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Universal cokriging of hydraulic heads accounting for boundary conditions

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SUMMARY

When contouring scalar potentials from point observations the process can often benefit from including the known effects of boundary curves with specified potential or gradient. Here we consider the hydraulic head in an aquifer and both no-flow and constant-head boundary conditions. We present a new approach to enforcing that equipotential contours be normal to no-flow boundaries. A constant-head boundary, with unknown head, can be included through the same process by rotating the boundary vector by 90°. Collocated observations of heads and boundaries can specify a constant-head boundary of known value. We estimate head given both head and boundary condition observations, cokriging with both types of information. Our new approach uses gradient vectors in contrast with previous approximate finite-difference methods that include boundary conditions in kriging. Either the approach given here or the finite-difference method must be implemented with smooth covariance models, e.g., Gaussian, generalized Cauchy, and Matérn.

Introduction

Kriging can be used to estimate hydraulic head between observation wells (e.g., on a grid) for the construction of 2D equipotential contour maps (Kitanidis, 1997). Although kriging is the best linear unbiased estimator, it does not include geologic or physical knowledge of the system (beyond structure embodied in the variogram), that a practitioner would likely use when contouring the same potentials by hand. We illustrate a method to include boundary condition information in the kriging of 2D potentials. These boundary conditions may include no-flow conditions along faults or hydrologic contacts, or constant head conditions.

Cokriging is the multi-variable extension to kriging, and was developed in mining to address the common problem of estimating an under-sampled variable (e.g., Chilés and Delfiner, 1999, Chapter 5). Often an allied variable is estimated more frequently than the variable of interest, and the correlation between the two is used to improve the quality of the final estimate (e.g., Chilés and Delfiner, 1999; Goovaerts, 1997; Isaaks and Srivastava, 1989; Kitanidis, 1997). Frequently the information contained in a second variable can be used to enhance estimates of the primary variable. The estimation of cross-covariance functions, which describe the spatial correlation between variables at different locations, is a hindrance to more widespread use of cokriging (Isaaks and Srivastava, 1989). Unless the dataset is exhaustive, cross-covariance models estimated solely from data are questionable.

Our approach derives the required cross-covariance functions from the mathematical relationship followed by a potential and its gradient. The benefits are twofold; first, only the direct covariance (or equivalent variogram) function need be estimated (as is done for single-variable kriging) and secondly, the cokriging now honors a portion of the underlying physical process (i.e., the spatial relationship between the potential and its gradient), which single-variable kriging cannot.

Pardo Igúzquiza and Chica Olmo (2004) and Brochu and Marcotte (2003) discuss covariance models which can be used to represent a function known to be second-order continuous, i.e., a potential governed by a second-order differential equation. The covariance model must be continuous at the origin (zero lag); most common covariance models do not satisfy this requirement (e.g., exponential and spherical), we will discuss three that do.

Chilés and Delfiner (1999, p. 319) introduced a finite-difference approximation to no-flow boundary condition information when kriging hydraulic heads, referring to an unpublished presentation by Delhomme from 1979. More recently Brochu and Marcotte (2003) give a finite-difference example in terms of a dual kriging formulation. We develop the cokriging equations using the true

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gradients of head and the cross-covariance models required from the covariance function used for heads. We compare and contrast this with the finite-difference approach.

True derivative approach

Cokriging is used to include boundary condition information when kriging potentials. Pardo Igúzquiza and Chica Olmo (2004, 2007) extended the related procedure of estimating the gradients using head data alone (Philip and Kitanidis, 1989), deriving the covariance and cross-covariance functions analytically from the Gaussian covariance which models the variability of head. The cokriging linear estimator, Z^*, is

$$Z^*(\mathbf{x}_0) = \sum_{\alpha=1}^{N} \lambda_\alpha Z(\mathbf{x}_\alpha) + \sum_{\beta=1}^{M} \delta_\beta [\hat{\nu}(\mathbf{x}_\beta) \cdot \nabla Z(\mathbf{x}_\beta)], \tag{1}$$

where $Z(\mathbf{x}_\alpha)$ is the potential observed at $\mathbf{x}_\alpha$ ($\mathbf{x}$ a 2D Cartesian coordinate), $\mathbf{x}_0$ is the location where the potential is to be estimated, λ_α and δ_β are cokriging weights, α and β are dummy variables, N and M are the number of head and boundary observations respectively, and $\hat{\nu}(\mathbf{x}_\beta)$ is a unit vector normal to the no-flow boundary (or tangent to a constant-head boundary), see Fig. 1. Using the shorthand notation $Z(\mathbf{x}_\alpha) = Z_\alpha$, we denote the directional derivative of Z_α, in the direction $\hat{\nu}$, as $(\hat{\nu} \cdot \nabla Z)_\alpha = Z_\alpha^{\hat{\nu}}$.

Kriging with a trend

The universal kriging drift is assumed to be polynomial in form, specified as

$$E[Z_0] = m(\mathbf{x}_0) = \sum_{\ell=0}^{L} \gamma_\ell f_0^\ell, \tag{2}$$

where E is the expectation operator, $m(\mathbf{x}_0)$ is the mean (a smooth function), γ_ℓ are free coefficients, L is the order of the polynomial approximation, and the monomial basis functions are $f^0 = 1,\ f^1 = x,\ f^2 = y,\ f^3 = x^2,\ f^4 = y^2,\ f^5 = xy$, etc. For $L = 0$, the universal kriging system simplifies to that of ordinary kriging (constant unknown mean). $L = 2$ corresponds to a linear trend, while $L = 5$ corresponds to a quadratic trend. Brochu and Marcotte (2003) indicate how other types of drift basis functions (e.g., the Thiem steady-state well solution) can be used in the contouring of hydraulic heads in special circumstances where additional information is known about the flow system.

Unbiasedness condition

The kriging weights λ_α and δ_α are sought to minimize the variance, while producing an unbiased solution. The unbiasedness condition is

$$E\left[Z_0^* - Z_0\right] = 0 \tag{3}$$

where Z_0 is the unknown true value at the desired estimation location. This can be expanded using (1) and (2) as

$$\begin{aligned} E[Z_0] &= \sum_\alpha \lambda_\alpha E[Z_\alpha] + \sum_\beta \delta_\beta E\left[Z_\beta^{\hat{\nu}}\right] \\ \sum_\ell \gamma_\ell f_0^\ell &= \sum_\ell \gamma_\ell \sum_\alpha \lambda_\alpha f_\alpha^\ell + \sum_\ell \gamma_\ell \sum_\beta \delta_\beta (\hat{\nu} \cdot \nabla f^\ell)_\beta \\ f_0^\ell &= \sum_\alpha \lambda_\alpha f_\alpha^\ell + \sum_\beta \delta_\beta (f^\ell)_\beta^{\hat{\nu}} \quad \ell = 0, \ldots, L \end{aligned} \tag{4}$$

where the $\hat{\nu}$ component of the gradient of the ℓth monomial drift term, $(f^\ell)_\beta^{\hat{\nu}}$, at location $\mathbf{x}_\beta$, can be computed explicitly. These gradients are $\nabla f_\beta^\ell = 0,\ \hat{\imath},\ \hat{\jmath},\ 2x\hat{\imath},\ 2y\hat{\jmath},\ y\hat{\imath} + x\hat{\jmath}$, for $\ell = 0, \ldots, 5$, where $\hat{\imath}$ and $\hat{\jmath}$ are the Cartesian unit vectors. These gradient vectors are projected onto $\hat{\nu}$. To ensure the expected value of the prediction is equal to the mean, $m(\mathbf{x})$, we enforce (4) while minimizing the estimation variance.

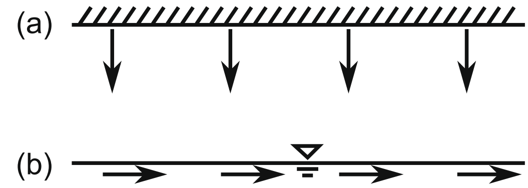

Fig. 1. No-flow (a) and constant head (b) boundary conditions, represented with boundary vectors (tail at point of application). Arrows offset from boundary for clarity.

Estimation variance

The variance of the estimation error R due to the linear estimator is

$$\mathrm{Var}[R] = E\{\left[Z_0^* - Z_0\right]^2\} \tag{5}$$

Following a procedure akin to that used to derive the standard kriging and cokriging equations (e.g., Goovaerts, 1997; Isaaks and Srivastava, 1989; Kitanidis, 1997), we substitute (1) and expand (5) as

$$\begin{aligned} \mathrm{Var}[R] = {} & \lambda_\alpha \lambda_\beta E[Z_\alpha Z_\beta] + \delta_\alpha \delta_\beta E\left[Z_\alpha^{\hat{\nu}} Z_\beta^{\hat{\nu}}\right] + E[Z_0 Z_0] + 2\lambda_\alpha \delta_\beta E\left[Z_\alpha Z_\beta^{\hat{\nu}}\right] \\ & - 2\lambda_\alpha E[Z_\alpha Z_0] - 2\delta_\alpha E\left[Z_0 Z_\alpha^{\hat{\nu}}\right] \end{aligned} \tag{6}$$

For brevity, Einstein summation convention is used; pairs of dummy subscripts within a product imply summation. The expected value of the product of random variables is their covariance, $C(h)$; here it is assumed the covariance is isotropic and only a function of the distance or lag h between the two points. For example, $E[Z_\alpha Z_\beta] = C(h_{\alpha\beta}) = \sigma_{\alpha\beta}$, where $\sigma_{\alpha\beta}$ is element (α, β) from the covariance matrix.

Parzen (1962, Section 3.3) illustrates how the expected value of the derivative of a stochastic process is the derivative of the expected value; the order of the E and ∇ operators can be switched, by assuming $m(\mathbf{x})$ is differentiable and the second derivative of the covariance exists. Doing so yields

$$\begin{aligned} \mathrm{Var}[R] = {} & \lambda_\alpha \lambda_\beta \sigma_{\alpha\beta} + \delta_\alpha \delta_\beta \sigma_{\alpha\beta}^{\hat{\nu}\hat{u}} + \sigma_{00}^2 + 2\lambda_\alpha \delta_\beta \sigma_{\alpha\beta}^{\hat{\nu}} - 2\lambda_\alpha \sigma_{\alpha 0} \\ & - 2\delta_\alpha \sigma_{0\alpha}^{\hat{u}} \end{aligned} \tag{7}$$

where $\sigma_{\alpha\beta}^{\hat{\nu}}$ and $\sigma_{\alpha\beta}^{\hat{\nu}\hat{u}}$ are the first and second directional derivatives of the covariance, respectively.

An objective function, Q, which incorporates both the minimization of the variance (7) and the unbiasedness condition (4), can be defined as (Chilés and Delfiner, 1999, p. 167)

$$Q = \mathrm{Var}[R] + 2\mu_\ell \left[\lambda_\alpha f_\alpha^\ell + \delta_\beta (f^\ell)_\beta^{\hat{\nu}} - f_0^\ell\right] \tag{8}$$

where $\mu_\ell : \ell = 0, \ldots, L$ are Lagrange multipliers.

Minimize variance of residual

To minimize Q, we take derivatives of (8) with respect to each weight and Lagrange multiplier (e.g., Chilés and Delfiner, 1999, Section 3.3.1)