A Solution for Order Relation Problems in Multiple Indicator Kriging

다분적 지시크리깅에 있어서 순서문제에 관한 연구

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요 지

Sullivan(1984)에 의한 제안과 모든 경계값에서의 추정분산값의 합을 최소화하는 개념을 포함하는 동시에, 다분적 지시크리깅에 있어서의 순서문제를 해결하기 위한 방법이 모색되었다. 최적화 문제를 이용함으로써 해결방법이 개발되었는데, 이는 원래 지시크리깅을 위해 요구되는 계산보다 약간의 계산을 더 함으로써 가능하다. 따라서 제안된 방법은 현재 많이 사용되는 다른 임시방편적인 해결방법들 보다 계산상 효율적인 동시에, 수학적으로도 모순되지 않는 명확한 추계적 원리에 근거를 둔 방법이다.

Abstract

Embracing a suggestion by Sullivan(1984) and minimizing the sum of the estimation variances at all thresholds, a rigorous solution to order relation problems in multiple indicator kriging is formulated. By utilizing the particular structure of the resulting optimization problem, a solution algorithm is developed that requires little computational effort beyond the initial indicator kriging. Thus, this proposed solution is computationally efficient, mathematically consistent, and based upon an explicit statistical foundation－unlike many of the ad hoc solutions currently in use.

1. Introduction

Multiple indicator kriging(MIK) uses indicator data and provides estimates of spatial distributions without assuming any particular form of the underlying distribution (Sullivan, 1984 : Journel, 1983, 1984).

For multiple indicator kriging, in practice, a common variability interval($[\alpha, \beta]$) is discretized by NT increasing thresholds :

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$$z_k,\ k=1,2,\cdots,NT \text{ with } \alpha < z_1 \le z_2 \le \cdots \le z_{NT} < \beta \tag{1}$$

NT indicator kriging estimates are calculated by solving the corresponding NT linear indicator kriging systems and the posterior cumulative density function(cdf) can be approximated by the NT indicator kriging estimates. In other words, the result of multiple indicator kriging is a probability column $F(z \mid n$ known samples) and can be used as a model for the uncertainty about the unknown value for the volume V(Journel, 1986).

The application of multiple indicator kriging can be found in many papers(Carr et al., 1986 ; Knudsen et al., 1989, Johnson et al., 1989, Alli et al., 1990, etc.). In practice, however, inadmissible estimates may occur, these are called order relation problems(Solow, 1986, Limic et al., 1984, Journel, 1982, 1983, 1986, Isaaks and Srivastava, 1989, p.447−448 ; Sullivan, 1984, etc.).

Two conditions must be satisfied for a valid estimate. First, the estimated proportion below any threshold cannot be less than 0 or greater than 1. Second, the estimated proportion below one threshold cannot be greater than the estimated proportion below higher threshold. From these two conditions, the order relation constraints can be written as follows :

$$0 \le F(z_1) \le F(z_2) \le \cdots \le F(z_{NT}) \le 1 \tag{2}$$

where NT is the number of thresholds,

z_k, $k=1, 2, \cdots, NT$, is the k-th threshold value, and

$F(z_k)$ is the indicator kriging estimate at the k-th threshold.

One way of meeting the first constraint is to use weighted linear combinations of the indicator data in which all of the weights are non-negative. Forcing all weights to be non-negative is a sufficient, but not necessary, condition for ensuring that all kriged estimates are positive(Journel 1986). Also one way of satisfying the second constraint is to use only non-negative weights that sum up to 1, and to use the same weights for the estimation at all thresholds(Isaaks and Srivastava, 1989, pp.447−448).

When order relation problems occur, a very simple but inexpensive method to evaluate them is to smooth the indicator kriging estimates by rounding to the nearest admissible values(Solow, 1986).

Two feasible methods to cope with order relation problems in multiple indicator kriging were proposed by Sullivan(1984). One method is to combine simple kriging systems for all thresholds into one giant system and minimize the sum of estimation variances. The fundamental drawback of this method is that the system of equations would be very large, hence the solution would be computationally expensive. The second method is to use the results given by the indicator kriging algorithm and fit a distribution from the optimal indicator kriging solution. For example, minimizing the sum of the squared deviation from the indicator kriging solution can be used for a fitting criterion.

In this paper, an alternate method of solving the order relation problems in multiple indicator kriging is described and the details of a computationally efficient algorithm are presented. The method embraces Sullivan's idea(1984) of minimizing the sum of the estimation variances at all thresholds(the total variance), but does so with little additional effort beyond the standard indicator kriging. Furthermore, for this presentation, ordinary indicator kriging is used, but simple indicator kriging can also be used by applying the same method.

2. Problem formulation

The ordinary kriging estimate for a volume V using n neighboring samples can be obtained by minimizing the associated estimation variance subject to the global unbiasedness constraint(Isaaks and Srivastava, 1989, p.279~284) :

$$\hat{z} = \mathbf{z}^T \mathbf{w}$$

such that

$$\underset{\mathbf{w}}{\text{Minimize}}\ \sigma_E^2 = \sigma_V^2 + \mathbf{w}^T \mathbf{A} \mathbf{w} - 2\mathbf{b}^T \mathbf{w},$$

subject to $\mathbf{1}^T \mathbf{w} = 1,$

where $\hat{z}$ is the estimated value of volume V,

$\mathbf{z}$ is the (nx1) vector of measured values, the superscript "T" indicates a vector transpose,

$\mathbf{w}$ is the (nx1) vector of weights to be determined,

σ_E^2 is the estimation variance for volume V using the n samples,

σ_V^2 is the dispersion variance of the volume V,

$\mathbf{A}$ is the (nxn) matrix of sample-to-sample covariances,

$\mathbf{b}$ is the (nx1) vector of covariances between the n samples and the volume V, and

$\mathbf{1}$ is the (nx1) vector of ones.

As for the ordinary kriging estimate, NT ordinary IK estimates for a volume V using n neighboring samples can be obtained at NT different thresholds :

$$F(z_k) = \mathbf{i}^T(z_k)\mathbf{w}(z_k), \quad k = 1, 2, \cdots, NT, \tag{3}$$

such that

$$\underset{\mathbf{w}(z_k)}{\text{Minimize}}\ \sigma_E^2 = \sigma_V^2(z_k) + \mathbf{w}^T(z_k)\mathbf{A}(z_k)\mathbf{w}(z_k) - 2\mathbf{b}^T(z_k)\mathbf{w}(z_k)$$

subject to $\mathbf{1}^T\mathbf{w}(z_k) = 1,$

where NT is the number of thresholds,

z_k is the k-th threshold value,

$F(z_k)$ is the ordinary IK estimate of the volume V at threshold k,

$\mathbf{i}(z_k)$ is the (nx1) vector of known indicator data at threshold k,

$\mathbf{w}(z_k)$ is the (nx1) vector of unknown weights at threshold k.

$\sigma_E^2(z_k)$ is the estimation variance for the volume using the n samples at threshold k,

$\sigma_V^2(z_k)$ is the dispersion variance of the volume at threshold k,

$\mathbf{A}(z_k)$ is the (nxn) matrix of sample-to-sample covariances at threshold k,

$\mathbf{b}(z_k)$ is the (nx1) vector of covariances between the n samples and the volume at threshold k, and

$\mathbf{1}$ is the (nx1) vector of ones.

In general, however, indicator kriging estimates violate the order relation constraints (Equation 2) and hence the indicator kriging estimates can not be directly used as a posterior cumulative distribution $F(z \mid n$ known samples).

Consider an extension of the indicator kriging problem where, in addition to the global unbiasedness condition, the algorithm is further constrained to satisfy the order relation constraints(Equation 2) at all thresholds. The different thresholds are further coupled in the multiple indicator kriging objective function by minimizing the sum of the estimation variances for all thresholds. This extended problem can be formalized by the followings constrained optimization problem :

$$\underset{\mathbf{w}(z_1),\cdots,\mathbf{w}(z_k)}{\text{Minimize}} \quad \sum_{k=1}^{NT} \left[\sigma_V^2(z_k)+\mathbf{w}^T(z_k)\mathbf{A}(z_k)\mathbf{w}(z_k)-2\mathbf{b}^T(z_k)\mathbf{w}(z_k)\right], \tag{4a}$$

subject to

$$\begin{aligned} 0 &\le \mathbf{i}^T(z_1)\mathbf{w}(z_1), \\ \mathbf{i}^T(z_k)\mathbf{w}(z_k) &\le \mathbf{i}^T(z_{k+1})\mathbf{w}(z_{k+1}),\ k=1, 2, \cdots, NT-1, \\ \mathbf{i}^T(z_{NT})\mathbf{w}(z_{NT}) &\le 1, \text{ and} \\ \mathbf{1}^T\mathbf{w}(z_k) &= 1, \quad k=1, 2, \cdots, NT \end{aligned} \tag{4b}$$

Note that there are NT equality constraints and NT+1 inequality constraints in Equation 4b.

3. Problem solution

As in traditional optimization problems with constraints, the indicator kriging weights satisfying order relation constraints are uniquely determined by the Kuhn-Tucker conditions from classical optimization theory(e.g. Luenberger, 1973, p.233) :

$$\mathbf{A}(z_k)\mathbf{w}(z_k)+\mu_k\mathbf{1}-(\lambda_k-\lambda_{k+1})\mathbf{i}(z_k)=\mathbf{b}(z_k) \tag{5a}$$

$$\mathbf{1}^T\mathbf{w}(z_k)=1, \text{ and} \tag{5b}$$

$$\begin{gathered} \lambda_1[0-\mathbf{i}^T(z_1)\mathbf{w}(z_1)]=0 \\ \lambda_{k+1}[\mathbf{i}^T(z_k)\mathbf{w}(z_k)]-\mathbf{i}^T(z_{k+1})\mathbf{w}(z_{k+1})]=0,\ k=1, 2, \cdots, NT-1 \\ \lambda_{NT+1}[\mathbf{i}^T(z_{NT})\mathbf{w}(z_{NT})-1]=0, \text{ and} \\ 0\le\mathbf{i}^T(z_1)\mathbf{w}(z_1)\le\mathbf{i}^T(z_2)\mathbf{w}(z_2)\le \cdots \le \mathbf{i}^T(z_{NT})\mathbf{w}(z_{NT})\le 1 \end{gathered} \tag{5c}$$

where μ_k, $k=1, 2, \cdots, NT$, are NT Lagrange multipliers associated with the global unbiasedness constraints, and

λ_k, $k=1, 2, \cdots, NT+1$, are NT+1 Lagrange multipliers for inequality constraints

Equation 5c shows that the indicator kriging estimate at a threshold is bounded by the two indicator kriging estimates at two neighboring thresholds which can be considered as a lower and a upper bound : if k is 1, $0 \leq F(z_1) \leq F(z_2)$, if $2 \leq k \leq NT-1$, $F(z_{k-1}) \leq F(z_k) \leq F(z_{k+1})$, or if k is NT, $F(z_{NT-1}) \leq F(z_{NT}) \leq 1$. These two bounds, however, may have to be updated themselves to satisfy the associated neighboring local order relation constraints. If the ordinary IK estimates violate any local order relation constraint, therefore, it should be solved globally rather than locally, for example, when $F(z_k)$ is greater than $F(z_{k+1})$, simply making $F(z_k)$ be equal to $F(z_{k+1})$ is not always appropriate.

On the other hand, if the order relation constraints are satisfied globally, all of the λ's will be zero from Equation 5c and the ordinary IK estimates do not have to be updated. Thus, if the ordinary IK estimates satisfy the order relation constraints globally, they are also the optimal solutions for the extended problem.

By eliminating $w(z_k)$ in Equation 5a and Equation 5b, the following μ_k is obtained :

$$\mu_k = c_k(\lambda_k - \lambda_{k+1}) + d_k, \tag{6}$$

where $c_k = \mathbf{1}^T\mathbf{A}^{-1}(z_k)\mathbf{i}(z_k) / \mathbf{1}^T\mathbf{A}^{-1}(z_k)\mathbf{1}$, and

$d_k = [\mathbf{1}^T\mathbf{A}^{-1}(z_k)\mathbf{b}(z_k) - 1] / \mathbf{1}^T\mathbf{A}^{-1}(z_k)\mathbf{1}$, $k = 1, 2, \cdots, NT$.

Substituting Equation 5a and 5 into Equation 5c, the following system of equations is established :

$$\begin{aligned} +\xi_1\lambda_1 - \xi_1\lambda_2 &= 0 - F(z_1), \\ -\xi_k\lambda_k + (\xi_k + \xi_{k+1})\lambda_{k+1} - \xi_{k+1}\lambda_{k+2} &= F(z_k) - F(z_{k+1}),\ k = 1, 2, \cdots, NT-1 \\ -\xi_{NT}\lambda_{NT} + \xi_{NT+1}\,\lambda_{NT+1} &= F(z_{NT}) - 1, \end{aligned} \tag{7}$$

where $\xi_k = \mathbf{i}^T(z_k)\mathbf{A}^{-1}(z_k)\mathbf{i}(z_k) - [\mathbf{1}^T\mathbf{A}^{-1}(z_k)\mathbf{i}(z_k)]^2 / \mathbf{1}^T\mathbf{A}^{-1}(z_k)\mathbf{1}$, $i = 1, 2, \cdots, NT$,

$\lambda_1, \lambda_2, \cdots$, and λ_{NT+1} are (NT+1) Lagrange multipliers, and

$F(z_k)$, $k = 1, 2, \cdots, NT$, are ordinary IK estimates before considering order relation problems.

In a matrix form, Equation 7 becomes

$$\begin{bmatrix} \xi_1 & \xi_1 & 0 & 0 & 0 & 0 \\ -\xi_1 & (\xi_1+\xi_2) & -\xi_2 & 0 & 0 & 0 \\ 0 & -\xi_2 & (\xi_2+\xi_3) & -\xi_3 & \cdots & 0 \\ \vdots & \vdots & \cdots & \cdots & \cdots & \vdots \\ 0 & 0 & \cdots & -\xi_{NT-1} & (\xi_{NT-1}+\xi_{NT}) & -\xi_{NT} \\ 0 & 0 & \cdots & 0 & -\xi_{NT} & \xi_{NT} \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \vdots \\ \lambda_{NT} \\ \lambda_{NT+1} \end{bmatrix} \tag{8}$$

$$\begin{bmatrix} 0 - F(z_1) \\ F(z_1) - F(z_2) \\ F(z_2) - F(z_3) \end{bmatrix}$$

$$\left[\begin{array}{c} \vdots \\ F(z_{NT-1})-F(z_{NT}) \\ F(z_{NT})-1 \end{array}\right]$$

Note that the coefficient matrix in Equation 8 is a tridiagonal matrix. The system can be readily solved by several methods, such as a Gaussian elimination method or Gauss–Seidel iteration scheme. However, these methods are not the most efficient for tridiagonal systems of equations. Rather, the solution can be expressed very concisely and it requires but 3(NT+1) steps (e.g., Carnahan et al., 1969, p.441~442). In brief, the complete algorithm for the solution of the above tridiagonal system(Equation 8) is given by

$$\lambda_{NT+1}=\nu_{NT+1}, \tag{9a}$$

$$\lambda_k=\nu_k+\frac{\xi_k\lambda_{k+1}}{\beta_k},\ k=NT,\ NT-1,\ \cdots,1, \tag{9b}$$

where the β's and ν's are determined from the recursive formulas

$$\beta_1=\xi_1,\ \nu_1=-\frac{F(z_1)}{\beta_1}, \tag{10a}$$

$$\beta_k=(\xi_{k-1}+\xi_k)-\frac{\xi_{k-1}^2}{\beta_{k-1}},\ k=2,\ 3,\ \cdots,\ NT, \tag{10b}$$

$$\beta_{NT+1}=\xi_{NT}-\frac{\xi_{NT}^2}{\beta_{NT}}, \tag{10c}$$

$$\nu_k=\frac{F(z_{k-1})-F(z_k)+\xi_{k-1}\nu_{k-1}}{\beta_k},\ k=2,\ 3,\ \cdots,\ NT, \tag{10d}$$

$$\nu_{NT+1}=\frac{F(z_{NT})-1+\xi_{NT}\nu_{NT}}{\beta_{NT+1}}. \tag{10e}$$

The difficulty to solve the system of equations is that the unknown values of λ_1, λ_2, $\cdots$, λ_{NT+1} should be guaranteed to be zeros when the corresponding local order relation constraints are satisfied. In other words, if $F(z_k)$ is less than $F(z_{k+1})$ in Equation 8, the system of equations should be established in such a way that λ_{k+1} is ensured to be zero. From Equation 9a and 9b, both ν_k and $\xi_k\lambda_{k+1}/\beta_k$ should be zeros to ensure λ_k to be zero. From Equation 10a, 10d, and 10e, it can be seen that ν_k becomes zero when β_k becomes large. Also, $\xi_k\lambda_{k+1}/\beta_k$ becomes zero when β_k becomes large. Therefore, a system of (NT+1) linear equations can be established to ensure λ_k to be zero by setting β_k equal to an infinity.

Once λ_1, λ_2, $\cdots$, and λ_{NT+1} are obtained, new weights satisfying local order relation constraint, $w^*(z_k)$, $k=1,\ 2,\ \cdots,\ NT$, can be computed by using Equation 5a and Equation 6. Therefore, new multiple IK estimates satisfying local order relation constraint, $F^*(z_k)$, can be obtained as follows :

$$\begin{aligned} F^* &= \mathbf{i}^T(z_k)\mathbf{w}^*(z_k) \\ &= F(z_k)+(\lambda_k-\lambda_{k+1})\ \xi_k,\ k=1,\ 2,\ \cdots,\ NT, \end{aligned} \tag{11}$$

where $F(z_k) = i^T(z_k)w(z_k)$, $k=1, 2, \cdots, NT$.

For general order relation problems, however, multiple cycles of calculation(Equation 8 and Equation 11) might be required before the order relation constraints are globally satisfied. Note that once ξ_k, $k=1, 2, \cdots, NT$, are calculated, their values remain same during any cycle because they are the function of $\mathbf{A}(z_k)$ and $i(z_k)$ which are given by the configuration of samples. Therefore, only $F(z_k)$ are needed to be updated during each cycle.

The following pseudo-code, which is based on the algorithm for general tridiagonal systems of equations given by Press et al. (1989, p.40), can be used for solving order relation problems in ordinary IK. Note that the algorithm will fail when β equals zero. However, β is the function of ξ's which are non-zero values. The algorithm fails only when the coefficient matrix becomes singular : e.g., if the same threshold value is used more than once in IK, the coefficient matrix may become singular. In most cases, however, the coefficient matrix becomes non-singular.

<u>Algorithm for the order relation problems in ordinary IK</u>

do $k = 1$, the number of thresholds(NT)
    Calculate ordinary IK estimate, $F(z_k)$
    Calculate ξ_k
enddo
do while(any local order relation constraint is violated)
    if($0 \le F(z_1)$) then
        $\beta = \infty$
    else
        $\beta = \xi_1$
    endif
    $\lambda_1 = -F(z_1/\beta)$
    do $k = 2$, NT *Decomposition and forward substitution*
        $v_k = -\xi_{k-1}/\beta$
        if($F(z_{k-1}) \le F(z_k)$)then
            $\beta = \infty$
        else
            $\beta = (\xi_{k-1} + \xi_k) + \xi_{k-1} * v_k$
        endif
        if($\beta = 0$) pause *Algorithm fails*
        $\lambda_k = (F(z_{k-1}) - F(z_k) + \xi_{k-1} * \lambda_{k-1})/\beta$
    enddo

    $v_{NT+1} = -\xi_{NT}/\beta$
    if($F(z_{NT}) \le 1.0$))then
        $\beta = \infty$

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        else
              β = ξ_NT + ξ_NT * ν_NT+1
        endif
        if(β=0) pause                                   Algorithm fails
        λ_NT+1 = (F(z_NT) - 1.0 + ξ_NT * λ_NT) / β
        do k = NT, 1, -1                                Backward substitution
              λ_k = λ_k - ν_k+1 * λ_k+1
        enddo
        do k = 1, NT
              Update F(z_k) using Equation 11
        enddo
enddo
stop
end
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4. An Example

Consider that seven boreholes are available from a tunnel site of interest which is discretized into 25(5×5) grid points. These boreholes will be used to characterize the geologic conditions according to the RMR classification scheme (Bieniawski, 1984, p.112~120). Table 1 gives the measured RMR values and locations(x and y coordinates). In general RMR values fall between 0 and 100. For indicator kriging analysis, five equally spaced thresholds(TH1, TH2, TH3, TH4, and TH5) between 0 and 100 are used: the corresponding RMR values are 16.67, 33.33, 50.00, 66.67, and 83.33 respectively. The same spherical variogram model (sill 10, nugget 0, and range 500) was inferred from the available information for five thresholds.

The ordinary IK estimates before and after performing order relation correction are shown at several locations in Table 2. Note that values on the first and second row at each point are the ordinary IK estimates before and after solving the order relation problems respectively.

Table 1 Sample locations and RMR values.

x	y	RMR value
0+00	1+00	33.00
1+00	3+00	58.00
2+00	0+00	5.00
2+00	2+00	70.00
3+00	1+00	42.00
3+00	3+00	83.00
4+00	2+00	90.00

Table 2 Ordinary IK estimates before and after solving order relation problems.

x	y	indicator kriged values at each threshold				
		TH1	TH2	TH3	TH4	TH5
0+00	0+00	.30970	1.04203	.98175	.95806	.94504
		.30970	.98615	.98615	.98615	.98615
0+00	1+00	.00000	1.00000	1.00000	1.00000	1.00000
		.00000	1.00000	1.00000	1.00000	1.00000
0+00	3+00	.00045	.29205	.28560	1.03643	.94125
		.00045	.28938	.28938	.97566	.97566
1+00	1+00	.26715	.73089	.76266	.81168	1.04721
		.26715	.73089	.76266	.81168	1.00000
3+00	0+00	.52365	.50826	.99222	1.02457	.90473
		.51612	.51612	.96251	.96251	.96251
3+00	2+00	−0.3115	−0.5930	.21902	.18661	.74921
		.00000	.00000	.20521	.20521	.74921
4+00	0+00	.29551	.32039	.80687	.89494	.66877
		.29551	.32039	.76897	.76897	.76897

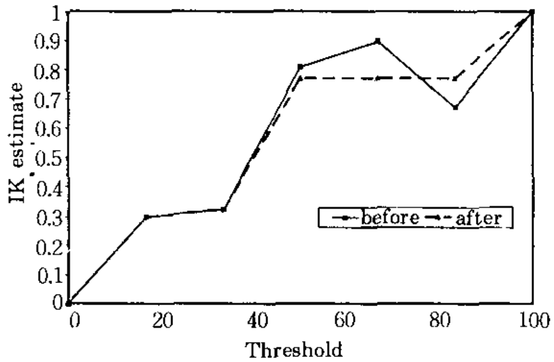

Figure 1 Cumulative density functions approximated by IK estimates before and after solving order relation problems.

Figure 1 shows the cumulative density functions approximated by IK estimates before and after solving order relation problems at location(4+00, 0+00).

5. Conclusions

By minimizing the total estimation variance (i.e., the sum of the estimation variances for all thresholds), a unique, defensible, solution for the order relation problem of multiple indicator kriging is proposed. If the standard multiple indicator kriging estimates satisfy all order relation constraints, they are also the optimal solution for the order relation problem. If the multiple indicator kriging estimates violate any order relation constraint, then the optimal solution can be obtained by establishing and solving a system of linear equations whose coefficient matrix is tridiagonal. If NT different thresholds are used, the size of the system to be solved is NT+1. The solution can be coded very concisely and it requires some 3(NT+1) steps(Carnahan et al., 1969, p.441~442). Also, a small number of iterations of calculation is enough to converge to the optimal global kriging estimates. This algorithm is, therefore, not an expensive one.

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