can see this in the application which follows.

[26] A few notes are given before proceeding. First, note that the mean length of the units is the same for each curve in Figure 6. Thus the near-origin behavior, which is defined by the mean length [see Carle and Fogg, 1996], is identical for each curve. However, the effective structural range is different among the curves. It increases as the $cv$ increases. The effective structural range of each of the functions shown for comparison in Figure 6 is given by $\phi(1 - P_i)l_i$, where $\phi = 1, 1.5,$ or 3 for the linear, spherical, and exponential models, respectively, and $l_i$ is the mean length of unit $i$ in the direction sampled [Ritzi, 2000]. Thus the structural range of transition probabilities, and of permeability semivariograms defined by them, will generally not equal the mean length of units [see also Lu and Zhang, 2002]. This is contrary to conventional wisdom (e.g., as in Figure 3.24 of Anderson and Woessner [1992, p. 76]).

[27] Second, although we focus on the semivariogram identity in the application below, the transition probabilities also control the shape of $C_Y(h)$ and $K_Y(h)$. The shape of

Figure 6. (a) Autotransition and (b) cross-transition probabilities for various $cv$. The $cv$ for the curves labeled a-e are a, 0.0; b, 0.2; c, 0.7; d, 0.9; and e, 1.3.
these identities will follow that of the autotransition probabilities. For example, for the case in Figure 5 the shape of either $\tilde{C}_Y(h)$ or $\tilde{K}_Y(h)$ will exactly match that of curve $a$ in Figure 6a. It will oscillate between $\frac{1}{4}(T_\alpha - T_\beta)^2$ and $\frac{1}{16}(T_\alpha - T_\beta)^2$ if computed for $\tilde{C}_Y(h)$ and between $\frac{1}{2}(T_\alpha^2 + T_\beta^2)$ and $T_\alpha T_\beta$ if computed for $\tilde{K}_Y(h)$. Thus the indicator correlation (either the autotransition or the cross-transition probabilities) can dictate the shape of the permeability correlation in any of its commonly used expressions (semivariogram and centered or noncentered covariance).

Finally, we note that if the transition probabilities can be represented with the sum of exponential functions then the identity in equations (1) or (2) can be posed elegantly in the canonical form of a Markov chain model [Carle and Fogg, 1997], as shown by Lu and Zhang [2002].

5. Application

We next explore the application of the identity in equation (2) to the set of synthetic permeability and lithofacies data developed by Scheibe and Freyberg [1995] shown in Figure 8. The domain represents a 1 m$^3$ cube centered on a mud drape within a point bar as depicted in Figure 1. The data represent the sedimentary units mapped and the permeability distributions measured in point bar deposits of the Wabash River (midwestern United States) by Pryor [1973] and Jackson [1976]. The microforms were created in a geometric simulation that drew from statistical distributions for various parameters (lengths, angles) that define their shapes. Permeability was mapped into the microforms, drawing from statistical distributions for permeability. The domain consists of 16,777,216 voxels, 256 along each axis, with permeability, microform type, and mesoscale type defined for each. Note that there is no vertical exaggeration in Figure 8; the avalanche bed and interbed microforms dip on the order of 25°, shoreward within the scroll bars ($S_a$ and $S_b$) and downstream within the trough sets ($T_a$ and $T_i$). The data set contains multiple scales of organization with complex geometries giving rise to variations in the length of sedimentary units in any given sampling direction, representing aspects of real deposits.

We will start by focusing within the scroll bar mesoform, which makes up the largest volume fraction of the deposit. The scroll bar mesoform has more complex cross stratification than conveyed in Figures 2, 5, or 7, with...
six microform types. The most abundant microforms are the avalanche and interbed types, $S_a$ and $S_i$, respectively (see Table 2), which repeat together in sets bounded by the $S_{ab}$ microform. These sets repeat within individual scroll bar cosets. Scroll bar cosets are bounded by planar beds comprising $S_{ap}$ and $S_{ip}$ microforms on the stoss side and are completely bounded by a scroll bar boundary microform, $S_b$. Thus the scroll bar mesoform contains complex nested cycles of microform types.

In the following sections we sample the scroll bar mesoform in different ways such that the variance in length for microform types within each sample is different. We first consider a small sample of microforms (analogous to that shown in Figure 5), a sample for which the length variance is low. We then consider larger samples (analogous to that shown in Figure 7) for which the length variance is progressively larger. In this way, we study how increased length variance affects the shape of the cross transition probabilities and the mesoform-scale semivariogram.

### 5.1. Limited Sample of Microforms

We sampled in one dimension along the arbitrarily selected line shown in Figure 8 within a portion of the scroll bar mesoform. The sample contains three microform types, $S_a$, $S_i$, and $S_{ab}$, with statistics summarized in Table 3. The permeability contrast arises mostly from the juxtaposition of either $S_a$ or $S_i$ microforms with relatively lower-permeability $S_{ab}$ microforms. The average of the $c_i$ for the lengths of these microform types is 0.5. The sample semivariogram for permeability is shown in Figure 9a. The identity on the far RHS of equation 2 with all summation terms exactly reproduces it, and the summation of only the cross-transition terms mostly reproduces it. The pre-

### 5.2. Exhaustive Sample of a Mesoform

Next we consider all possible lines of sampling in the $+y$ direction through all parts of the data set that are scroll bar mesoform. Figure 10a gives the mesoform-scale sample semivariogram. Again, the identity using all summation terms exactly reproduces it, and the summation of only the cross-transition terms mostly reproduces it. The pre-

## Table 2. Statistics From Exhaustively Sampling the Numerical Point Bar

<table>
<thead>
<tr>
<th>Microform</th>
<th>$N_b$</th>
<th>$p$</th>
<th>$i$</th>
<th>$\sigma_i$</th>
<th>$C_i$</th>
<th>$k$</th>
<th>$\sigma_k$</th>
<th>$\ln(K)$</th>
<th>$\sigma_{\ln(K)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$S_a$</td>
<td>4</td>
<td>0.352</td>
<td>0.085</td>
<td>0.056</td>
<td>0.657</td>
<td>147.29</td>
<td>2.12</td>
<td>$-1.950$</td>
<td>0.0001</td>
</tr>
<tr>
<td>$S_i$</td>
<td>3</td>
<td>0.371</td>
<td>0.121</td>
<td>0.030</td>
<td>0.250</td>
<td>112.69</td>
<td>113.30</td>
<td>$-2.222$</td>
<td>0.0087</td>
</tr>
<tr>
<td>$S_{ab}$</td>
<td>3</td>
<td>0.277</td>
<td>0.090</td>
<td>0.061</td>
<td>0.676</td>
<td>67.30</td>
<td>0.00</td>
<td>$-2.733$</td>
<td>0.00</td>
</tr>
</tbody>
</table>

*aGlobal $\sigma_k^2 = 1034.83$, and global $\sigma_{\ln(K)}^2 = 0.0996$.
Most important is the comparison of the result in the $y$ direction to results in the $x$ and $z$ directions as shown in Figure 11. Contrast in permeability arises across the same microform types in all three directions. However, the average of the $c_i$ for lengths of these microform types sampled along $z$ is lowest (0.6), so the semivariogram in the $+z$ direction has the greatest periodicity. The average of the $c_i$ is highest in the $x$ direction (0.9), and so the semivariogram in the $+x$ direction has the least periodicity and approaches the sill in the most exponential-like fashion. We see in this result that a sufficient condition for an exponential-like semivariogram structure is the existence of repeated unit types with permeability contrasts and a relatively large variance in their lengths.

These results show anisotropy in the range. The mean length among microform types is least along the $z$ direction so the range is least. The mean length is greatest along the $x$ direction, so the range is longest.

Importantly, the results also show anisotropy in the shape of the semivariogram. Anisotropy in shape is often noticed but seldom incorporated into models. In this case the reason for the anisotropy in the shape of the correlation structure is that the variance in the length of the microform types changes with direction.

Note that the same general relationships occur with equivalent sampling of the trough set mesoform, but for lack of space we do not include those results. Furthermore, the permeability data used here are from the “low-variance mapping” of permeability to microforms by Scheibe and...
Freyberg [1995], which represent the permeability distributions measured in the field. Scheibe and Freyberg also used a high-variance mapping to create a second data set. Because the shape of the semiavgaram is largely controlled by the shape of the cross-transition probabilities, the high-variance mapping generally only changes the sill of the semivariogram, not the shape. We do not show these results here but this effect can be seen in comparing the semivariograms from high- and low-variance data mapped in two-dimensional slices of the numerical aquifer by Scheibe [1993].

5.3. Scale of a Macroform and Beyond

In equation (2), i and j can be shifted to represent mesoforms in order to compute the macroform-scale semivariogram. This is not a satisfying exercise with the Scheibe and Freyberg [1995] data set because of its limited extent. Figure 1 shows that a point bar at the scale of tens to hundreds of meters contains laterally adjacent mesoforms. Lateral sampling at this scale would involve transitions across mesoforms with larger variation in permeability than in the transitions across microforms within them. This would be true for transitions from mud drape to either scrolI bar or trough set mesoforms.

Such lateral transitions are not represented within the 1 m³ extent of the Scheibe and Freyberg [1995] data set. At this scale, the mesoforms are essentially layered. Thus lateral auto-transitions are essentially unity and the lateral cross-transition probabilities are essentially zero. The lateral sample semivariogram determined within the 1 m³ data set is not expected to represent a point bar at the larger scale of interest, even though it does contain each of the mesoforms of the larger point bar.

Note that because the global variance represents the contrast in mean permeability across mesoforms (equation (A20)) but the lateral semivariogram from the 1 m³ domain does not, the sill of the semivariogram is significantly below the variance. This type of zonal anisotropy was also noted and explained in the study of a layered system by Barrash and Clemo [2002]. Also note that the 1 m³ data set does not fully represent sampling the point bar of Figure 1 in the z direction. For example, there are no transitions from mud drape to trough set mesoforms in the +z direction. In addition, the variance in the thickness of units is probably underrepresented. Both of these characteristics affect the shape of the cross-transition probabilities.

Because they have little significance in this light, we do not present the analyses of data at this scale. However, these considerations suggest that the global semivariogram is strongly influenced by the size of the domain sampled. This brings into question the practice of sampling some small fraction of a domain containing each of the smaller-scale units of interest in order to infer a permeability length scale for the domain. The transition probabilities for higher-contrast units within the sample must be representative of those at the larger scale of interest.

For the full point bar deposit, the variance in the lengths of higher-contrast mesoforms could largely dictate the shape of the mesoform cross-transition probabilities and thus the shape of the point bar semivariogram. The global semivariogram at a still-larger scale that includes multiple macroforms (e.g., point bars, channel fills, and overbank fines) might be governed by the variance in the lengths of macroforms if the predominant permeability contrast is that arising across macroforms. So we can think in this way about how correlation might evolve with scale.

However, at some scale the permeability will likely become strongly multimodal with the univariate variance of the natural log of hydraulic conductivity greatly exceeding unity and violating the assumptions of analytically derived stochastic transport models [see Kitanidis, 1988; Bellin et al., 1992; Chin and Wang, 1992; Follin, 1992; Glimm et al., 1993; Rubin, 1995; Lu and Zhang, 2002]. At this scale it is likely that the representation of preferential flow pathways and low permeability regions is paramount in any meaningful modeling exercise, making the lumped measure of spatial variation that the global semivariogram represents inappropriate. The analysis herein shows that such strongly multimodal permeability could give rise to an exponential-like global semivariogram structure, although such lumped representation may have little value in simulation.

6. Discussion

We began with the question of why a cross-stratified deposit might have an exponential-like permeability correlation structure (or any other shape). We see that the shape of the correlation structure is largely determined by the shape of the transition probabilities for those strata that have the largest contrast in permeability and that occur in non-negligible proportions. Indeed, within our study of a scroll bar mesoform the biggest permeability contrasts were between the higher permeability S₀ or Sᵢ microforms and the lower permeability Sₘ₀ or Sᵢ microforms, and these microforms made up the majority of the deposit. We can explain much of the global semivariogram if we only know the cross-transition probabilities for those microform types and the univariate statistics (mean and variance) for permeability within them. This can be seen by first writing the cross-semivariograms as:

$$\gamma_{ij}(h) = \frac{\sigma_{ij}^2(h)}{2} + \frac{1}{2} (\bar{m}_{ij}(h) - \bar{m}_{ij}(h))^2 - C_{ij}(h), \ i \neq j$$

(3)
see Deutsch and Journel [1998, p. 60] and the note following equation (A22) in Appendix A) and then making some approximations. Under the condition that $C_{ij}$ is small, it can be neglected. If the univariate statistics within lag classes are approximately equal to the univariate statistics for the microform (i.e., $m_{ij}(h) \approx m_{ij}^2$, $\sigma_{ij}^2(h) \approx \sigma_{ij}^2$, $P_i(h) \approx P_i$), we can use the microform statistics. (Similar approximations were considered by Barrash and Clemo [2002] in a different context.) Substitution of (3) into (2) with these approximations and ignoring the autotransition terms gives:

$$g_{ij}(h) \approx \sum_{i,j=1}^{n} \frac{1}{2} [\sigma_{ij}^2 + (m_{ij} - m_{ij})^2] P_i \delta(h);$$

$$i,j = S_a, S_i, S_{ab}, S_b$$

(4)

In Figure 12 we compare this approximation to the global sample semivariogram in the $+x$ direction. Equation (4) explains the general shape and range of the semivariogram and most of the sill. The difference between the approximation and the global semivariogram represents the additional information gained from including the autotransition terms, the full microform semivariograms, the variation of univariate statistics with lag class, and the terms representing other microforms. Indeed, much of the global semivariogram structure can be inferred without this information and by knowing just the univariate permeability statistics and the cross-transition probabilities for the high-contrast units. [46] This analysis suggests that the most important things to get right in field studies are the univariate statistics for permeability and the proportions and cross-transition probabilities of the sedimentary units with larger permeability contrasts.

[47] Note that the literature contains a number of studies showing how transition probabilities can be developed from general geologic knowledge along with statistical attributes of the architecture including proportions, mean length, variance in length, and relative number of occurrences of unit types. [48] We raised the question of what scales contribute most to the shape of the correlation structure. If permeability modes can be defined with a hierarchical organization and if the difference between the permeability modes at level N are always much greater than between those at level N-1, then the scaling is as described by Dagan [1986]. In that case, the shape of the global sample correlation structure is predominantly determined by the transition probabilities for the units defined at the highest hierarchical level at which the data are subdivided. However, as Rubin [1995] noted, permeability modes may not always scale in this way and in some sedimentary deposits the disparity between the modes defined from one hierarchical level to another may not be large. In such cases the hierarchical correlation identity in equation (1) might be used to represent multiple hierarchical levels together in developing macrodispersivity models. Some extensions of the derivation of macrodispersivity models in this direction are given by Dai et al. [2004].

7. Conclusions

[50] 1. Cross-stratified deposits can give rise to a hierarchy of permeability modes, across scales, corresponding to a hierarchy of sedimentary unit types. Thus the modes for unit types defined at hierarchical level N are made up of modes defined for smaller scale units defined at level N-1. We can write the identities for spatial correlation of permeability in a corresponding form.

[51] 2. In such deposits, the shape of the global semivariogram determined in a particular direction of sampling can be largely governed by the shape of the cross-transition probabilities for the unit types having the greatest contrast in permeability. The shape of those cross-transition probabilities can, in turn, be determined largely by the variance for the lengths of those unit types in that direction. If so, the shape lies somewhere along a spectrum from a periodic, piecewise linear structure to an aperiodic exponential-like structure. With larger length variance, the cross-transition probabilities lose periodicity, rise asymptotically toward a sill, and increase in effective range. The effective range of the correlation structure generally will not equal the mean of the lengths of unit types. Anisotropy in the shape of spatial correlation can occur because of anisotropy in length variance.

[52] 3. A sufficient condition for an exponential-like semivariogram structure, often assumed in macrodispersivity models, is the existence of repeated unit types with permeability contrasts and a relatively large length variance.
In field studies of such deposits, sample semi-vario-grams will not represent the true correlation structure unless the sample cross-transition probabilities defined at permeability data locations are representative of the true sedimentary architecture.

The most important things to get right in these field studies are the univariate permeability statistics, the proportions, and the cross-transition probabilities for the sedimentary units with larger permeability contrasts.

Appendix A

Here we derive a general form of the identity for hierarchical spatial correlation. The derivation follows Isaaks and Srivastava [1988] in distinguishing between deterministic vs. probabilistic frameworks in characterizing spatial continuity. Their approach is here modified to account for hierarchical organization of space and is generalized for various functions that represent spatial correlation. To briefly review, in the probabilistic framework the correlation of \(Y(x), Y(x')\) is developed assuming second order stationarity and is viewed as the expected value or ensemble average. The probabilistic notation is extremely convenient in deriving relationships among geostatistical attributes, hence its predominance in the literature. However, most problems encountered in application are within a well-defined, finite domain and involve computing sample statistics in a deterministic framework [Journel, 1985; Gardner, 1986, p. 53; Cressie, 1993]. We first derive equations (1) and (2) with the deterministic approach, which is more involved but leads to a more general result. We then re-derive those equations with the probabilistic approach. The same general functions result. Their subtle differences become apparent when working with real data sampled from a specific domain. These differences are especially significant when attempting to equate calculations of global sample statistics to functions that combine calculations of sample statistics from smaller scale regions at lower hierarchical levels. There will not be exact equality unless the deterministic form is used.

Here the notation developed by Isaaks and Srivastava [1988] is continued. This notation, as noted by those authors, is tedious compared to that of the probabilistic framework but precise and is needed in applications. Consider the bounded domain, \(D\), of any dimension. The symbol \(S\) will be used to refer to the set of sample locations within \(D\):

\[
S : \{x | Y(x) \text{ is known and } x \in D\} \tag{A1}
\]

Consider a lag vector, \(h\), for defining pairs in \(S\) with tail at \(x\) and head at \(x'\). We denote translations of sample locations (Figure A1):

\[
S_{i} \pm h : \{x \pm h | Y(x) \text{ is known and } x \in D\} \tag{A2}
\]

\[
S \pm h : \{x \pm h | Y(x) \text{ is known and } x \in D\} \tag{A3}
\]

Focusing now on the set \(S \cap S_{\pm h}\), it is not simply the subset of sample locations that fall within \(D \cap D_{\pm h}\) as shown in Figure A1.

Figure A1. (a) Definition of the domain, \(D\), and the set of points sampled within it, \(S\). (b) Translation of \(D\) and \(S\). Modified from Isaacs and Srivastava [1989] (with permission of Kluwer Academic Publishers) to represent organization of sample points into units within \(S\).

In the example in Figure A1 there are two pairs formed among the eight data with the lag vector shown.

\([56]\) \(S_{i}\) is the set of sample locations from \(S\) taken in facies \(i\), among \(n_{f}\) facies. The interest is in defining transition pairs from facies \(i\) to facies \(j\): i.e., the sets \(S_{i} \cap S_{j} \pm h\) for \(+h\). The number of pairs is given by

\[
N_{i}(h) = N_{j}(h) = \sum_{m=1}^{\lfloor |S_{j}\cap S_{i}|-1 \rfloor} 1 \tag{A4}
\]

and

\[
\sum_{i} \sum_{j} N_{i}(h) = N_{i}(h). \tag{A6}
\]

Note that \(N_{i}(+h)\) and \(N_{i}(-h)\) can be unequal (asymmetric) and commonly will be in applications within finite and bounded domains.
[57] We use the circumflex in the following equations to denote sample statistics. The sample mean of \( Y_i \) among the tail and head data are a function of lag, as follows:

\[
m_{Y_i}(h) = \frac{1}{N_i(h)} \sum_{m=1}^{N_i(h)} Y_i(x_m) \quad \text{(A7)}
\]

\[
m_{Y_j}(h) = \frac{1}{N_j(h)} \sum_{m=1}^{N_j(h)} Y_j(x'_m). \quad \text{(A8)}
\]

The sample mean of \( I_i(x) \) among the tail data gives the proportion of tail samples in facies \( i \), \( \hat{P}_i(h) \)

\[
m_{Y_i}(h) = \hat{P}_i(h) = \frac{1}{N_i(h)} \sum_{m=1}^{N_i(h)} I_i(x_m). \quad \text{(A9)}
\]

and for heads

\[
m_{Y_j}(h) = \hat{P}_j(h) = \frac{1}{N_j(h)} \sum_{m=1}^{N_j(h)} I_j(x'_m). \quad \text{(A10)}
\]

Note the difference in the summation limits between the functions of \( Y, \) defined only in \( S_i \), vs. functions of \( I \), which are defined over all \( S \).

[58] The global noncentered sample covariance on \( [Y(x), \ Y(x')] \) is defined by

\[
\hat{K}_Y(h) = \frac{1}{N(h)} \sum_{m=1}^{N(h)} Y(x_m)Y(x'_m). \quad \text{(A11)}
\]

and the local noncentered sample covariance for \( [Y(x), \ Y(x')] \), is defined by

\[
\hat{K}_{Y_i}(h) = \frac{1}{N_i(h)} \sum_{m=1}^{N_i(h)} Y_i(x_m)Y_i(x'_m). \quad \text{(A12)}
\]

and for \( [I_i(x), \ I_j(x')] \) by

\[
\hat{K}_{I_i}(h) = \frac{1}{N_i(h)} \sum_{m=1}^{N_i(h)} I_i(x_m)I_j(x'_m) = \frac{N_{ij}(h)}{N_i(h)}. \quad \text{(A13)}
\]

and thus

\[
\sum_i \sum_j \hat{K}_{I_i}(h) = 1. \quad \text{(A14)}
\]

The theorem

\[
\hat{K}_Y(h) = \sum_i \sum_j \hat{K}_{I_i}(h)\hat{K}_{I_j}(h) \quad \text{(A15)}
\]

is proven by simple substitution of (A12) and (A13) which yields the definition in (A11). There are many alternate ways to write this basic identity. To start with, the sample transition probability is defined by

\[
\hat{p}_i(h) = \frac{1}{N_i(h)} \sum_{m=1}^{N_i(h)} I_i(x_m)I_j(x'_m). \quad \text{(A16)}
\]

and from definitions in (A9) and (A13)

\[
\hat{p}_j(h) = \frac{\hat{K}_{I_i}(h)}{\hat{P}_j(h)}. \quad \text{(A17)}
\]

Substitution of (A17) into (A15) gives

\[
\hat{K}_Y(h) = \sum_i \sum_j \hat{K}_{I_i}(h)\hat{P}_j(h)\hat{p}_j(h). \quad \text{(A18)}
\]

[59] Following from the development of (A18) we see that the global computation of any bivariate sample statistic for \( [Y(x), \ Y(x')] \) can be written as a function of those computed on \( [I_i(x), \ I_j(x')] \). Considering the centered covariance gives:

\[
\hat{C}_Y(h) = \frac{1}{N(h)} \sum_{m=1}^{N(h)} Y(x_m)Y(x'_m) - \hat{m}_Y(x)\hat{m}_Y(x'). \quad \text{(A19)}
\]

Note that from (A19), with \( h = 0 \), the variance is given by

\[
\sigma_Y^2 = \sum_i \hat{p}_i \hat{p}_j + \sum_i \sum_j \hat{p}_i \hat{p}_j (\hat{m}_Y - \hat{m}_Y)^2. \quad \text{(A20)}
\]

The classical semivariogram equation is defined by

\[
\hat{\gamma}_Y(h) = \frac{1}{2N(h)} \sum_{m=1}^{N(h)} (Y(x_m) - Y(x'_m))^2 \quad \text{(A21)}
\]

\[
\hat{\gamma}_{Y_i}(h) = \frac{1}{2N_i(h)} \sum_{m=1}^{N_i(h)} (Y_i(x_m) - Y_i(x'_m))^2. \quad \text{(A22)}
\]

Note that alternate forms for the cross-semivariogram are defined elsewhere, e.g., equation III.2 of *Deutsch and Journel* [1998]; however, this form is required when comparing local structure to global structure. Thus

\[
\hat{\gamma}_Y(h) = \sum_i \sum_j \hat{\gamma}_{Y_i}(h)\hat{p}_i(h)\hat{p}_j(h). \quad \text{(A23)}
\]

[60] The summation terms in the identity can be written to span any number of levels of hierarchical organization. For example, we can expand to three levels as in equation (1) by considering microform \( k \) is one of \( n_k \) microforms in mesoform \( o \), which is one of \( n_o \) mesoforms in macroform \( r \),
one of $n_r$ macroforms. The number of translation pairs formed from region $rok$ to region $spm$ for $h$ is given by

$$N_{rokspm}(h) = \sum_{i=1}^{\lfloor y \rfloor} I_{rok}(\underline{x}) I_{spm}(\underline{x}'); \quad k, m = 1, 2 \ldots n_k;$$

$$o, p = 1, 2 \ldots n_o; \quad r, s = 1, 2 \ldots n_r$$

(A24)

and the total number of pairs is given by

$$N_r(h) = \sum_r \sum_o \sum_k \sum_s \sum_p \sum_m N_{rokspm}(h).$$

(A25)

The noncentered covariance equations are

$$K_{rokspm}(h) = \frac{1}{N_{rokspm}(h)} \sum_{i=1}^{N_{rokspm}(h)} Y_{rok}(\underline{x}) Y_{spm}(\underline{x}').$$

(A26)

$$K_{rokspm}(h) = \frac{1}{N_r(h)} \sum_{i=1}^{N_r(h)} I_{rok}(\underline{x}) I_{spm}(\underline{x}').$$

(A27)

and thus

$$\hat{K}_h(h) = \sum_r \sum_o \sum_k \sum_s \sum_p \sum_m K_{rokspm}(h) Pr(h) I_{rokspm}(h).$$

(A28)

The development of the related equations for the centered covariance or variogram follow as above and also involve just an expansion of the summation terms corresponding to the number of hierarchical levels desired.

[61] Note that the global variance can now be decomposed as

$$\sigma^2_h = \sum_r \sum_o \sum_k \sum_s \sum_p \sum_m \sigma_r^2 Pr_{com}(\hat{m}_{rok} - \hat{m}_{com})^2$$

$$+ \sum_r \sum_o \sum_k \sum_s \sum_p \sum_m P_{com}(\hat{m}_{rok} - \hat{m}_{com})^2$$

$$+ \sum_r \sum_o \sum_k \sum_s \sum_p \sum_m \sum_{m'} \sum_{m''} P_{com}(\hat{m}_{rok} - \hat{m}_{com})^2.$$ 

(A29)

The first term gives the contribution due to variance within microform types. The second term gives the contribution arising from mean differences across microform types within the same mesoform and macroform type, the third term gives the contribution arising from mean differences across mesoforms within the same macroform, and the fourth term gives the contribution arising from mean differences across macroforms.

[62] The equations can also be derived in probabilistic form. For simplicity, again consider the moving frame of reference spanning two hierarchical levels, and translations from facies $i$ to facies $j$ at the lower level. We develop the conditional expectation by applying Baye’s Theorem [Rubin, 2003]:

$$\langle A \rangle = \int \int A f(A) dA f(B) dB$$

(A30)

or in the discrete case

$$\langle A \rangle = \sum_i \sum_j A Pr(A|B_i) Pr(B_j).$$

(A31)

Expanding the definition of the ensemble $K_\theta(h)$ with the discrete form we obtain

$$K_\theta(h) = \langle Y(\underline{x}) Y(\underline{x}') \rangle = \sum_i \sum_{i'} \langle Y(\underline{x}) Y(\underline{x}') \rangle I_i(h) = 1$$

and $I_j(h) = 1) Pr\{I_j(h) = 1 \text{ and } I_j(h') = 1\}$

(A32)

and because

$$K_{ij}(h) = \langle Y(\underline{x}) Y(\underline{x}') \rangle I_i(h) = 1 \text{ and } I_j(h') = 1 \}$$

(A33)

$$K_{ij}(h) = Pr\{I_i(h) = 1 \} \text{ and } I_j(h') = 1 \}$$

(A34)

we can write

$$K_\theta(h) = \sum_i \sum_j K_{ij}(h) K_{ij}(h).$$

(A35)

The ensemble transition probability is defined as

$$t_{ij}(h) = \frac{Pr\{I_i(h) = 1 \} \text{ and } I_j(h') = 1 \} \Pr\{I_j(h) = 1 \}$$

(A36)

and assuming ergodicity and stationarity so that $Pr\{I_i(h) = 1 \} = P_i$

$$K_\theta(h) = \sum_i \sum_j K_{ij}(h) P_{ij}(h).$$

(A37)

Here $P_{ij}(h)$ simply represents the joint probability of $[I_i(h) = 1, I_j(h') = 1]$. Forms written for the centered covariance or variogram follow in the same way.

[63] If written for just two levels, and in the form of the centered covariance, with ergodicity and stationarity assumed within the probabilistic framework, the expression is in the form used by Lu and Zhang [2002]. If the expression by Lu and Zhang is limited to two modes, it reduces to the form used by Rubin [1995]. If the form of the semivariogram is used, written for one lower level, it can be equated to the deterministic identity used by Barash and Clemo [2002], with their weighting functions being the equivalent of any of the forms of indicator correlation. Davis et al. [1997] and Di Federico and Neuman [1997] give fractal scaling models for the semivariogram, which do not represent cross-semivariograms between units $i$ and $j$ with $i \neq j$. Neuman [2003, equation 53] also assumes that cross-semivariograms can be ignored. The application in this paper shows the importance of the cross-transition terms in certain geologic settings.

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