Improving permeability semivariograms with transition probability models of hierarchical sedimentary architecture derived from outcrop analog studies

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[1] As analogs for aquifers, outcrops of sedimentary deposits allow sedimentary units to be mapped, permeability to be measured with high resolution, and sedimentary architecture to be related to the univariate and spatial bivariate statistics of permeability. Sedimentary deposits typically can be organized into hierarchies of unit types and associated permeability modes. The types of units and the number of hierarchical levels defined on an outcrop might vary depending upon the focus of the study. Regardless of how the outcrop sediments are subdivided, a composite bivariate statistic like the permeability semivariogram is a linear summation of the autosemivariograms and cross semivariograms for the unit types defined, weighted by the proportions and transition probabilities associated with the unit types. The composite sample semivariogram will not be representative unless data locations adequately define these transition probabilities. Data reflecting the stratigraphic architecture can often be much more numerous than permeability measurements. These lithologic data can be used to better define transition probabilities and thus improve the estimates of the composite permeability semivariogram. In doing so, bias created from the incomplete exposure of units can be reduced by a Bayesian approach for estimating unit proportions and mean lengths. We illustrate this methodology with field data from an outcrop in the Española Basin, New Mexico.


1. Introduction

[2] Outcrops provide an opportunity for observing and mapping sedimentary architecture and for measuring permeability with high resolution. Outcrop analogs have been used in both reservoir and aquifer characterization [e.g., Goggin et al., 1992; Davis et al., 1993, 1997; White and Willis, 2000; Ritzi et al., 2002; Dai et al., 2003; Gaud et al., 2004]. In these studies, sedimentary units were mapped and permeability was measured with high resolution within and across the units using air permeameters. The spatial variation of permeability was linked to attributes of the sedimentary deposit.

[3] Spatial variation in permeability is a predominant control on contaminant plume spreading. Stochastic models relate statistics that characterize the spatial variation of permeability to statistics that characterize the spatial distribution of mass in a spreading plume (see review by Rubin [1997]). For example, Lagrangian-based macrodispersivity models use second-order spatial bivariate statistics, such as the semivariogram, to characterize the spatial variation of permeability [e.g., Woodbury and Sudicky, 1991]. These models are derived assuming the variance of log permeability is less than 1.0. In this paper we focus on sites for which this is true, and we consider outcrop analog studies for defining the semivariogram for log permeability.

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[4] Recently, attention has been focused on linking semivariograms to permeability modes and to facies architecture [Davis et al., 1993, 1997; Allen-King et al., 1998; Ritzi et al., 2004; Dai et al., 2004a; Gaud et al., 2004]. In related work, expressions have been developed for bivariate spatial statistics, including the semivariogram in bimodal domains [Rubin, 1995], multimodal domains [Lu and Zhang, 2002; Zhang, 2002; Barrash and Clemo, 2002], and hierarchical multimodal domains [Ritzi et al., 2002, 2004; Dai et al., 2004b]. Importantly, Lu and Zhang [2002] and Ritzi et al. [2004] related the spatial bivariate statistics for permeability to transition probabilities that represent the aquifer architecture [Carle and Fogg, 1996, 1997]. Ritzi et al. [2004] examined such relationships for cross-stratified deposits having hierarchical permeability modes and showed that the shape and range of the composite sample semivariogram can be determined largely by the cross-transition probabilities for those unit types that create large permeability contrasts and that occur in greater proportions. Ritzi [2000] showed that a sufficient condition for exponential-like cross-transition probabilities is a relatively large coefficient of variation in the lengths of these units in the direction for which the sample semivariogram is determined.

[5] Gaud et al. [2004] showed that outcrop analog studies can be used to define and map lithofacies, to define permeability modes, and to show the correspondence between these permeability modes and the lithofacies. This
was shown in a study of the Skull Ridge Member of the Tesuque Formation in New Mexico. In this paper we revisit these data as we consider how permeability data and lithologic data from outcrops can be used to define the permeability semivariogram. In doing so, we address three issues.

[6] The first issue we address is that there is not a unique hierarchy for classifying sediments at any given site, even when considering quantified textural attributes and permeability modes. We will examine how different classification schemes lead to different relationships between architectural attributes and the semivariogram shape.

[7] The second issue we address is that measuring permeability with high resolution on outcrops (e.g., with an air permeameter) has practical limitations. Field studies have usually generated fewer than 2000 permeability data, a number that is a small fraction of that which could be considered exhaustive sampling. However, maps of the exposed sedimentary units can be used to generate data indicating lithology. These data represent essentially an exhaustive sampling of the exposed units at the level of the detail mapped and are of a number that is commonly orders of magnitude larger than the number of permeability data. We show how these data can be used to generate transition probability models for the sedimentary architecture, models that can be used to improve equivocal sample semivariograms.

[8] The third issue we address is that sedimentary units are often only partially exposed in outcrops. White and Willis [2000] discussed how this biases estimates of proportion and of the mean and variance for length, and they presented a Bayesian method for improving these estimates. Here we discuss how incomplete exposure also biases the shape of the cross-transition probabilities and thus the shape of the sample semivariogram. We present a method for reducing this bias that builds on the method of White and Willis [2000]. We demonstrate how this method improves the estimation of the semivariogram and discuss the limitations of the method.

2. Conceptual Frameworks for Sedimentary Architecture

[9] The Tesuque Formation occurs within the Rio Grande rift basin, New Mexico, as shown in Figure 1, and is an important aquifer [Smith, 2000; Kuhle and Smith, 2001; Gaud et al., 2004]. An outcropping of the Skull Ridge Member of the Tesuque Formation is shown in Figure 2. These sediments were deposited on an alluvial slope draining the Santa Fe Range, as described by Smith [2000]. The sediments represent both channel and interchannel deposits, are both ribbon-form and tabular in shape, and vary in grain size from clay to sandy gravel. Channel depths were less than 3 m. Sediment-transporting flows were rapid, shallow, and markedly unsteady [Gaud et al., 2004]. Upper flow regime sedimentary structures and abundant scours and-fill structures dominate the channel deposits. Deposition between channels included eolian redistribution of channel sand so that not all interchannel deposits are mud.

[10] Gaud et al. [2004] surveyed the exposed lithofacies and measured permeability at 1748 points as shown in Figure 2. The outcrop is about 380 m long, aligned approximately north-south, and is perpendicular to the general flow direction during deposition. About 30 m of stratigraphic thickness is exposed. Importantly, there are many gaps between the exposed areas because of talus and vegetative cover and thus individual units are only partially exposed. The locations at which permeability was measured are referenced by the location vector \( x_k \). The mapped lithology was digitized (approximately a 0.5 m \( \times \) 0.5 m grid) and coded with integer indicators giving 14,860 lithologic data. These data represent an essentially exhaustive sampling of the exposed areas in Figure 2. These locations are referenced by the location vector \( x_f \). Note that \( x_k \) is a subset of \( x_f \). We will first analyze the permeability and lithologic data only at \( x_k \), and then incorporate the additional lithologic information defined at \( x_f \) to better model some of the univariate and bivariate statistics.

[11] The sediments can be subdivided in different ways using different criteria. Gaud et al. [2004] divided the sediments into unit types based primarily on texture. Eight of these are given in Figure 3 under the column labeled “level I.” Furthermore, Gaud et al. [2004] found that these unit types have statistically significant differences in permeability modes (see Figure 4a). The existence of separate permeability modes is a common criterion that...
hydrogeologists use in dividing sediment into hydrofacies. However, the categorization of Gaud et al. [2004] is not unique when using this criterion. Subdividing the sediments to a greater or lesser extent might still result in unit types with separate permeability modes. Grouping the level I unit types into four larger-scale unit types (SG, S, SF, and F in Figure 3) results in the distinct permeability modes shown in Figure 4b. Grouping the same level I units differently into channel and interchannel unit types (Figure 3) also results in distinct permeability modes as shown in Figure 4c.

Figure 2. Map of the outcropping of the Skull Ridge Member of the Tesuque Formation divided into (a) left and (b) right sides, which join along the broken line (modified from Gaud et al. [2004], reprinted with permission of SEPM Society for Sedimentary Geology). Permeability measurement locations, $x_k$, are shown with stars (1748 locations among Figures 2a and 2b). Labels on photo insets are from field notes and are not referred to in this article. See color version of this figure at back of this issue.
Furthermore, it is likely that unit types still smaller in scale than the level I units can be defined as having distinct permeability modes [e.g., Ritzi et al., 2004]. Whether distinctions in permeability need to be made at any given scale depends on the context: what might be parsimonious for one purpose may not have enough detail for another.

Sedimentary deposits are often conceptualized as having hierarchical organization and the conceptual hierarchy can be linked to permeability modes [e.g., Ritzi et al., 2004]. There may be contexts in which using a hierarchy of units is beneficial. However, as we see from this discussion, the hierarchy we might apply to subdivide sediments is not unique.

To illustrate the ramifications of using alternate hierarchies for categorizing the sediment, we will consider the two hierarchies in Figure 3 as examples. We will analyze and compare each of these in the following sections, and consider the issue of parsimony within the context of defining the permeability semivariogram.

At level I, the smallest scale delineated by Gaud et al. [2004], the units are defined texturally. The units at level I are defined the same in either of the two hierarchies. Table 1a gives their proportions. Note that there are three additional units mapped by Gaud et al. [2004] in Figure 2: Ss, Fl, and A. Of these units only A (ash) occurs in an appreciable proportion. Because there are no permeability measurements for Ss and Fl, they are excluded from the analysis. Ash bounds the other units above and below, and, by excluding it, our analysis is thus of one succession between two ash deposits.

Compared to the units at level I, the units at level II are larger features representing the cumulative effect of multiple depositional events over a longer period of time. In the first hierarchy, level II units are defined as textural categories that are broader than those at level I (see Figure 3). In that units at both levels are defined by texture, this hierarchy will be referred to as the textural-textural (TT) hierarchy. The exposed areas indicate that sand and fine sand dominate as a volume fraction of the deposit in this hierarchy (see Table 1b). It is possible that estimates of unit proportions are biased by the incomplete exposure of units, a point that is examined below.

In the second hierarchy, the units at level II are defined by their inferred location of deposition as either channel or interchannel units (see Figure 3). This will be referred to as the depositional-textural (DT) hierarchy. The exposed areas indicate that the interchannel deposits dominate...
as a volume fraction of the deposit (see Table 1b). Again, the possibility of bias in these results is examined below.

Figure 3 shows that in the TT hierarchy, the level II units contain level I units having similar permeabilities. In contrast, the level II units in the DT hierarchy contain level I units with diverse permeabilities. This contrast is important in explaining the differing results using the two hierarchies.

3. Relevant Spatial Bivariate Statistics

Itzi et al. [2004] showed how the semivariogram can be written for a hierarchical system with any number of levels. Here we write it for three hierarchical levels. Consider a domain at level III (the composite interash succession) made up of level II units filling space in mutually exclusive occurrences. The level II regions are themselves made up of level I units, also filling space and not overlapping. A measurement of log permeability at sample location \( x \) is given by \( Y(x) \).

Two points \( x \) and \( x' \) are separated by a vector \( h \). Point \( x \) occurs in level I unit type \( r \) which is in level II unit type \( o \) and point \( x' \) is within level I unit type \( i \) which is in level II unit type \( j \). The identity for the sample semivariogram can be written as

\[
\hat{\gamma}(h) = \frac{1}{2N_u(h)} \sum_{a} (Y(x_a) - Y(x'_a))^2
\]

According to Itzi et al. [2004], (1) can be rewritten as the sum of four terms:

\[
\hat{\gamma}(h) = \sum_{i} \sum_{j} \hat{\gamma}_{ijij}(h) \hat{p}_{ij}(h) \hat{p}_{ij}(h)
\]

\[
+ \sum_{i} \sum_{j} \sum_{k} \hat{\gamma}_{ijkj}(h) \hat{p}_{ik}(h) \hat{p}_{jk}(h)
\]

\[
+ \sum_{i} \sum_{j} \sum_{k} \hat{\gamma}_{ijik}(h) \hat{p}_{ik}(h) \hat{p}_{jk}(h)
\]

\[
+ \sum_{i} \sum_{j} \sum_{k} \hat{\gamma}_{ikij}(h) \hat{p}_{ik}(h) \hat{p}_{jk}(h)
\]

where \( \hat{\gamma}(h) \) is the composite sample semivariogram, \( N_u(h) \) is the number of pairs defined by lag \( h \), \( \hat{\gamma}_{ij}(h) \) is the sample semivariogram for transitions between region types.
or and \( \text{ji} \) (autosemivariogram if \( or = \text{ji} \)), \( p_{or}(h) \) is the proportion of region type \( or \), and \( i_{or,ji}(h) \) is the sample transition probability for transitioning from region \( or \) to region \( \text{ji} \).

[20] In essence, the expansion in expression (2) subdivides the lag pairs according to the unit types into which the tails and heads of a data pair fall. The first term on the right-hand side of expression (2) includes contributions from pairs that represent autotransitions with tail and head in the same level II unit type and the same level I unit type. We will refer to this as the \( \alpha \alpha \) (auto-auto) term. The second term on the right-hand side of expression (2) includes contributions from pairs defining transitions with tail and head in the same level II unit type but across different level I unit types. We will refer to this as the \( \alpha \chi \) cross-transition term. The third term on the right-hand side of expression (2) includes contributions from pairs defining transitions with tail and head in different level II unit types but the same level I unit type (\( \chi \alpha \) terms). Note that there are no such transitions in the case study and so we will not refer to them below. The fourth term on the right-hand side of expression (2) includes contributions from pairs defining transitions with tail and head in different unit types at both hierarchical levels, and will be referred to as the \( \chi \chi \) cross-transition term.

4. Hierarchical Variography

4.1. Vertical Variography in TT Hierarchy

[21] The composite sample semivariogram computed in the vertical direction from permeability data sampled at \( x_k \) locations is shown in Figure 5a. It is not particularly smooth and leads to equivocal choices for the sill and range. This equivocal result occurs because the sample locations are limited. We overcome some of this limitation below when using the \( x_I \) data. Before doing so, we first decompose the composite semivariogram according to equation (2) and analyze the contributions of the various terms. Through this
decomposition and analysis we show that the composite sample semivariogram from data at \( x_k \) is not representative of the permeability correlation.

[22] Figure 5a also shows the sum of all the terms of equation (2) under the TT hierarchy, which exactly matches equation (1). Note that the \( \alpha \alpha \) and \( \alpha \chi \) terms plotted individually in Figure 5a contribute in a minor way to the composite semivariogram. The shape and range are determined to a much greater extent by the \( \chi \chi \) terms. Thus, in the TT hierarchy there is significantly less contribution from data pairs representing transitions among the same level II unit type than from pairs representing transitions across two different level II unit types. This suggests that if the outcrop is delineated by level II textural unit types (SG, S, SF and F), there is little added value for defining the semivariogram in further delineating the outcrop into level I textural unit types.

[23] Note that we do not attempt to show all 64 \( \gamma_{\chi \chi}(h) \) or all 64 \( \gamma_{\alpha \chi}(h) \) individually. More insight can be gained by analyzing certain groups of these in the following analysis.

[24] We first examine transition probabilities as weighted by proportions. The expression \( \gamma_{\alpha \chi}(h) \) defines the proportion of lag pairs that start in region type \( c \) and end in region type \( \chi \) [Ritzi et al., 2004]. In Figure 5b we plot the sum of \( \gamma_{\alpha \chi}(h) \) terms associated with all cross transitions, just \( \alpha \chi \) cross transitions, and just \( \chi \chi \) cross transitions. The \( \chi \chi \) terms make up the greater proportion of cross transitions. This fact and some further insights described below explain why the \( \chi \chi \) terms in equation (2) dominate the composite semivariogram.

[25] Ritzi et al. [2004] showed that the sample semivariogram can be approximated using only cross-transition probabilities and the univariate statistics (mean and variance) for permeability within unit types. This can be seen by first writing the cross semivariograms as

\[
\gamma_{\alpha \chi}(h) = \frac{\gamma_{\alpha \chi}^2(h) + \gamma_{\chi \chi}^2(h)}{2} + \frac{1}{2} (m_{\alpha \chi}(h) - m_{\chi \chi}(h))^2 - C_{\alpha \chi}(h)
\]

where \( m_{\alpha \chi}(h) \) and \( \gamma_{\alpha \chi}^2(h) \) are the sample mean and variance within the lag class (see Deutsch and Journel [1998, p. 60] and the note following equation (A22) of Ritzi et al. [2004]) and then making some approximations. Under the condition that the cross covariance \( C_{\alpha \chi}(h) \) is small, it can be neglected. If the univariate statistics within lag classes are approximately equal to the univariate statistics for the unit types (i.e., \( m_{\alpha \chi}(h) \approx m_{\alpha \chi}, \gamma_{\alpha \chi}^2(h) \approx \gamma_{\alpha \chi}^2, P_{\alpha \chi}(h) \approx P_{\alpha \chi} \)), the latter statistics can be used (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

\[
\hat{\gamma}_{\alpha \chi}(h) \approx \sum_o \sum_j \sum_r \sum_{i \neq r} [\gamma_{\alpha \chi}^2(h) + \gamma_{\chi \chi}^2(h) + (m_{\alpha \chi} - m_{\chi \chi})^2] \hat{P}_{\alpha \chi}(h) \]

(4)

Figure 5a compares this approximation to the composite sample semivariogram. Indeed, equation (4) explains the general shape of the composite sample semivariogram and thus is a good approximation. The difference between the approximation and the composite sample semivariogram represents the additional information gained from including the autotransition terms, the semivariograms for units, and the differences that may exist in univariate statistics among lag classes. Much of the composite semivariogram structure can be inferred without this information and by knowing just the univariate permeability statistics and the cross-transition probabilities. Ritzi et al. [2004] observed similar results for another type of sedimentary deposit and noted that such results suggest that the most important things to quantify correctly in field studies are the univariate statistics for permeability and the proportions and cross-transition probabilities of the sedimentary unit types creating large permeability contrasts.

[26] The \( \chi \chi \) transition probabilities define the shape and range in the plot of equation (4) and the univariate statistics, surrogates for the cross semivariograms, scale the curve and define the sill. We can deduce that within the expression \( \sum_{\alpha \chi} \sum_{\chi \chi} \gamma_{\alpha \chi}(h) \) \( P_{\alpha \chi}(h) \) for \( \alpha \chi \) transition terms, the products \( P_{\alpha \chi}(h) \) for cross-transition terms, in large part, determine the shape and range of the composite sample semivariogram, whereas \( \gamma_{\chi \chi}(h) \) for cross-transition terms act to scale the curve and define the sill.

4.2. Improving the Estimate of the Composite Semivariogram Using Lithologic Data

[27] The insights gained above lead to a method for incorporating information from the abundant lithologic data defined at the \( x_k \) locations, even though they are not accompanied by permeability data. These data were used to recompute the proportions and the cross-transition probabilities and to replot the \( \tilde{P}_{\alpha \chi}(h) \) terms as determined at \( x_k \) locations. The result is shown in Figure 5d, are smoother, have more of an asymptotic-like rise, and have a less equivocal range and sill than the curves in Figure 5b. The \( x_k \) data clearly represent the cross transitions of units better than the \( x_k \) data, especially over lag distances between 1 m and 6 m. Furthermore, because the shape of the composite sample semivariogram is largely determined by the shape of the \( \gamma_{\alpha \chi}(h) \) cross-transition curves, we conclude that the composite sample semivariogram is not well defined by the \( x_k \) locations.

[28] Accordingly, the composite sample semivariogram can be improved by recomputer it using equation (4) and \( \tilde{P}_{\alpha \chi}(h) \) terms as determined at \( x_k \) locations. The result is shown in Figure 5c (as \( \alpha \chi + \chi \chi \)). This estimate of the composite semivariogram incorporates more information about the architecture of the deposit than is represented by the \( x_k \) data. Furthermore, the sum of only the \( \alpha \chi \) cross-transition terms is also plotted and is very small for all lags. This indicates that there is little added value in including \( \alpha \chi \) cross transitions; the \( \chi \chi \) cross transitions are most important within the TT hierarchy.

[29] If this is accepted as an improved estimate of the composite semivariogram, one approach to model it is to first develop a model for the cross-transition probabilities. However, the transition probabilities can be further improved by reducing the bias introduced by the partial exposure of the units in the outcrop. As shown by Ritzi [2000] and Dai et al. [2004b], the cross-transition probabilities are related to statistics that characterize the thickness of unit types. In the following analysis we first
develop statistics for thickness of unit types that account for incomplete exposure and then use those statistics to create a model for cross-transition probabilities.

4.3. Improving the Estimate of the Composite Semivariogram Using Thickness Statistics

As is commonly the case, many of the occurrences of the units in the outcrop are not exposed over their full thickness. When the map in Figure 2 is sampled along closely spaced vertical lines (as represented in the \( x \) lithologic data), there are often fewer than two terminations (i.e., one exposed upper boundary and one exposed lower boundary) per unit (see Table 2). Because the units are not fully exposed, the mean thickness computed for unit types using the \( x \) data has bias, as does the computed proportion of unit types. To reduce this bias we use a method of estimation based upon termination frequencies and a Bayesian updating algorithm modified from White and Willis [2000]. Details of the estimation procedure are given in Appendix A; the estimates are given in Table 2.

If the unit types were to repeat in equal numbers (so that proportion is only a function of mean length) and were to have exponential cross-transition probabilities, those frequencies and a Bayesian updating algorithm modified from White and Willis [2000]. Details of the estimation procedure are given in Appendix A; the estimates are given in Table 2.

4.4. Vertical Variography in the DT Hierarchy

We used the DT hierarchy (as given in Figure 3) and repeated each of the steps used above in analyzing the vertical semivariogram. Thus we first used the \( x \) data and computed the autotransition and cross-transition terms in equation (2). The results in Figure 6a show that the \( \alpha \alpha \) terms contribute little to the composite sample semivariogram. The shape and range of the composite sample semivariogram are determined to a much greater extent by cross-transition terms, as was the case using the TT hierarchy (Figure 5a). However, while the \( \alpha \alpha \) term was rather inconsequential within the TT hierarchy, the \( \alpha \chi \) and the \( \chi \chi \) cross terms both contribute equally within the DT hierarchy. This is as we would expect, knowing that in the DT hierarchy there are significant differences in permeability modes among level I unit types occurring within the same level II regions (e.g., SFi and SGr within channel regions; see Figure 3).

Figure 6b shows the sum of \( \tilde{P}_{\text{tr}}(h)I_{\text{tr},i,j}(h) \) cross-transition terms, including \( \alpha \chi \) cross transitions, \( \chi \chi \) cross transitions, and the sum of both. The number of data pairs defining \( \chi \chi \) transitions is smaller than for \( \alpha \chi \) cross transitions. However, permeability differences in the \( \chi \chi \) cross transitions must, in general, be greater than those in \( \alpha \chi \) cross transitions given the almost equal contributions of \( \alpha \chi \) and \( \chi \chi \) cross-transition terms in Figure 6a.

Note that the level I units are defined the same way in the TT and the DT hierarchies so that the sum of all cross-transition terms in equations (2), (4), and (5) are the same in

### Table 2. Statistics Associated With Modeling the Vertical Transition Probabilities

<table>
<thead>
<tr>
<th>Level I Unit Types</th>
<th>SGr</th>
<th>SGt</th>
<th>SFi</th>
<th>Sm</th>
<th>Sw</th>
<th>SFn</th>
<th>SFm</th>
<th>P</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of occurrences</td>
<td>258</td>
<td>216</td>
<td>80</td>
<td>914</td>
<td>114</td>
<td>463</td>
<td>1128</td>
<td>416</td>
</tr>
<tr>
<td>Termination count</td>
<td>411</td>
<td>398</td>
<td>146</td>
<td>1115</td>
<td>218</td>
<td>613</td>
<td>1265</td>
<td>729</td>
</tr>
<tr>
<td>Observed proportion</td>
<td>0.047</td>
<td>0.041</td>
<td>0.022</td>
<td>0.309</td>
<td>0.023</td>
<td>0.220</td>
<td>0.288</td>
<td>0.050</td>
</tr>
<tr>
<td>Observed mean thickness, m</td>
<td>0.65</td>
<td>0.63</td>
<td>0.72</td>
<td>2.34</td>
<td>0.93</td>
<td>1.56</td>
<td>2.15</td>
<td>0.58</td>
</tr>
<tr>
<td>Inferred proportion</td>
<td>0.045</td>
<td>0.040</td>
<td>0.021</td>
<td>0.313</td>
<td>0.022</td>
<td>0.220</td>
<td>0.291</td>
<td>0.048</td>
</tr>
<tr>
<td>Inferred mean thickness, m</td>
<td>0.78</td>
<td>0.66</td>
<td>0.77</td>
<td>3.75</td>
<td>0.86</td>
<td>2.14</td>
<td>3.68</td>
<td>0.64</td>
</tr>
</tbody>
</table>

\[ a_{\omega} = 3l_{\omega}(1 - p_{\omega}), \text{ m} \]

The unit types do not occur in equal numbers in the outcrop and the terms \( 3l_{\omega}(1 - p_{\omega}) \) computed in Table 2 have some difference but are of the same order of magnitude and we take their average for the model. For most unit types, the inferred mean thicknesses are greater than observed on outcrop and the inferred proportions are less than observed. Both of these differences increase \( 3l_{\omega}(1 - p_{\omega}) \) from what it would be if computed from the observed mean thicknesses and proportions. The average \( 3l_{\omega}(1 - p_{\omega}) \) computed from the inferred statistics is 3.92 m. The model using this value as an effective range is plotted in Figure 5c. Figure 5c shows that the model semivariogram (equation (5)) is generally similar to the semivariogram computed using equation (4) but has a slightly larger effective range. Thus, by accounting for the incomplete exposure of units when inferring the proportions and thicknesses of unit types, and by developing a semivariogram model based on those estimates, we arrive at a model with a greater correlation range.
either hierarchy. Furthermore, all curves among Figures 5 and 6 that represent the sum of all cross transitions are the same in either hierarchy. Accordingly, the sum of all cross-transition terms explains most of the composite semivariogram in the DT hierarchy just as it did in the TT hierarchy, and the shape of these cross-transition terms is, in turn, determined largely by the shape of the sample cross-transition probabilities. A difference is that the sample cross-transition probabilities for \( \alpha \times \) cross transitions are more important in the DT hierarchy than they are in the TT hierarchy.

The results using the lithologic data defined at the \( x_i \) locations and using the DT hierarchy are given in Figures 6c and 6d. The sums of \( \rho_{or}(h)\rho_{or,ji}(h) \) for cross-transition terms are smoother, have more of an asymptotic-like rise, and have a less equivocal range and sill than the curves in Figure 6b. The composite sample semivariogram using equation (4) and these better defined \( \rho_{or}(h)\rho_{or,ji}(h) \) is shown in Figure 6c (as \( \alpha\chi + \chi\chi \)). Figure 6c also shows the model computed using equation (5) and the inferred statistics for proportion and thickness (Table 2 and Appendix A). The model is generally similar to the sample semivariogram but has a slightly larger effective range. The larger range occurs because the transition probability models are based on estimates for proportion and thickness that account for incomplete exposure of the units. Therefore the model is a better representation of the spatial correlation of log permeability within the deposit than is the sample semivariogram.

Comparing results from the TT and DT hierarchies shows that the semivariogram is sensitive to those unit types having large permeability contrasts. It is necessary, when using equation (5), to recognize those types of units and to characterize their cross-transition probabilities and their univariate statistics for permeability. In the DT hierarchy, both the \( \alpha\chi \) and the \( \chi\chi \) terms of the model are significant; it is important to recognize unit types at both hierarchical levels I and II. In the TT hierarchy, only

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**Figure 6.** Analysis of the vertical semivariogram; DT hierarchy. (a and b) Using data at \( x_k \) locations. (c and d) Incorporating data at \( x_I \) locations. In Figures 6b and 6d, \( F = \sum_a \sum_j \sum_r \sum_{i,pr} \rho_{or}(h)\rho_{or,ji}(h) \).
the $\chi \chi$ terms are significant in defining the semivariogram; it is important to recognize level II unit types. In this context the most parsimonious hierarchy is the one that defines the higher contrast permeability modes with the least number of unit types and hierarchical levels, as is done by defining only level II unit types within the TT hierarchy.

[39] Field work using outcrop analogs facilitates the study of permeability modes and their correspondence to conceptual models for the sedimentary architecture (hierarchies of unit types). Thus outcrop studies can facilitate the development of a parsimonious hierarchy when categorizing the sediment into unit types.

4.5. Lateral Variography

[40] The composite sample semivariogram computed in the horizontal direction with the $x_k$ data is shown in Figure 7. The approximation using equation (4) and the $x_k$ data is also shown. In both cases the approximation includes all cross terms and so is the same within either the TT or the DT hierarchy. As in the vertical direction, the approximation is almost identical to the composite sample semivariogram, indicating that the shape of the lateral sample semivariogram is mostly defined by the shape of the sample cross-transition probabilities.

[41] As in the vertical direction, the cross-transition probabilities are not well defined by the $x_k$ data locations. Indeed, when the composite horizontal semivariogram is estimated using the more abundant $x_I$ data and equation (4), the semivariogram has a less equivocal range and sill, as shown in Figure 7.

[42] When the outcrop map in Figure 2 is sampled along closely spaced horizontal lines (as represented in the $x_I$ data) very few units have two terminations exposed (Table 3). There are slightly more than one termination per occurrence for most of the unit types. Those occurrences having two terminations tend to have a relatively short length. The bias in mean length due to incomplete exposure is more severe in the horizontal direction than in the vertical. In Appendix A we develop estimates for horizontal mean length using the termination frequencies and Bayesian updating to reduce this bias. The results are given in Table 3.

[43] However, these estimates may still have significant bias. It seems plausible that these deposits contain a population of units with long horizontal lengths that has not been represented. Figure 2 shows that the thicker units such as SFn and Sm could be continuous across the gaps in the middle and beyond the boundaries of the exposure. If so, units could be sampled along many horizontal lines extending for hundreds of meters if they were fully exposed. If this population of long samples were to be included in the Bayesian updating procedure, the estimates of mean length for these units would increase significantly.

[44] Assuming exponential transition probabilities and unit types in equal numbers, and thus that all cross transition probabilities have the same range [Dai et al., 2004b], we can use equation (5) to understand how the horizontal semivariogram would change if it reflected the occurrence of longer units. If the mean lengths for SFn and Sm are really of the order of $100 \text{ m}$, the semivariogram with a range computed using $3/l_{or} (1 - p_{or})$ has an effective range of the order $200 \text{ m}$ as shown in Figure 7. Thus, if some units are continuous across the gaps in the exposure and beyond it, then the semivariogram would have a significantly longer range than does the sample semivariogram computed using the $x_k$ or $x_I$ data locations.

5. Discussion

[45] The results presented above show that in order to characterize the composite semivariogram for log perme-

<table>
<thead>
<tr>
<th>Level I Unit Types</th>
<th>SGr</th>
<th>SGt</th>
<th>SFi</th>
<th>Sm</th>
<th>Sw</th>
<th>SFn</th>
<th>SFm</th>
<th>P</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of occurrences</td>
<td>55</td>
<td>20</td>
<td>26</td>
<td>177</td>
<td>22</td>
<td>60</td>
<td>188</td>
<td>35</td>
</tr>
<tr>
<td>Termination count</td>
<td>59</td>
<td>22</td>
<td>30</td>
<td>181</td>
<td>25</td>
<td>60</td>
<td>190</td>
<td>39</td>
</tr>
<tr>
<td>Observed proportion</td>
<td>0.047</td>
<td>0.041</td>
<td>0.022</td>
<td>0.309</td>
<td>0.023</td>
<td>0.220</td>
<td>0.288</td>
<td>0.050</td>
</tr>
<tr>
<td>Observed mean length, m</td>
<td>6.34</td>
<td>14.88</td>
<td>5.92</td>
<td>13.01</td>
<td>6.84</td>
<td>27.61</td>
<td>11.55</td>
<td>9.88</td>
</tr>
<tr>
<td>Inferred proportion</td>
<td>0.047</td>
<td>0.042</td>
<td>0.022</td>
<td>0.304</td>
<td>0.023</td>
<td>0.228</td>
<td>0.284</td>
<td>0.051</td>
</tr>
<tr>
<td>Inferred mean length, m</td>
<td>9.60</td>
<td>21.03</td>
<td>8.41</td>
<td>20.75</td>
<td>9.73</td>
<td>42.23</td>
<td>18.61</td>
<td>14.24</td>
</tr>
<tr>
<td>$a_{or} = 3/l_{or} (1 - p_{or})$, m</td>
<td>27.45</td>
<td>60.45</td>
<td>24.69</td>
<td>43.32</td>
<td>28.53</td>
<td>97.80</td>
<td>39.99</td>
<td>40.53</td>
</tr>
</tbody>
</table>

Figure 7. Analysis of the lateral semivariogram.
ability within sediments having a multimodal distribution of log permeability, we must adequately characterize the cross-transition probabilities for unit types that correspond to those modes. This is consistent with results presented by Ritzi et al. [2004]. The present results for alternate but equally justifiable hierarchical classifications of unit types show that this is also true for alternate subdivisions of the same sediment deposit. Indeed, if the cross-transition probabilities are known along with the univariate statistics for the permeability modes, then equation (4) provides a very good approximation for the composite semivariogram. This implies that the composite permeability semivariogram can be characterized by (1) sampling permeability within some representative occurrences of each unit type to characterize the permeability modes, and (2) sampling the broader exposure for lithology to characterize the cross-transition probabilities. However, to characterize these cross-transition probabilities in a particular direction, the sample locations must represent the distribution of lengths for each unit type. In this study we see that outcrop exposures may not be adequate to characterize these cross-transition probabilities.

This study was based upon a very large and extensive outcrop with fairly exhaustive lithologic sampling of the exposed units. However, the units themselves are large and may be much more laterally extensive than the exposures in the outcrop. As a result, we could not satisfactorily characterize the lateral lengths of units, and the cross-transition probabilities are equivocal. Thus the lateral length scale of outcrop exposures must be much larger than the lateral scale of the units exposed in order to characterize the length distributions of the unit types, their cross transition probabilities, and the permeability semivariogram. Our experience suggests that many outcrop exposures are not large enough for this type of characterization.

Accordingly, we expect that many outcrops would not allow direct characterization of lateral permeability semivariograms, even if they were to be exhaustively sampled. Furthermore, outcrop studies are limited in that they commonly involve exposures of the sediments in essentially two dimensions. In the current example, the sediments are exposed along a direction perpendicular to the general direction of flow during deposition. In deposits such as these that were dominated by fluvial processes, the mean lengths of many of the unit types are expected to be shortest in this direction. Mean lengths can be expected to be longer in other directions and therefore the semivariogram can be expected to be anisotropic in its range. Such anisotropy cannot be determined directly from a two-dimensional outcrop.

The vertical succession of units is better revealed in the Skull Ridge outcrop than is the lateral succession of units. Because this is commonly the case, cross-transition probabilities and semivariograms determined from field studies are expected to be better defined in the vertical than in the lateral directions.

Though many outcrops are inadequate to fully characterize the lengths of unit types, their cross-transition probabilities, or the composite permeability semivariogram in directions other than vertical, outcrop analog studies are still important. The study of the Skull Ridge deposits illustrates that outcrop analog studies can lead to a hierarchy in which the sediments are parsimoniously delineated into unit types with permeability contrasts.

6. Conclusions

The major conclusions of this study are as follows. The hierarchy used for conceptually organizing specific sediments may not be unique. Even so, the composite sample semivariogram for permeability can be written as a function of terms that correspond to unit types in whatever hierarchy is chosen. In the context of defining the composite semivariogram, the parsimonious hierarchy is the one that represents unit types having the most significant permeability contrast with the least number of unit types and hierarchical levels. A primary benefit from an outcrop analog study is that it provides information for the development of such a hierarchy.

Within a given hierarchy, the shape of the composite semivariogram may largely be determined by the shape of the sum of $P_{or \ Tor}$ (h) for unit types that have significant permeability contrasts (shown here and also by Ritzi et al. [2004]). Here we conclude that one can use lithologic data, independent of permeability measurements, to improve estimates of $P_{or \ Tor}$ (h) and thus to improve estimates of the permeability semivariogram.

The shape of $P_{or \ Tor}$ (h) will not represent the sedimentary architecture unless the units are sampled along their full length and in their proper proportions. Outcrop exposures often do not allow this, and if not, the shape of the sample composite semivariogram is not representative (i.e., is biased).

The composite permeability semivariogram can be modeled without fitting a curve to what might be a biased sample semivariogram. Instead, the model can be based on statistics for proportion and mean length of unit types. Furthermore, a Bayesian approach can be used for improving estimates of proportion and mean length by accounting for less than full exposure of units. Doing so leads to less biased models for the composite semivariogram. This method should be useful for modeling the vertical composite semivariogram in many outcrop-analog studies.

The method cannot correct bias if there are no exposed unit terminations or if they are insufficient for inferring length distributions. This may often be true of outcrop exposures when sampling in the lateral direction. Still, equation (5) can be used to explore how the range of an exponential composite semivariogram model would change as a function of the mean length of unit types.

Appendix A: Estimation of Mean Length From Sparse Data

The distribution of unit lengths can be modeled with an Erlangian probability density function based on termination frequency [White and Willis, 2000]. Termination frequency, $f_{or}$, can be calculated from outcrop observations even if the sedimentary units are incompletely exposed:

$$f_{or} = \frac{M_{or}}{N_{Tor}} \sum_{m=1}^{M_{or}} \frac{N_{Tor}}{L_{form}}$$

(A1)
where \( M_{or} \) is the number of the occurrences, \( N_{\text{Form}} \) is the number of terminations for occurrence \( m \) of level II type \( o \) and level I type \( r \) (\( N_{\text{Form}} = 0, 1 \) or 2), and \( l_{\text{orm}} \) is the observed length of the \( m \)th occurrence.

The occurrences of different sedimentary units can be partitioned into families using conditional probabilities and Bayes’ theorem [White and Willis, 2000]. The probabilities for all observed lengths are calculated, conditional to occurrence \( m \) being a member of the family \( U_{or} \). The families are assumed to have second-order Erlangian length distributions. For occurrence \( m \), if zero or one termination is observed on the outcrop (\( N_{\text{Form}} = 0 \) or 1),

\[
\text{prob}(l_{\text{orm}}|m \in U_{or}) = \int_{l_{\text{orm}}}^{\infty} f_{or}^2 \cdot e^{-f_{or}l} dl, \tag{A2}
\]

whereas if the occurrence is completely observed (\( N_{\text{Form}} = 2 \),

\[
\text{prob}(l_{\text{orm}}|m \in U_{or}) \propto f_{or}^2 l_{\text{orm}} e^{-f_{or}l_{\text{orm}}}. \tag{A3}
\]

The probability of membership in \( U_{or} \) is computed using Bayes’ theorem:

\[
\text{prob}(m \in U_{or}|l_{\text{orm}}) = \frac{p_{or} \cdot \text{prob}(l_{\text{orm}}|m \in U_{or})}{\sum_{m=1}^{M_{or}} \sum_{l=1}^{L} p_{or} \cdot \text{prob}(l_{\text{orm}}|m \in U_{or})}. \tag{A4}
\]

Updated family proportions are

\[
p_{or} = \frac{\sum_{m=1}^{M_{or}} \text{prob}(m \in U_{or}|l_{\text{orm}})}{M_{or}}. \tag{A5}
\]

The updated probabilities of family membership (equations (A2) and (A3)) are used to weight the lengths and termination counts used in calculating the termination frequency. Then, equation (A1) becomes

\[
f_{or} = \frac{\sum_{m=1}^{M_{or}} \text{prob}(m \in U_{or}|l_{\text{orm}})N_{\text{Form}}}{\sum_{m=1}^{M_{or}} \text{prob}(m \in U_{or}|l_{\text{orm}})l_{\text{orm}}}. \tag{A6}
\]

The conditional probability in equation (A4) is updated for each unit every time a new distribution model is generated. The unit proportions (equation (A5)) and the termination frequency (equation (A6)) are then reevaluated. The loop of the iteration is terminated when the change in the probability

### Table B1. Statistics Associated With the Variance Within Each Level I Unit and Their Percent Contribution to Composite Variance

<table>
<thead>
<tr>
<th>Level I</th>
<th>SGr</th>
<th>SGr</th>
<th>SFI</th>
<th>Sm</th>
<th>Sw</th>
<th>SFn</th>
<th>SFm</th>
<th>P</th>
</tr>
</thead>
<tbody>
<tr>
<td>Proportion</td>
<td>0.05</td>
<td>0.04</td>
<td>0.02</td>
<td>0.31</td>
<td>0.02</td>
<td>0.22</td>
<td>0.29</td>
<td>0.05</td>
</tr>
<tr>
<td>Variance</td>
<td>1.12</td>
<td>1.02</td>
<td>0.74</td>
<td>0.39</td>
<td>0.17</td>
<td>0.36</td>
<td>0.34</td>
<td>0.48</td>
</tr>
<tr>
<td>Percent</td>
<td>6.14</td>
<td>4.97</td>
<td>1.89</td>
<td>14.87</td>
<td>0.46</td>
<td>9.65</td>
<td>12.05</td>
<td>2.81</td>
</tr>
</tbody>
</table>

### Table B2. Percent Contribution to Composite Variance Arising From Differences in the Mean Log Permeability Among Level I Units

<table>
<thead>
<tr>
<th>Level I</th>
<th>SGr</th>
<th>SGr</th>
<th>SFI</th>
<th>Sm</th>
<th>Sw</th>
<th>SFn</th>
<th>SFm</th>
<th>P</th>
</tr>
</thead>
<tbody>
<tr>
<td>Proportion</td>
<td>0.05</td>
<td>0.04</td>
<td>0.02</td>
<td>0.31</td>
<td>0.02</td>
<td>0.22</td>
<td>0.29</td>
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<td>14.87</td>
<td>0.46</td>
<td>9.65</td>
<td>12.05</td>
<td>2.81</td>
</tr>
</tbody>
</table>

### Appendix B: Decomposition of the Sample Variance of ln(k)

By using the expression for hierarchical variance from Ritzi et al. [2004] or Dai et al. [2004a, 2004b],

\[
\sigma_{ij}^2 = \sum_{\alpha} \sum_{\beta} \sum_{\gamma} \rho_{\alpha} \rho_{\beta} (\bar{m}_{or} - \bar{m}_{or})^2 + \frac{1}{2} \sum_{\alpha} \sum_{\beta} \sum_{\gamma} \rho_{\alpha} \rho_{\beta} (\bar{m}_{or} - \bar{m}_{or})^2 + \frac{1}{2} \sum_{\alpha} \sum_{\beta} (\bar{m}_{or} - \bar{m}_{or})^2 \tag{B1}
\]

we can decompose the composite sample variance of ln(k) and in doing so analyze the contribution arising within and across unit types defined at level I and level II. The first term on the right is the variance arising within each unit type (an \( \alpha \alpha \) term, analogous to the first term on the right-hand side of equation (2)). The second term is the variance arising from differences in the mean between different level I unit types occurring within the same level II unit type (an \( \alpha \chi \) term). The third term is the variance arising from differences in the mean between different level I units occurring in different level II unit types (a \( \chi \chi \) term). Taking each term on the right and dividing by \( \sigma_{ij}^2 \) gives the percent contribution of each term to the composite sample variance.

The proportions inferred from Bayes’ theorem are more representative of the volume fractions of the sedimentary units as compared to the observed proportions listed in Table 2. Therefore equation (B1) was used with the proportions inferred from Bayes’ theorem to recompute the composite variance. In doing so, the composite variance is computed to be 0.821.

The \( \alpha \alpha \) term in either the DT or the TT hierarchy is 0.434 or 52.8% of the composite variance. Table B1 lists the variance within each level I unit. Because of their larger proportions, Sm, SFn and SFm have relatively larger contributions to the composite variance.

Table B2 lists the percentage of variance arising from differences in the mean log permeability among level I units. The lower parts of the table are not written out because they are symmetrical to the upper parts. The sum (representing the sum of contributions from \( \alpha \chi \) and \( \chi \chi \) terms) is 47.2% of the composite variance. The elements in
Table B2 combine differently into $\alpha_X$ and $\chi_X$ terms when considering the DT or the TT hierarchies.

[61] In the DT hierarchy the $\alpha_X$ term is 0.146 or 17.7% of the composite variance. The $\chi_X$ term is 0.242 or 29.5% of the composite variance. Therefore both the $\alpha_X$ and $\chi_X$ terms have significant contributions to the composite variance in the DT hierarchy.

[62] In contrast, in the TT hierarchy only the $\chi_X$ term makes a significant contribution to the composite variance. The $\chi_X$ term is 0.384 or 46.8% of the composite variance. Note that over 20% of the composite variance arises from differences in the mean between SG and SF. The $\alpha_X$ term is only 0.0028 or 0.35% of the composite variance.

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References


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Figure 2. Map of the outcropping of the Skull Ridge Member of the Tesuque Formation divided into (a) left and (b) right sides, which join along the broken line (modified from Gaud et al. [2004], reprinted with permission of SEPM Society for Sedimentary Geology). Permeability measurement locations, $x_k$, are shown with stars (1748 locations among Figures 2a and 2b). Labels on photo insets are from field notes and are not referred to in this article.