

Ordinary kriging in terms of the covariance function

The model:

The model assumption is:

$$Z(s) = \mu + \delta(s)$$

where $\delta(s)$ is a zero mean stochastic term with variogram $2\gamma(\cdot)$.

The Kriging System

The predictor assumption is

$$\hat{Z}(s_0) = \sum_{i=1}^n w_i Z(s_i)$$

It is a weighted average of the sample values, and $\sum_{i=1}^n w_i = 1$ to ensure unbiasedness. The w_i 's are the weights that will be estimated.

Kriging minimizes the mean squared error of prediction

$$\min \sigma_e^2 = E[(Z(s_0) - \hat{Z}(s_0))^2]$$

or

$$\min \sigma_e^2 = E \left[\left(Z(s_0) - \sum_{i=1}^n w_i Z(s_i) \right)^2 \right]$$

For second order stationary process the last equation can be written as:

$$\sigma_e^2 = C(0) - 2 \sum_{i=1}^n w_i C(s_0, s_i) + \sum_{i=1}^n \sum_{j=1}^n w_i w_j C(s_i, s_j) \quad (1)$$

See next page for the proof:

Let's examine $(Z(s_0) - \sum_{i=1}^n w_i Z(s_i))^2$:

$$\begin{aligned} \left(z(s_0) - \sum_{i=1}^n w_i z(s_i) + \mu - \mu \right)^2 &= \\ \left\{ [z(s_0) - \mu] - \sum_{i=1}^n w_i [z(s_i) - \mu] \right\}^2 &= \\ [z(s_0) - \mu]^2 - 2 \sum_{i=1}^n w_i [z(s_i) - \mu][z(s_0) - \mu] + \sum_{i=1}^n \sum_{j=1}^n w_i w_j [z(s_i) - \mu][z(s_j) - \mu]. \end{aligned}$$

If we take expectations on the last expression we have

$$E[z(s_0) - \mu]^2 - 2 \sum_{i=1}^n w_i E[z(s_i) - \mu][z(s_0) - \mu] + \sum_{i=1}^n \sum_{j=1}^n w_i w_j E[z(s_i) - \mu][z(s_j) - \mu]$$

The expectations above are the covariances:

$$C(0) - 2 \sum_{i=1}^n w_i C(s_0, s_i) + \sum_{i=1}^n \sum_{j=1}^n w_i w_j C(s_i, s_j)$$

Therefore kriging minimizes

$$\begin{aligned} \sigma_e^2 &= E[(Z(s_0) - \sum_{i=1}^n w_i Z(s_i))]^2 = \\ C(0) - 2 \sum_{i=1}^n w_i C(s_0, s_i) + \sum_{i=1}^n \sum_{j=1}^n w_i w_j C(s_i, s_j) & \\ \text{subject to} & \\ \sum_{i=1}^n w_i &= 1 \end{aligned}$$

The minimization is carried out over (w_1, w_2, \dots, w_n) , subject to the constraint $\sum_{i=1}^n w_i = 1$. Therefore the minimization problem can be written as:

$$\min C(0) - 2 \sum_{i=1}^n w_i C(s_0, s_i) + \sum_{i=1}^n \sum_{j=1}^n w_i w_j C(s_i, s_j) - 2\lambda \left(\sum_{i=1}^n w_i - 1 \right) \quad (2)$$

where λ is the Lagrange multiplier. After differentiating (2) with respect to w_1, w_2, \dots, w_n , and λ and set the derivatives equal to zero we find that

$$\begin{aligned} 2 \sum_{j=1}^n w_j C(s_i, s_j) - 2C(s_0, s_i) - 2\lambda &= 0, \quad i = 1, \dots, n \\ \sum_{j=1}^n w_j C(s_i, s_j) - C(s_0, s_i) - \lambda &= 0, \quad i = 1, \dots, n \end{aligned}$$

and

$$\sum_{i=1}^n w_i = 1$$

Using matrix notation the previous system of equations can be written as

$$\mathbf{C}\mathbf{W} = \mathbf{c}$$

Therefore the weights w_1, w_2, \dots, w_n and the Lagrange multiplier λ can be obtained by

$$\mathbf{W} = \mathbf{C}^{-1}\mathbf{c}$$

where

$$\mathbf{W} = (w_1, w_2, \dots, w_n, -\lambda)$$

$$\mathbf{c} = (C(s_0, s_1), C(s_0, s_2), \dots, C(s_0, s_n), 1)'$$

$$\mathbf{C} = \begin{cases} C(s_i, s_j), & i = 1, 2, \dots, n, \quad j = 1, 2, \dots, n, \\ 1, & i = n+1, \quad j = 1, \dots, n, \\ 1, & j = n+1, \quad i = 1, \dots, n, \\ 0, & i = n+1, \quad j = n+1. \end{cases}$$

The variance of the estimator:

So far, we found the weights and therefore we can compute the estimator: $\hat{Z}(s_0) = \sum_{i=1}^n w_i Z(s_i)$. How about the variance of the estimator, namely σ_e^2 ?

We multiply

$$\sum_{j=1}^n w_j C(s_i, s_j) - C(s_0, s_i) - \lambda = 0, \quad i = 1, \dots, n$$

by w_i and we sum over all $i = 1, \dots, n$ to get:

$$\sum_{i=1}^n \sum_{j=1}^n w_i w_j C(s_i, s_j) - \sum_{i=1}^n w_i C(s_0, s_i) - \sum_{i=1}^n w_i \lambda = 0$$

Therefore,

$$\sum_{i=1}^n \sum_{j=1}^n w_i w_j C(s_i, s_j) = \sum_{i=1}^n w_i C(s_0, s_i) + \lambda$$

If we substitute this result into equation (1) we finally get:

$$\sigma_e^2 = C(0) - \sum_{i=1}^n w_i C(s_i, s_0) + \lambda \tag{3}$$

The kriging system in terms of covariance

$$\begin{pmatrix} C(s_1, s_1) & C(s_1, s_2) & C(s_1, s_3) & \dots & C(s_1, s_n) & 1 \\ C(s_2, s_1) & C(s_2, s_2) & C(s_2, s_3) & \dots & C(s_2, s_n) & 1 \\ \dots & \dots & \ddots & \dots & \dots & 1 \\ \vdots & \vdots & \vdots & \ddots & \dots & 1 \\ C(s_n, s_1) & C(s_n, s_2) & C(s_n, s_3) & \dots & C(s_n, s_n) & 1 \\ 1 & 1 & \dots & \dots & 1 & 0 \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \\ \vdots \\ \vdots \\ w_n \\ -\lambda \end{pmatrix} = \begin{pmatrix} C(s_0, s_1) \\ C(s_0, s_2) \\ \vdots \\ \vdots \\ C(s_0, s_n) \\ 1 \end{pmatrix}$$

Again we observe that the matrix \mathbf{C} must be positive definite and this ensured by a choice of a model covariance function.

Short code for ordinary kriging in terms of variogram:

```
a <- read.table("kriging_1.txt", header=TRUE)
b <- read.table("kriging_11.txt", header=TRUE)

x <- as.matrix(cbind(a$x, a$y))

x1 <- rep(rep(0,8),8)           #Initialize
dist <- matrix(x1,nrow=8,ncol=8) #the distance matrix

for (i in 1:8){
  for (j in 1:8){
    dist[i,j]=((x[i,1]-x[j,1])^2+(x[i,2]-x[j,2])^2)^.5
  }
}

c0 <- 0
c1 <- 10
alpha <- 3.33

x1 <- rep(rep(0,8),8)           #Initialize
G <- matrix(x1,nrow=8,ncol=8)   #the GAMMA matrix

for(i in 1:8){
  for (j in 1:8){
    G[i,j]=c1*(1-exp(-dist[i,j]/alpha))
    if(i==j){G[i,j]=0}
    if(i==8){G[i,j]=1}
    if(j==8){G[i,j]=1}
    if(i==8 & j==8) {G[i,j]=0}
  }
}

g <- rep(0,8)                   #Initialize
                                #the g vector

for(j in 1:8){
  g[j]=c1*(1-exp(-dist[8,j]/alpha))
  if(j == 8) {g[j]=1}
}

w <- solve(G) %*% g             #Obtain the weights and the Lagrange parameter

z_hat <- w[-8] %*% b$z          #Compute the estimate
var_z_hat <- t(w) %*% g         #Compute the variance of the estimate
```