

adjustment can be easily calculated by

$$(3) \quad n \cdot R = \frac{1}{4} \frac{\partial^3 f_2}{\partial \nu_1^3} \left/ \left(\frac{\partial f_2}{\partial \nu_1} \right)^2 \right. - \frac{1}{4} \frac{\partial^3 f_1}{\partial \nu_2^3} \left/ \left(\frac{\partial f_1}{\partial \nu_2} \right)^2 \right. - \frac{1}{2} \frac{\partial^3 f_1}{\partial \nu_1^2 \partial \nu_2} \left/ \left(\frac{\partial f_2}{\partial \nu_1} \frac{\partial f_1}{\partial \nu_2} \right) \right. \\ + \frac{1}{3} \left(\frac{\partial^2 f_1}{\partial \nu_2^2} \right)^2 \left/ \left(\frac{\partial f_1}{\partial \nu_2} \right)^3 \right. - \frac{5}{12} \left(\frac{\partial^2 f_2}{\partial \nu_1^2} \right)^2 \left/ \left(\frac{\partial f_2}{\partial \nu_1} \right)^3 \right. \\ + \frac{1}{2} \left(\frac{\partial^2 f_2}{\partial \nu_1^2} \frac{\partial^2 f_1}{\partial \nu_1 \partial \nu_2} \right) \left/ \left(\left(\frac{\partial f_2}{\partial \nu_1} \right)^2 \frac{\partial f_1}{\partial \nu_2} \right) \right. + \frac{1}{4} \left(\frac{\partial^2 f_1}{\partial \nu_1 \partial \nu_2} \right)^2 \left/ \left(\frac{\partial f_2}{\partial \nu_1} \left(\frac{\partial f_1}{\partial \nu_2} \right)^2 \right) \right.$$

The Bartlett adjustment is invariant under reparameterization and (3) can be used to calculate R for all parameter versions in the two-parameter exponential family.

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CROSS-VALIDATION AND VARIOGRAM ESTIMATION

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One of the methods used for the interpolation of spatially correlated data is known as kriging, which is a regression technique. Consider a model of the form $Z(x)$, a random function defined in p -dimensional space satisfying a weak stationarity condition as follows:

(i) $E[Z(x+h) - Z(x)] = 0$ for all x, h ;

(ii) $\gamma(h) = 0.5 \text{Var}\{Z(x+h) - Z(x)\}$ exists and depends only on h .

The objective is to estimate $Z(x_0)$ or Z_v where Z_v is a spatial average over a p -dimensional volume given by data $Z(x_1), \dots, Z(x_n)$. The estimator is a linear function of the data $\sum \beta_i(x_0)Z(x_i)$, the coefficients being determined by requiring that the estimator be unbiased and that the estimation error have minimum variance resulting in a linear system of equations:

$$\sum \beta_i(x_0)\gamma(x_i - x_j) + \mu(x_0) = \gamma(x_0 - x_j); \quad j = 1, \dots, n, \\ \sum \beta_i(x_0) = 1.$$

The minimized variance is computed from the variogram model, which, in turn, must be estimated and modeled from the data. In the case of the estimation of a spatial average the terms on the right-hand side are replaced by averages.

The system of equations and the estimator can be rewritten in an equivalent form

$$Z^*(x_0) = \sum b_i \gamma(x_0 - x_i) + a, \\ \sum b_i \gamma(x_i - x_j) + a = Z(x_j); \quad j = 1, \dots, n, \quad \sum b_i = 0,$$

in which it is seen that any function having the requisite positive-definiteness property will ensure invertibility of the coefficient matrix in the system and hence a unique solution for the coefficients in the estimator (for that variogram). The minimized variance is not a discriminator between model selections.

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Because distributional assumptions are generally lacking and because of the spatial correlation, the statistical behavior of various variogram estimators is not adequately known. It is not sufficient to estimate the values of the variogram (or in the case of the stronger assumption of second-order stationarity, the values of the (auto-) covariance function), rather it is necessary to select a valid model. Because the variogram estimation process is generally not adequate to relate the model to the data, it is common in geostatistics to use some form of validation and in particular cross-validation. While the smoothing spline is related to the kriging estimator, the purpose of cross-validation and the method are quite different when applied to kriging. The technique depends on the exactness property of the kriging estimator, i.e., the estimated value at data location is the observed value if that data value is utilized. Moreover, the weights in the kriging estimator (not the alternative form) do not depend on the data values rather only on the data location pattern and the spatial correlation function. Similarly the minimized variance does not depend on the data values and finally any valid variogram will result in a unique choice of the coefficients in the kriging estimator. By jackknifing the data one can obtain estimated and observed values for each data location. A number of statistics may be defined which characterize the fit of the variogram to the data independently of the variogram estimator. These include the following:

$$\begin{aligned} T_1 &= (1/n) \sum [Z(x_i) - Z^*(x_i)], & T_2 &= (1/n) \sum [Z(x_i) - Z^*(x_i)]^2, \\ T_3 &= (1/n) \sum \left\{ [Z(x_i) - Z^*(x_i)] / \sigma \right\}^2, & T_4 &= \text{Correl} \{ Z(x_i), Z^*(x_i) \}, \\ T_5 &= \text{Correl} \left\{ [Z(x_i) - Z^*(x_i)] / \sigma, Z^*(x_i) \right\}. \end{aligned}$$

It is easy to show that $E\{T_1\} = 0$, $E\{T_3\} = 1$, and although $E\{T_4\}$ and $E\{T_5\}$ depend on the values of the Lagrange multipliers they are "approximately" 1 and 0, respectively. These should not be viewed as test statistics in which one can test a hypothesis but rather for comparison between different choices for the variogram.

The ability of these statistics to discriminate between hypothesized variograms is related to the sensitivity and robustness of the solution vector for the kriging equations to changes in the variogram model. The changes can be quantified in at least two different ways: definition of a topology on the space of variograms (by defining a neighborhood system) or by changes in the values of the parameter(s) in a particular form of the variogram. At least three different neighborhood definitions have been considered, none of which is best possible. The robustness or continuity of the solution vector is also affected by the variogram model, the use of local (spatial) neighborhoods in the kriging step, and the degree of complexity permitted in the model. In some cases the geometry of the data location pattern is more important than all other factors. This property and the nonconsistency between cross-validation statistics is easily seen from numerical examples using an interactive software package such as GeoEAS available in the public domain for use on a PC compatible microcomputer.

The kriging estimator has been generalized to a multivariate form wherein the random function is vector-valued and the variogram is matrix-valued, i.e., the entries are variograms on the diagonal and cross-variograms off diagonal. In general the entries must be separately estimated but the cross-variograms must be modeled jointly with the associated variograms and they can only be cross-validated jointly with those variograms. Analogous cross-validation statistics can be defined using cokriging.

While the form of stationarity assumed in the model is weaker than that of second-order stationarity, it implicitly assumes that the mean is (spatially) constant. The kriging estimator has been extended to the case of a nonconstant mean and the same cross-validation statistics can be used.

Numerical results: using GeoEAS (EPA-Public domain) and the example data set supplied with the software. The variable is Cadmium with values at 60 points in 2-space.

1. The model consisted of a nugget of 4.5 and an anisotropic exponential model with a sill 13.5 and ranges of 300, 100. The search radius was 59.4, using a minimum of 1 point and

a maximum of 8 points:

$$T_1 = .312, \quad T_3 = 1.103, \quad T_4 = .442, \quad T_5 = .171.$$

2. All choices the same as in #1 except with ranges of 300, 300:

$$T_1 = .303, \quad T_3 = 1.318.$$

3. The model consisted of three components; a nugget 3.0, a spherical model with a sill of 5 and ranges of 100, 100 and a spherical model with a sill of 10 with ranges of 300, 300. The search radius was 59.4 using a minimum of 1 point and a maximum of 8 points:

$$T_1 = .258, \quad T_3 = 1.613, \quad T_4 = .501, \quad T_5 = .041.$$

4. Same as #3 except with a search radius of 150:

$$T_1 = .231, \quad T_3 = 1.618.$$

5. Same as #4 except using a maximum of 15 points instead of 8:

$$T_1 = .118, \quad T_3 = 1.573.$$

6. Same as #5 except using a search radius of 300:

$$T_1 = .118, \quad T_3 = 1.573, \quad T_4 = .541, \quad T_5 = .013.$$

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