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Geostatistical modelling on stream networks: developing valid covariance matrices based on hydrologic distance and stream flow

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SUMMARY

1. Geostatistical models based on Euclidean distance fail to represent the spatial configuration, connectivity, and directionality of sites in a stream network and may not be ecologically relevant for many chemical, physical and biological studies of freshwater streams. Functional distance measures, such as symmetric and asymmetric hydrologic distance, more accurately represent the transfer of organisms, material and energy through stream networks. However, calculating the hydrologic distances for a large study area remains challenging and substituting hydrologic distance for Euclidean distance may violate geostatistical modelling assumptions.
2. We provide a review of geostatistical modelling assumptions and discuss the statistical and ecological consequences of substituting hydrologic distance measures for Euclidean distance. We also describe a new family of autocovariance models that we developed for stream networks, which are based on hydrologic distance measures.
3. We describe the geographical information system (GIS) methodology used to generate spatial data necessary for geostatistical modelling in stream networks. We also provide an example that illustrates the methodology used to create a valid covariance matrix based on asymmetric hydrologic distance and weighted by discharge volume, which can be incorporated into common geostatistical models.
4. The methodology and tools described supply ecologically meaningful and statistically valid geostatistical models for stream networks. They also provide stream ecologists with the opportunity to develop their own functional measures of distance and connectivity, which will improve geostatistical models developed for stream networks in the future.
5. The GIS tools presented here are being made available in order to facilitate the application of valid geostatistical modelling in freshwater ecology.

Keywords: functional distance, geographical information system, geostatistical model, hydrologic distance, streams

Introduction

Stream data sets are notoriously sparse because data are costly and time consuming to physically collect (Olsen & Ivanovich, 1993; Herlihy *et al.*, 2000; USEPA, 2001). Many data sets contain single survey sites from spatially independent watersheds (USEPA, 2001), while others are limited to samples from a single linear feature, such as the mainstem of a stream network (Dent & Grimm, 1999). These samples

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provide valuable information about the ecological condition at distinct points, but may not provide all of the information necessary to investigate processes and interactions at a network or regional-scale.

Recently, researchers have recognised that some principle themes in landscape ecology, such as hierarchy theory, may also be relevant in freshwater ecology (Fausch *et al.*, 2002; Ward *et al.*, 2002; Wiens, 2002). This trend has sparked an exciting new set of research questions, which are related to multi-scale biological, ecological and physical processes, such as habitat utilisation by aquatic species (Kneib, 1994). It is difficult to recognise multi-scale patterns in a freshwater environment based on sparse site-scale data and it is prohibitively costly to collect a continuous regional sample throughout space. Therefore, we propose that geostatistical models be used to investigate spatial patterns in streams data and to make predictions throughout stream networks.

Geostatistical models are commonly used to quantify spatial patterns in the terrestrial environment, but have been applied less frequently to aquatic systems such as lakes (Altunkaynak, Ozger & Sen, 2003), estuaries (Little, Edwards & Porter, 1997; Rathbun, 1998), and streams (Kellum, 2002; Yuan, 2004). Freshwater ecologists might have found little utility in geostatistical models because they are typically based on Euclidean (also known as straight-line) distance. Euclidean distance may not be ecologically meaningful because it fails to represent the spatial configuration, connectivity, directionality and relative position of sites in a stream network. Therefore, it may not be a suitable distance measure for most chemical, physical and biological studies of freshwater streams (Olden, Jackson & Peres-Neto, 2001; Benda *et al.*, 2004; Ganio, Torgersen & Gresswell, 2005). Recently, freshwater ecologists have begun to explore spatial patterns in stream networks using hydrologic distance measures (Dent & Grimm, 1999; Gardner, Sullivan & Lembo, 2003; Legleiter *et al.*, 2003; Torgersen, Gresswell & Bateman, 2004; Ganio *et al.*, 2005). In addition, new geostatistical methodologies have recently been developed that rely on valid covariances based on directional hydrologic distance measures (Cressie *et al.*, 2006; Ver Hoef, Peterson & Theobald, 2006). This provides ecologists with a variety of distance measures to choose from and makes geostatistical modelling an ecologically relevant tool.

Our objective is to discuss and demonstrate methods used to create valid covariance matrices based on hydrologic distance measures. Geostatistical modelling assumptions are reviewed and the statistical consequences of substituting hydrologic distance measures for Euclidean distance will be explained. We also describe a methodology to generate a valid covariance matrix based on asymmetric hydrologic distance weighted by discharge volume.

Background

Distance measures for use in geostatistical models

Two types of distances are often used to represent physical and ecological processes in stream ecosystems: symmetric and asymmetric distance classes. These distances are used to model connected sites that have a quantifiable influence upon one another. Symmetric distance allows movement between sites in all directions (or both on a stream). Euclidean distance (Fig. 1a) is symmetric and all locations within a study area are connected. Hydrologic distance can be either symmetric or asymmetric and is simply the distance between two locations when movement is restricted to the stream network. Symmetric hydrologic distance is the shortest hydrologic distance between two sites when movement is not limited by flow direction (Fig. 1b). In other words, movement in both the upstream and downstream direction may take place. Thus, all sites located within a single stream network are connected. In contrast, asymmetric hydrologic distance requires that water flow from one location to another for two sites to be connected (Fig. 1c). Movement is restricted to either the upstream or the downstream direction and movement in both directions is not permitted. Models based on asymmetric hydrologic distance can be dramatically different from models based on Euclidean or symmetric hydrologic distance.

Additive measures that represent relative network position based on stream conditions, such as flow volume, Shreve's stream order, or watershed area, can be used to weight hydrologic distance measures to make them more ecologically representative. They should also represent an ecological relationship between sites to ensure that they are ecologically valid.

It seems reasonable to represent terrestrial processes using Euclidean distance because the terrestrial

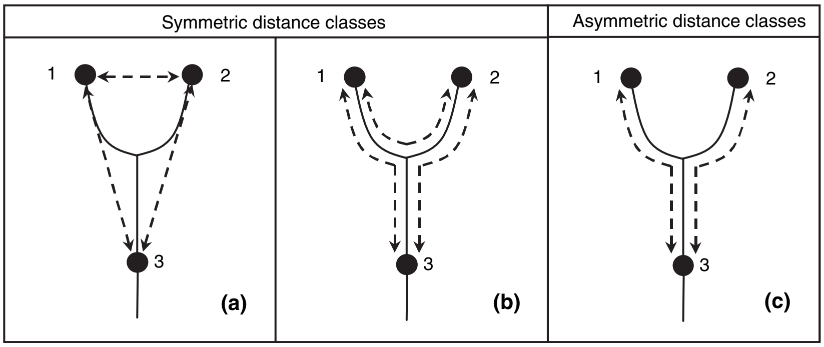


Fig. 1 Symmetric and asymmetric distance classes. The stream network is represented by a solid line, while distance measurements are represented with dotted lines. Symmetric hydrologic distance measures include Euclidean distance (a) and symmetric hydrologic distance (b). Sites 1, 2, and 3 are all neighbours to one another when these distance measures are used. Asymmetric distance classes include upstream and downstream asymmetric hydrologic distance (c). Sites 1 and 2 are neighbours to site 3, but not to each other.

landscape is commonly represented as a two-dimensional surface where any two sites may be connected. At times, it may also be appropriate to apply Euclidean distance to stream ecosystems. For example, an aquatic response variable may be significantly influenced by a continuous landscape variable, such as geology type (Kellum, 2002) or by broad-scale factors, such as acid precipitation (Driscoll *et al.*, 2001).

We recognise that freshwater systems have four dimensions: longitudinal (along the flow line), lateral (across the flow line), vertical (depth), and temporal (Ward, 1989), but we focus solely on the longitudinal dimension. In this case, a two-dimensional representation of distance may not always be appropriate as streams are represented as linear features and typically the movement of material is strongly influenced by unidirectional flow. For example, some fish move both up and downstream, but cannot move across the terrestrial landscape. Other materials, such as seeds or chemicals, are passive movers primarily affected by longitudinal transport. In these cases, movement is restricted to the network, but occurs primarily in the downstream direction.

The relative position in the network also affects the condition of a site (Pringle, 2001; Benda *et al.*, 2004) and reflects the influence that it will have on other sites (Cumming, 2002). For instance, a site located on a small tributary may have little influence on a downstream site located on the mainstem because of substantial differences in discharge volume (Benda *et al.*, 2004). Clearly, physical characteristics of the stream network provide a vast amount of information about conditions at unobserved sites and therefore, functional distances based on hydrology should also be considered.

Geostatistical modelling in stream networks

Linear statistical models traditionally have two components: the deterministic mean (also known as trend) and random errors, which are usually assumed to be normally distributed, homoscedastic (constant variance), and independent, so that a random error at one site is not influenced by that of another site. Streams data commonly violate the assumption of independence as stream networks are hierarchically structured, with nested watersheds, and stream segments that are connected by flow. Geostatistical models can be seen as a generalisation of traditional linear statistical models with a deterministic mean function; however, they relax the assumption of independence and allow spatial autocorrelation in the errors (Ver Hoef *et al.*, 2001). Local deviations from the mean are modelled using the covariance between nearby sites. The mean, variance and autocorrelation structure of the error term are assumed to be stationary or similar across a study area (Cressie, 1993).

The covariance represents the strength of spatial autocorrelation between two sites given their separation distance (h) (Olea, 1991). The separation distance is simply the distance travelled from one location to a second location and can be calculated using a variety of distance measures. The covariance is the joint variation of the values ($Y(s_i)$, $Y(s_j)$) at two locations (s_i, s_j) about their means ($\mu(s_i)$, $\mu(s_j)$) and provides a quantitative measure of the way sites co-vary in space.

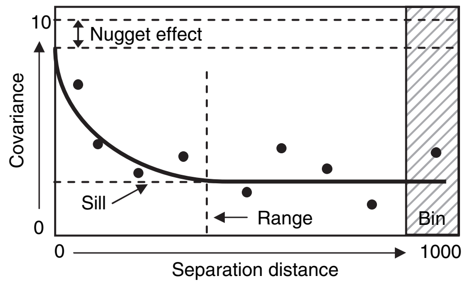


Fig. 2 Covariograms are generated by grouping the separation distances into bins, calculating a mean covariance for each bin, and plotting them in ascending order. Each mean covariance is represented by a single point. The covariogram is used to derive visual estimates of the nugget, range and sill.

The covariance of a spatial stochastic process $\{Y(s), s \in R\}$ at any two locations within a study area (R) is defined as:

$$C(s_i, s_j) = E\{[Y(s_i) - \mu(s_i)][Y(s_j) - \mu(s_j)]\}, \quad (1)$$

where $E(\cdot)$ represents the expectation (Bailey & Gatrell, 1995).

There are more covariances than data in (Eqn 1) because we cannot observe a response continually in space. Therefore, we make simplifying assumptions by using an autocovariance function, which typically has three parameters (θ), the nugget effect, sill and range. These must be estimated in order to fit the function to the empirical covariances (Fig. 2). The nugget effect represents the variation between sites as their separation distance approaches zero. It can result from experimental error or could indicate that a substantial amount of variation occurs at a scale finer than the sampling scale. The autocovariance asymptote is called the sill and it represents variance found among uncorrelated data. The range parameter describes how fast the autocovariance decays with distance. Some common methods that can be used to estimate the autocovariance parameters include maximum likelihood, restricted maximum likelihood (REML), weighted least-squares (Cressie, 1993), or Markov Chain Monte Carlo in a Bayesian framework (Handcock & Stein, 1993). The mathematical structure of the fitted autocovariance function provides a way to estimate the local deviation from the mean value at an unobserved site using observed values at nearby sites. Thus, geostatistical models are typically able to model more variability in the response variable and provide more accurate predictions at unobserved sites when spatial autocorrelation is present in the data (Isaaks & Srivastava, 1989).

In general, covariance matrices contain the covariance between each site and every other site. They have n rows and n columns, where n is the total number of sample sites. In geostatistics, these covariances are obtained from the fitted autocovariance function. Not all functions are valid because the covariance matrix must be symmetric, positive-definite, and all diagonal elements must be non-negative (Cressie, 1993). However, a review of methods used to examine these assumptions is beyond the scope of this manuscript. See Isaaks & Srivastava (1989) for a detailed discussion of positive-definite matrices and rules used to test them.

A few notable efforts have used symmetric hydrologic distance to explore spatial autocorrelation in stream networks. Their results indicate that patterns of spatial autocorrelation in biological (Torgersen *et al.*, 2004; Ganio *et al.*, 2005), chemical (Dent & Grimm, 1999; Gardner *et al.*, 2003), and physical (Legleiter *et al.*, 2003) streams data can be represented using symmetric hydrologic distance. However, the exponential model is the only known autocovariance function that is valid when making predictions at unobserved locations using covariance matrices based on symmetric hydrologic distance (Ver Hoef *et al.*, 2006). When symmetric hydrologic distance is substituted for Euclidean distance in other commonly used geostatistical autocovariance functions, the covariance matrix may contain negative eigenvalues, it may produce negative variance estimates, it is not guaranteed to be positive-definite, and therefore it is not valid. To our knowledge, there have been no valid predictions generated using geostatistical models solely based on symmetric hydrologic distance measures.

An asymmetric hydrologic distance measure may more accurately characterise passive movement in riverine systems because ecological and physical stream processes are strongly influenced by network configuration and flow direction (Olden *et al.*, 2001; Fagan, 2002). However, pure asymmetric distance measures (unweighted) do not produce symmetric covariance matrices, which are required for geostatistical modelling. Here we describe how to generate valid covariance matrices based on a weighted asymmetric hydrologic distance (WAHD). These should be ecologically interesting because they more accurately represent the connectivity and flow relationships in stream networks, and they provide a useful tool for geostatistical modelling in stream networks. Next, we develop spatial autocovariance models using moving average constructions based on asymmetric hydrologic distances that are both statistically and ecologically valid for stream networks (Cressie *et al.*, 2006; Ver Hoef *et al.*, 2006).

Autocovariance models using hydrologic distances

Stream processes and conditions are not necessarily random in an ecological sense because they result from ecologically complex interactions; however, we model our lack of knowledge about such processes with random variables. In that sense, a single stream sample is one realisation from a distribution of possible sample values, but that sample can have autocorrelation among its values. Our goal is to create autocorrelated models for stream networks. Barry & Ver Hoef (1996) show that a large class of autocovariance functions can be developed by creating random variables as the integration of a moving average function over white noise random process:

$$Z(s) = \int_{-\infty}^{\infty} g(x - s|\theta) W(x) \mathrm{d}x, \tag{2}$$

where $W(x)$ is the white noise random process and $g(x{-}s \mid \theta)$ is the moving average function. The moving average construction allows a valid autocovariance to be expressed as:

$$C(h|\theta) = \begin{cases} \int_{-\infty}^{\infty} [g(x|\theta)]^2 \mathrm{d}x + \theta_0 & \text{if } h = 0 \\ \int_{-\infty}^{\infty} g(x|\theta) g(x - h|\theta) \mathrm{d}x & \text{if } h > 0, \end{cases} \tag{3}$$

where θ_0 is the nugget effect and h is the separation distance. We also assume that the integral exists. This idea will now be developed for stream networks.

It is useful to establish a mathematical framework and notation before describing the moving average construction of a valid autocovariance model for stream networks. For our purposes, a stream segment is defined as a single line feature in a vector data set. A group of segments with a common stream outlet, or pour point, form a stream network. It is possible to measure the distance upstream of any segment from the stream outlet within a single network. We refer to this as the 'distance upstream.' The outlet's distance upstream to itself is zero. The stream segments within a network are indexed arbitrarily with $i = 1, 2, \ldots, m$. We denote each location as x_i, which is the distance upstream on the ith stream segment, to uniquely define each location. Similarly, we denote the most downstream location on the ith segment as l_i, and the most upstream location as u_i, where u_i is ∞ if there are no stream segments upstream of the ith segment. Stream segments within a network are connected and therefore, $l_i = u_j$ when the ith segment is directly upstream from the jth segment. Let the index set of stream segments upstream of x_i, excluding i, be U_{x_i}, and let B_{x_i, s_j} be the index set of segments *between* downstream location x_i and upstream location s_j, excluding the downstream segment but including the upstream segment. In a similar way, let $B_{x_i,[j]}$ be the index set between a downstream location and an upstream segment j (for more details, see Ver Hoef *et al.*, 2006).

For the unique conditions in a stream network, a moving average construction that is equivalent to Eqn 2 is used to create the random variable $Z(s_i)$ at stream location s_i:

$$\begin{aligned} Z(s_i) = &\int_{s_i}^{u_i} g(x_i - s_i|\theta) W(x_i) \mathrm{d}x_i \\ &+ \sum_{j \in U_{s_i}} \left(\prod_{k \in B_{s_i,[j]}} \sqrt{\omega_k} \right) \int_{l_j}^{u_j} g(x_j - s_i|\theta) W(x_j) \mathrm{d}x_j, \end{aligned} \tag{4}$$

where $g(x \mid \theta)$ is the moving average function that depends on parameters θ. It can be non-zero for positive values, but must be zero for all negative values. $W(x_i)$ is the white noise process on the ith stream segment and ω_k is a segment weight equal to the proportion that a stream segment contributes to the segment directly downstream. This general formulation is given by Ver Hoef *et al.* (2006). If weights on stream segments are a sum of the weights on the two segments directly above it, a special case of Eqn 4 is given by Cressie *et al.* (2006). Special care has been taken with the weights to ensure that all random variables have the same variance, however such a construction could allow for non-stationary variances.

An interpretation of Eqn 4 is that we construct the random variable segment by segment, starting with the ith segment and move upstream. However, as we go upstream, the moving average function must branch with each stream segment j. To keep a constant variance, the moving average function must be apportioned at each branch. The multiplication of weights (between 0 and 1) ensures that influence decreases as we move upstream, but we can also control which branches have more influence through the weights themselves.

We use the definition given in Eqn 4 to build valid autocovariance models for stream networks:

$$C(s_i, s_j|\theta) = \begin{cases} 0 & \text{locations are not flow connected,} \\ C_1(0) + \theta_0 & \text{if location 1 = location 2,} \\ \prod\limits_{k \in B_{s_i, s_j}} \sqrt{\omega_k} C_1(|s_i - s_j|) & \text{otherwise.} \end{cases} \tag{5}$$

and

$$C_1(h) = \int_{-\infty}^{\infty} g(x|\theta) g(x - h|\theta) \mathrm{d}x,$$

where s_i and s_j represent two spatial locations on the stream network and $|s_i–s_j|$ is the hydrologic distance between them. Once the asymmetric hydrologic distance data have been weighted appropriately, the exponential, linear with sill, spherical, or Mariah autocovariance functions (Ver Hoef *et al.*, 2006) can be fit to the empirical covariances using one of the parameter estimation methods mentioned previously. Ver Hoef *et al.* (2006) used REML for several models, while Cressie *et al.* (2006), used weighted least squares for a spherical autocovariance. A valid covariance matrix produced using the moving average autocovariance functions can be used as input for a variety of kriging equations, such as simple, ordinary, or universal kriging (Cressie, 1993; Bailey & Gatrell, 1995).

Moving average autocovariance functions for stream networks are a new statistical development and therefore, few geostatistical models based on WAHD have been generated. Ver Hoef *et al.* (2006) developed the methodology for the WAHD models and provided an example using a spatially dense subset of sulphate (meq L^{-1}). Peterson *et al.* (2006) used a large data set to compare patterns of spatial autocorrelation in eight water chemistry variables: dissolved oxygen, sulphate, nitrate-nitrogen, temperature, dissolved organic carbon, pH, acid-neutralising capacity and conductivity, using three distance measures: Euclidean, symmetric hydrologic, and WAHD. Cressie *et al.* (2006) developed a geostatistical model for daily change in dissolved oxygen based on a mixture of covariances, which is exciting because it demonstrates how multiple patterns of spatial autocorrelation can be represented in one geostatistical model. For example, a broad-scale landscape process that is not constrained by watershed boundaries, such as the weathering of parent material or coarse climatic conditions, might produce a primary pattern of spatial autocorrelation that is better described using Euclidean distance. In contrast, an instream process, such as nutrient spiraling or fish movement, could produce a secondary pattern at a different scale that may be better described using a hydrologic distance measure.

GIS, hydrologic distances and spatial weights

The ability to generate covariance matrices based on a moving average construction makes it possible to create a variety of valid geostatistical models for stream networks, but calculating distances and spatial weights along stream networks remains challenging. A handful of geographical information system (GIS) tools have been developed to calculate hydrologic distance, including the National Hydrography Dataset (NHD) ARCVIEW Toolkit version 7.0 from the United States Geological Survey (USGS, 2004a) and ARC HYDRO Tools from the Environmental Systems Research Institute (ESRI, 2001). However, each of these tools has practical and theoretical limitations. The NHD ARCVIEW Toolkit allows the user to calculate the hydrologic distance between two sites based on flow direction, but does not provide a tool to calculate the spatial weights. The code is encrypted, which makes it impossible to automate the tool so that processing large data sets is difficult and time consuming. In addition, the toolkit is not compatible with ESRI ARCGIS version 8.0 (ESRI, 2002) and higher. The ARC HYDRO Tools can be used with more recent versions of ARCGIS, but cannot be used to calculate the hydrologic distance between sites or the spatial weights without extensive data preprocessing and programmatic modification. Other researchers have developed their own scripts, written in AVENUE, ARC MACRO Language, or VISUAL BASIC, to calculate the hydrologic distance between sample sites (Rathbun, 1998; Theobald, 2002; Dussault & Brochu, 2003; Gardner *et al.*, 2003; Torgersen *et al.*, 2004), but they were not designed to calculate the spatial weights for the stream network. We believe that some practical and accessible tools are needed to generate the hydrologic distance matrices and spatial weights matrices in a cost-efficient manner. Now we describe the methodology and tools in order to facilitate valid geostatistical modelling in freshwater riverine systems.

Methods

We detail how to calculate a valid covariance matrix based on asymmetric hydrologic distance and weighted by stream discharge. There are three steps: (i) data preprocessing, (ii) generating the hydrologic distance and spatial weights matrices, and (iii) creating a statistically valid covariance matrix. We also provide an example to illustrate these methods.

Preprocessing stream data

One challenge of working with GIS data is that sample sites collected within a stream are not always located directly on a stream segment, even though they should be. This is a common phenomenon that can result for a variety of reasons. Although GPS-based points are differentially corrected, they still have some error and do not always fall directly on a vertex or line segment representing a stream. Some stretches of river can move (e.g. meander) slightly from their mapped position. Streams are often represented on a map by lines and so samples collected on the banks of a large river may not fall directly on a line segment. When streams are represented at coarser scales the digital streams data sets may contain mapping errors and generalisations, such as the absence of small tributaries and the homogenisation of form. Regardless of the error source, the sample sites must fall exactly on a stream line. Our solution is to 'snap' the sites to the nearest stream segment and manually examine each site to ensure that it is located on the correct stream segment. However, a refinement might be to move the site to the nearest stream segment and automatically compare attributes, such as stream name or upstream watershed area, to ensure that it lies in the correct location (Mixon, 2002). In contrast, the NHD Reach Indexing Tool (USEPA, 2002) uses dynamic segmentation to relate features to NHD reaches without moving the feature or altering the reach.

Calculating hydrologic distance measures

We developed a program in VISUAL BASIC Applications for ARCGIS version 8.3 (ESRI, 2002) to locate the path between survey sites and to compute the hydrologic distance between geographical locations. The total distance traversed in the downstream direction is recorded in a distance table (Fig. 3b), which provides sufficient information to calculate symmetric and asymmetric hydrologic distance measures. Flow direction is retained by recording the downstream distance in both directions. For example, in Fig. 3a,b the downstream distance from site B to site C = 13 and the downstream distance from site C to site B = 15. The upstream distance between two sites is found by switching the direction of the path (e.g. upstream distance from B to C = 15 and upstream distance from C to B = 13). The symmetric hydrologic distance is calculated by summing the two downstream distances (e.g. B to C and C to B = 13 + 15 = 28). Asymmetric hydrologic distance is restricted to flow-connected sites, which are identified by comparing the downstream distances between sites. If the distance is greater than zero in one direction and equal to zero in the other, then the two sites are connected by flow (e.g. downstream distance A to B = 0 and downstream distance B to A = 28). They are not connected by flow if the downstream distance is equal to zero in both directions (e.g. D to A, D to B, D to C) or the downstream distance is greater than zero in both directions (e.g. B to C, C to B). The symmetric or asymmetric hydrologic distance measures are calculated and recorded in an $n \times n$ hydrologic distance matrix and output as a text file, which is compatible with most statistical software.

Calculating the spatial weights

The proportional influence (PI) is defined as the influence of an upstream location on a downstream location and is used to create a spatial weights matrix. It is based on discharge volume, which can be calculated using regression equations (Vogel, Wilson & Daly, 1999; USGS, 2004b) or process-based models such as the Soil and Water Assessment Tool (Neitsch *et al.*, 2002). We use watershed area as a surrogate for discharge, which appears to be a viable alternative as it is correlated to mean annual discharge in every region of the United States (Vogel *et al.*, 1999). We

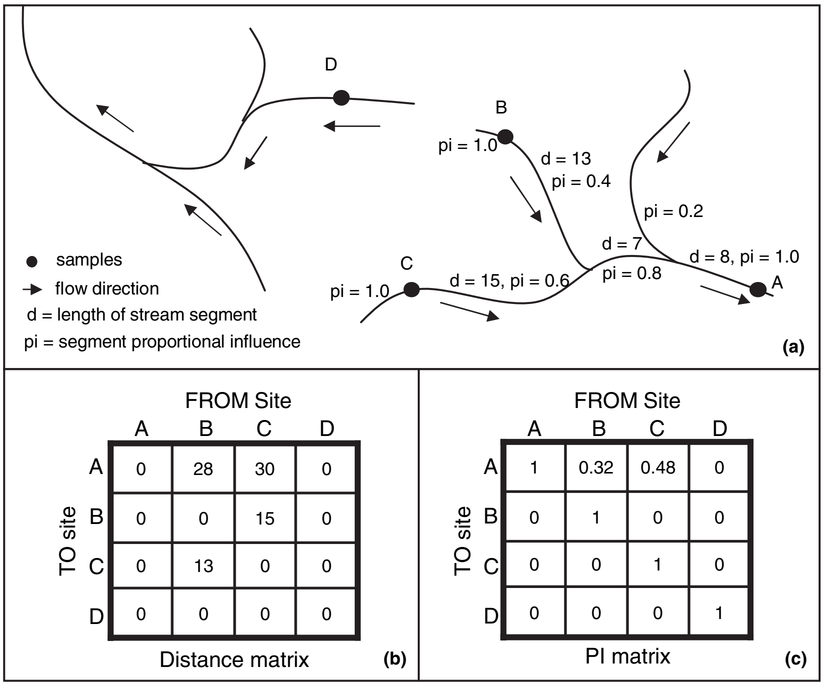
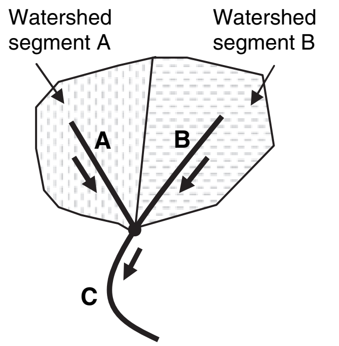


Fig. 3 The $n \times n$ hydrologic distance and proportional influence (PI) matrices represent the spatial connectivity and neighborhood relationships in a stream network (a). The hydrologic distance matrix (b) only contains the downstream distance between sites (B $\rightarrow$ C = 13; C $\rightarrow$ B = 15), but contains sufficient information to calculate a variety of hydrologic distance measures. The PI matrix (c) represents the proportion of water at a downstream site that comes from an upstream site. The PI for a pair of sites is equal to the product of the segment PIs found in the path between them (PI B $\rightarrow$ A = 0.4 $\times$ 0.8 $\times$ 1.0 = 0.32).

calculated the upstream watershed area for each stream segment in the network using a GIS. Again, a stream segment is defined as a single line feature in a vector data set. The area was stored as a segment attribute in the streams data set and represents the watershed area for the downstream node of the stream segment.

Calculating the PI of one sample site on another is a two-step process. First, the PI of each stream segment on the segment directly downstream must be calculated and recorded in the streams attribute table (Fig. 4). This was accomplished using a VBA program implemented in ARCGIS version 8.3 (ESRI, 2002). At each node in the network, the incoming segment(s) are identified. The total incoming area is calculated by summing the cumulative watershed area for the incoming stream segments. Then, the PI for each incoming segment is calculated by dividing its cumulative watershed area by the total incoming area. The PIs of the incoming segments always sum to one because they are proportions. When the program is complete, each segment in the streams data set has a PI value stored in its attribute table.

The second step is to use the segment PIs to calculate the PI for each pair of flow-connected sites (Fig. 3c). The PI for a pair of sites is equal to the product of the segment PIs found in the downstream path between them. The PI of a site to itself is equal to 1 and two sites that are not flow connected receive a PI value equal to zero. The site PI for each pair of sample sites in the data set are output as an $n \times n$ PI matrix.



$$\text{Segment PI of A} = \frac{\text{Watershed area A}}{\text{Watershed area A+B}}$$

Fig. 4 The segment proportional influence represents a segment's proportional influence on the segment directly downstream. It is calculated by dividing the segment's cumulative watershed area by the total incoming area at its downstream node.

Developing a valid covariance matrix based on hydrologic distance and flow

The asymmetric hydrologic distance and PI matrices must be reformatted before they can be used to create a statistically valid covariance matrix. A matrix, W, is computed by taking the square root of the PI matrix. A symmetric spatial weights matrix is created by taking $A = W + W'$. Then, the asymmetric hydrologic distance matrix, D, is forced into symmetry by computing the symmetric hydrologic distance between all flow-connected sites. Unconnected sites retain a distance or spatial weight equal to zero, while pairs of flow-connected sites are assigned an identical distance or spatial weight in both directions. This may seem counterintuitive because the matrices are intended to represent asymmetric flow relationships. Nevertheless, there is a symmetric correlation between flow-connected sites. Even though a downstream site does not affect upstream sites, the conditions at the downstream site are, in part, a result of those found upstream. This concept also applies to autoregressive models in time series, where the model is constructed with later time events depending on earlier ones. Although time flows in one direction, the correlation between two time events is symmetric. If we want to predict forward in one unit of time from a single observed event the prediction would be the same as if we went back one unit of time (Barnett, 2004). However, there is an added twist to stream networks because the positive spatial autocorrelation only includes flow-connected sites (Fig. 1c). This unique characteristic makes a model based on asymmetric hydrologic distance dramatically different from models based on Euclidean or symmetric hydrologic distance. Flow connectivity is preserved in the symmetric distance matrix, while the strength of the spatial autocorrelation between flow-connected sites is represented by the spatial weights and the hydrologic distance.

To our knowledge, the exponential autocovariance function is the *only* function that can be used to create a statistically valid covariance matrix based purely on symmetric hydrologic distance. However, the exponential, spherical, linear with sill, and Mariah moving average autocovariance functions (Ver Hoef *et al*., 2006) can be fit to the asymmetric hydrologic distance data (which has been forced into symmetry) because the spatial weights ensure its validity. Practically, autocovariance parameters are estimated from data in order to generate a covariance matrix, V, from an autocovariance function, $\rho(h)$. The distance (h) may be scaled by the range parameter (θ_2), $\rho(h)$ can be multiplied by the partial sill (θ_1), and the nugget effect (θ_0) added when the distance is greater than zero (Eqn 6). We recorded a distance equal to zero when two sites were not flow-connected, but a true distance of zero only occurs on the diagonal of the distance matrix when we measure the distance between a site and itself. We use the distance matrix D to compute a matrix V, where each element of V uses the hydrologic distance between each pair of locations, h (from D), in

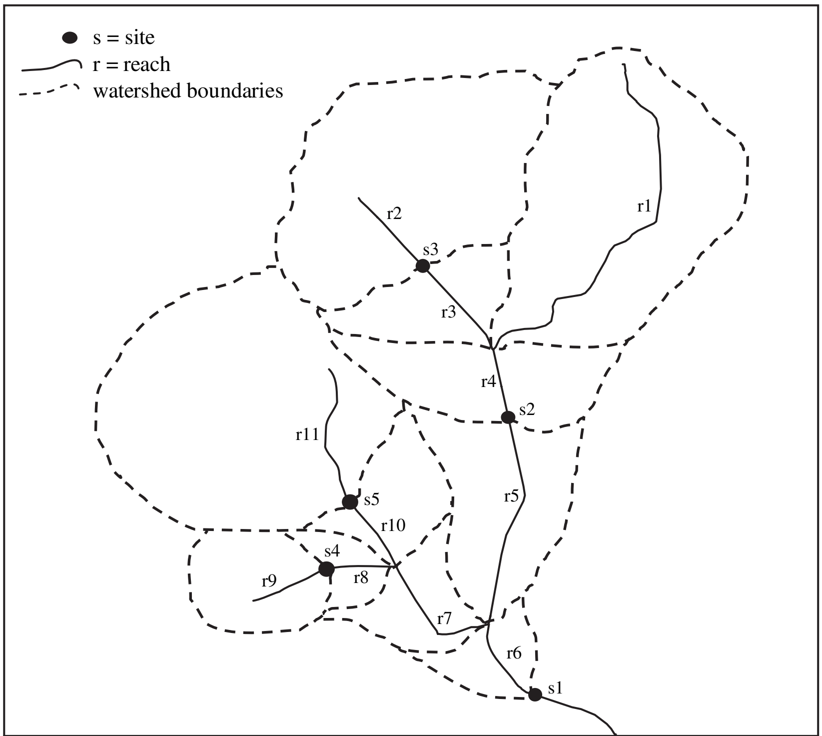
$$C_1(h|\theta) = \begin{cases} \theta_0 + \theta_1 & \text{if } h = 0 \\ \theta_1 \rho(h/\theta_2) & \text{if } h > 0 \end{cases} \qquad (6)$$

The Hadamard (element-wise) product, $\Sigma = A \odot V$, is applied to the two matrices and the product is a covariance matrix that meets the statistical assumptions necessary for geostatistical modelling (Cressie *et al*., 2006; Ver Hoef *et al*., 2006).

Logically, the next step would be to generate a geostatistical model based in part on a WAHD covariance matrix. However, we decided to limit our discussion here because the geostatistical modelling methods have been clearly described in the literature. For an overview of geostatistical modelling please see Isaaks & Srivastava (1989), Cressie (1993), or Bailey & Gatrell (1995). Cressie *et al.* (2006), Ver Hoef *et al.* (2006) and Peterson *et al.* (2006) described, in detail, the statistical methods that they used to generate geostatistical models based on WAHD covariance matrices. In addition, Peterson *et al.* (2006) discuss how alternative distance measures affect the way that spatial relationships are represented in a geostatistical model.

Example

We provide an example using data from a hypothetical basin to illustrate the methods used to calculate a valid covariance matrix based on WAHD. Fig. 5 contains information about a small stream network with five sample sites and 11 stream segments, which will be referred to throughout this example. The segment lengths and watershed areas were calculated using a GIS (Fig. 5). We generated a 5×5 asymmetric hydrologic distance matrix and forced it into symmetry by assigning the one-directional asymmetric distance to both upstream and downstream flow directions for sites s1–s5:



Segment	r1	r2	r3	r4	r5	r6	r7	r8	r9	r10	r11
Length (m)	1000	230	280	180	540	190	450	190	290	260	520
Watershed area (km^2)	275	220	265	600	708	1000	262	53	28	187	160
Segment PI	0.51	1.00	0.49	1.00	0.73	1.00	0.27	0.22	1.00	0.78	1.00

Fig. 5 The data derived from this small stream network with five sample sites (s1–s5) and 11 stream segments (r1–r11) was used to calculate a valid covariance matrix based on asymmetric hydrologic distance weighted by watershed area, which is used as a surrogate for discharge volume. The watershed boundaries are delineated for the downstream node of each stream segment. They are nested and so the cumulative watershed area includes the entire upstream drainage area. The length and true watershed area are recorded in the table above. The segment proportional influence values are computed using watershed area and are also recorded above.

$$\begin{pmatrix} 0 & 730 & 1190 & 830 & 900 \\ 730 & 0 & 460 & 0 & 0 \\ 1190 & 460 & 0 & 0 & 0 \\ 830 & 0 & 0 & 0 & 0 \\ 900 & 0 & 0 & 0 & 0 \end{pmatrix}. \tag{7}$$

The segment PI was calculated for each of the 11 stream segments based on the watershed areas in the network (Fig. 5). The PI for each pair of sites was computed and recorded in the PI matrix, which was also forced into symmetry:

$$\begin{pmatrix} 1 & 0.73 & 0.36 & 0.06 & 0.21 \\ 0.73 & 1 & 0.49 & 0 & 0 \\ 0.36 & 0.49 & 1 & 0 & 0 \\ 0.06 & 0 & 0 & 1 & 0 \\ 0.21 & 0 & 0 & 0 & 1 \end{pmatrix}. \tag{8}$$

Matrix V was generated using the exponential autocovariance function for the data (h) contained in the hydrologic distance matrix, D:

$$C(D;\theta_0,\theta_1,\theta_2) = \begin{cases} \theta_0 + \theta_1 & \text{if } h = 0, \\ \theta_1 \exp(-h/\theta_2) & \text{if } 0 < h. \end{cases} \tag{9}$$

The covariance parameters can be estimated using a variety of methods, which were mentioned previously, but we set the covariance parameters, $\theta_0 = 0.1$, $\theta_1 = 0.7$, $\theta_2 = 750$, to maintain the simplicity of the example.

We created matrix A by taking the square root of the PI matrix (Eqn 8) and then applied the Hadamard (element-wise) product to the two matrices, $\Sigma = A \odot V$, to obtain a valid covariance matrix:

$$\begin{pmatrix} 0.800 & 0.226 & 0.086 & 0.057 & 0.097 \\ 0.226 & 0.800 & 0.265 & 0 & 0 \\ 0.086 & 0.265 & 0.800 & 0 & 0 \\ 0.057 & 0 & 0 & 0.800 & 0 \\ 0.097 & 0 & 0 & 0 & 0.800 \end{pmatrix} \tag{10}$$

Discussion

The ability to efficiently calculate hydrologic distances and spatial weights provides the opportunity to create more ecologically meaningful distance measures for geostatistical modelling in stream networks. Until recently, Euclidean distance has been the primary distance measure used in geostatistical models. However, the physical characteristics of streams, such as network configuration, connectivity, flow direction, and position within the network, demand more functional, process-based measures. Stream ecologists will be able to choose models that are more appropriate for testing ecological hypotheses. In addition, different patterns of spatial autocorrelation may occur at coarse and fine scales, which could warrant modelling each pattern using a different distance measure.

Current models can be based on a variety of distance measures, but it may also be possible to create other more ecologically relevant distance measures that incorporate physical characteristics such as flow velocity, stream gradient, or physical structures that better reflect the energy an organism expends to move from one location to another. Network connectivity could also include chemical, physical and biological barriers, such as pH, waterfalls and predators, to make the potential movement of organisms and material more realistic. Given the complexity of stream ecosystems, there is unlikely to be one measure of distance and connectivity that is most appropriate for all situations. Instead, providing a variety of functional measures will facilitate exploration so that stream ecologists can select or develop a measure appropriate for their hypotheses.

As new functional distance measures are developed, it is imperative to be aware of the statistical assumptions on which geostatistical models are based. Stream ecologists and statisticians must ensure that geostatistical models for stream networks are both ecologically meaningful and statistically valid.

The tools and methodologies presented here provide an example of how to calculate the hydrologic distances and spatial weights needed for geostatistical modelling in stream networks. The tools described here have been further developed as an ESRI ARCGIS toolbox called the Functional Linkage of Watersheds and Streams (FLoWS) (Theobald *et al*., 2005) and have been made freely available to the public (http://www.nrel.colostate.edu/projects/starmap/).

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