

A Note on Programs Performing Kriging with Nonnegative Weights¹

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This note deals with the problem of solving kriging systems with nonnegative weights. Mathematically the question is considered as a case of quadratic programming. Hints concerning computational approaches and software are given.

KEY WORDS: Kriging under constraints, quadratic programming, software.

As is well known, kriging (point kriging) gives an optimal linear estimator of a phenomenon described by a regionalized variable in the sense of Matheron (cf. Journel and Huijbregts, 1978, p. 568ff): The data are considered as realization of a random process (under a stationary or intrinsic hypothesis). The value y_0 at a point x_0 is estimated by

$$y_0^* = \sum_{i=1}^n \lambda_i y_i, \quad \lambda_i \in \mathbb{R} \quad (1)$$

where y_i are measured values at points x_i in a suitable neighborhood of x_0 ($i = 1, \dots, n$). Weights λ_i are determined such that the estimation variance

$$\text{var}(y_0^* - y_0) \quad (2)$$

is minimal and the estimation is unbiased.

Note that, in the estimation, negative coefficients may occur. In some applications, however, the geologic setting of the problem requires an estimator involving only nonnegative weights.

Given nonnegative data y_i , nonnegativity of weights λ_i is a sufficient, but not a necessary, condition to gain nonnegative estimates [examples are found easily, in opposition to Limić and Mikelić (1984, p. 425)].

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For instance, in resource exploration, geologic layers should always have nonnegative thicknesses and hanging and foot walls must not cross each other.

If nonnegative weights are required, kriging has to be performed subject to the additional condition

$$\lambda_i \geq 0, \quad i = 1, \dots, n \quad (3)$$

This amounts to a problem that may be considered in the wider context of convex programming.

The function f in point kriging is denoted,

$$f(\lambda_1, \dots, \lambda_n) = \sum_{i,j=1}^n \lambda_i \lambda_j C(x_i - x_j) - 2 \sum_{i=1}^n \lambda_i C(x_i - x_0) + C(0) \quad (4)$$

where C is the covariance function.

Function f has to be minimized with respect to the unbiasedness condition

$$\sum_{i=1}^n \lambda_i - 1 = 0 \quad (5)$$

and nonnegativity conditions (3). (The use of a positive definite covariance model C or variogram γ and of pairwise different data points ensures that the matrix constructed by $[C(x_i - x_j)]_{i,j=1,\dots,n}$ is strictly positive definite (Journel and Huijbregts, 1978, p. 307-308), and, consequently, f is in fact a convex function.) Herzfeld (1988) provides the theoretical background.

In this form, software is available that does the major part of the optimization in nonnegative kriging; these procedures involve either modified simplex-type methods derived from the Kuhn-Tucker optimality conditions to solve the above problem of convex programming Eqs. (3)-(5) (e.g., Limić and Mikić 1984) or projection methods on active sets of constraints (Goldfarb and Idnani, 1983). The "active constraints" constitute the subset of constraints $\{\lambda_i \geq 0, i = 1, \dots, n\}$ characterized by the following property: If the active constraints are satisfied as exact data (i.e., $\lambda_i = 0$ for i in the active set), all other constraints are satisfied as well. As soon as the set of active constraints is known, the solution of kriging under constraints is equivalent to (usual) kriging relying on the original (exact) data plus the active constraints taken as exact data.

To avoid the computational effort of quadratic optimization, Barnes and Johnson (1984) use the latter property of the active set concept and develop a fast algorithm that first solves the ordinary point kriging system and then stepwise eliminates components with negative weights. Though it serves the most likely practical cases, however, it might yield a solution that is not consistent with the theoretical optimal one (Barnes and Johnson, 1984, p. 240).

Szidyrovsky et al. (1987) base their algorithm on the property of the active constraints mentioned above. They generate the power set (set of all subsets)

of the set of indices $\{1, \dots, n\}$ of the constraints, and carry the whole kriging procedure through for any member of the power set. This is a costly method (the power set has 2^n members). Their routine presented to cut down the effort consists mainly in counting and track keeping of previous calculations and does not attack the real problem. The kriging system need not be solved in all cases, so it should be worthwhile to compare the efficiency with that of a standard program of quadratic optimization that uses the active set concept. Such a routine solves the associated problem of convex programming and selects the set of active constraints; in our case, it gives a solution of the kriging system and takes care of the nonnegativity conditions (cf., Goldfarb and Idnani, 1983; Kostov and Dubrule, 1986; Limić and Mikelić, 1984).

A practicable routine for quadratic optimization with constraints can be found in most general-purpose software libraries (for example, the Harwell Subroutine Library (1985, Sect. VE), Kostov and Dubrule (1986) use the MINOS.5 optimization package). To extend a kriging program to one that allows additional constraints, such a routine has to be installed in the place where the matrix is inverted (kriging system solved); in standard kriging; everything else remains unchanged essentially.

REFERENCES

- Szidarovsky, F., Baafi, E. Y., and Kim, Y. C., 1987, Kriging Without Negative Weights: *Math. Geol.* v. 19, p. 549-559.
- Barnes, R. J., and Johnson, T. B., 1984, Positive Kriging: p. 231-240 in G. Verly (ed.), *Geostatistics for Natural Resources Characterization, Part 1: Reidel, Dordrecht, The Netherlands.*
- Kostov, C., and Dubrule, O., 1986, An Interpolation Method Taking into Account Inequality Constraints: II. Practical Approach: *Math. Geol.*, v. 18, p. 53-75.
- Goldfarb, D., and Idnani, A. 1983, A Numerically Stable Dual Method for Solving Strictly Convex Quadratic Programs: *Math. Program.*, v. 27, p. 1-33.
- Harwell Subroutine Library, 1985, A Catalogue of Subroutines: Harwell Laboratory, Oxfordshire, England.
- Herzfeld, U. C., 1988, A Method of Interval-Valued Kriging: *Sci. Terre, Série Inf.* (in press).
- Journel, A. G., and Huijbregts, C. J., 1978, *Mining Geostatistics*: Academic Press, London, 600 p.
- Limić, N., and Mikelić, A., 1984, Constrained Kriging Using Quadratic Programming: *Math. Geol.*, v. 16, p. 423-429.
- MINOS.5, Optimization package: Stanford University, Department of Operations Research, Stanford, California.