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Statistics C173/C273 **Instructor: Nicolas Christou**

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

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

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

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

See next page for the proof:

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

$$\left(z(s_0) - \sum_{i=1}^n w_i z(s_i) + \mu - \mu\right)^2 =$$

$$\left\{[z(s_0) - \mu] - \sum_{i=1}^n w_i [z(s_i) - \mu]\right\}^2 =$$

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

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

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

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

subject to

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

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

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

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

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

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

and

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

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

$$\mathbf{CW} = \boldsymbol{c}$$

Therefore the weights $w_1, w_2, ..., w_n$ and the Lagrange multiplier λ can be obtained by

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

where

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

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

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

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

We multiply

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

by w_i and we sum over all $i = 1, \cdots, n$ 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

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

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

Ordinary kriging using the covariance function:

The same example as in the previous handout (ordinary kriging using variogram) is solved using the covariance function: $C(h) = 10e^{-\frac{h}{3.33}}$. Reminder: The corresponding semivariogram function was $\gamma(h) = 10(1 - e^{-\frac{h}{3.33}})$.

$$\boldsymbol{W} = \boldsymbol{C^{-1}c} = \begin{pmatrix} 10 & 5.103 & 0.435 & 0.199 & 0.489 & 0.259 & 0.048 & 1 \\ 5.103 & 10 & 0.362 & 0.202 & 0.905 & 0.489 & 0.061 & 1 \\ 0.435 & 0.362 & 10 & 2.902 & 0.199 & 0.111 & 0.362 & 1 \\ 0.199 & 0.202 & 2.902 & 10 & 0.244 & 0.152 & 1.222 & 1 \\ 0.489 & 0.905 & 0.199 & 0.244 & 10 & 5.103 & 0.224 & 1 \\ 0.259 & 0.489 & 0.111 & 0.152 & 5.103 & 10 & 0.193 & 1 \\ 0.048 & 0.061 & 0.362 & 1.222 & 0.224 & 0.193 & 10 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 & 1 & 0 \end{pmatrix}^{-1} \begin{pmatrix} 2.612 \\ 3.382 \\ 0.889 \\ 0.579 \\ 1.333 \\ 0.682 \\ 0.176 \\ 1 \end{pmatrix}.$$

The answer is:

$$\boldsymbol{W} = \begin{pmatrix} 0.174 \\ 0.317 \\ 0.129 \\ 0.086 \\ 0.151 \\ 0.057 \\ 0.086 \\ -0.906 \end{pmatrix} = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \\ w_5 \\ w_6 \\ w_7 \\ -\lambda \end{pmatrix}.$$

We observe that the weights are same as before when we used the variogram, and therefore

$$\hat{z}(s_0) = \sum_{i=1}^{n} w_i z(s_i) = 0.174(477) + \cdots + 0.086(783) = 592.59.$$

The Lagrange multiplier is now $\lambda = -0.907$. However the variance of the estimator is the same as before because:

$$\sigma_e^2 = C(0) - \sum_{i=1}^{n} w_i C(s_i - s_0) + \lambda = 8.96.$$

Short code for ordinary kriging in terms of covariance:

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

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
C <- matrix(x1,nrow=8,ncol=8)     #the C matrix

for(i in 1:8){
for (j in 1:8){
C[i,j]=c1*exp(-dist[i,j]/alpha)
                if(i==j){C[i,j]=c0+c1}
if(i==8){C[i,j]=1}
if(j==8){C[i,j]=1}
if(i==8 & j==8) {C[i,j]=0}
}
}

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

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

w <- solve(C) %*% c     #Obtain the weights and the Lagrange parameter

z_hat <- w[-8] %*% b$z         #Compute the estimate
var_z_hat <- c0+c1 - t(w) %*% c  #Compute the variance of the estimate
```

File `kriging_1.txt`: All the coordinates (observed data points plus the point to be predicted).

```
x  y
61 139
63 140
64 129
68 128
71 140
73 141
75 128
65 137
```

File `kriging_11.txt`: Observed data points and their coordinates.

```
x  y   z
61 139 477
63 140 696
64 129 227
68 128 646
71 140 606
73 141 791
75 128 783
```