Problem class sheet 2

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Exercise 1. Let $(Z_s)_{s \in \mathcal{S}}$ be a specified statistical model. Assume that $(Z_s)_{s \in \mathcal{S}}$ is weakly stationary with unknown constant mean $\mu = \mathrm{E}(Z(s))$ and known covariogram $c(\cdot)$. Assume there is available a dataset $\{(s_i, Z_i := Z(s_i))\}_{i=1}^{n}$ and assume they are realizations of $(Z_s)_{s \in \mathcal{S}}$. Assume that the matrix C such as $[C]_{i,j} = c(\|s_i - s_j\|)$ has an inverse. Consider the "Kriging" estimator μ_{KM} of μ as the BLUE (Best Linear Unbiased Estimator)

$$\mu_{\mathrm{KM}} = \sum_{i=1}^{n} w_i Z(s_i) = w^{\top} Z,$$

for some unknown $\{w_i\}$ that we need to learn.

(1) Find sufficient conditions on $w = (w_1, ..., w_n)$ so that the Kriging estimator μ_{KM} to be unbiased.

(2) Assume C is invertable. Compute the MSE of μ_{KM} as a function of $w = (w_1, ..., w_n)$ and C

(3) Derive the Kriging estimator μ_{KM} of μ as a function of C

(4) Derive the Kriging standard error as $\sigma_{\mathrm{KM}} = \sqrt{\mathrm{E}(\mu_{\mathrm{KM}} - \mu)^2}$ as a function of C

Solution 2. The method is called Kriging the Mean, and hence we denote it as KM.

(1) It is

$$\mu_{\mathrm{KM}} = \sum_{i=1}^{n} w_i Z(s_i) = w^{\top} Z,$$

where $\{w_i\}$ is a set of unknown weights to be learned.

We assume that assume zero systematic error (unbiasness), hence

$$\mathrm{E}(\mu_{\mathrm{KM}} - \mu) = \mathrm{E}\left(\sum_{i=1}^{n} w_i Z(s_i) - \mu\right) = \sum_{i=1}^{n} w_i \underbrace{\mathrm{E}(Z(s_i))}_{= \mu} - \mu$$

which is satisfied given the assumption

$$\sum_{i=1}^{n} w_i = 1 \iff 1^{\top} w = 1 \quad \text{(ASSUMPTION)}$$

(2) It is

$$E \left(\mu_{\text{KM}} - \mu \right)^2 = E \left(\mu_{\text{KM}}^2 + \mu^2 - 2\mu_{\text{KM}}\mu \right) = \sum_{i=1}^{n} \sum_{j=1}^{n} w_i w_j E \left(Z \left(s_i \right) Z \left(s_j \right) \right) - \sum_{i=1}^{n} \overset{=1}{\cancel{w_i}} \sum_{j=1}^{n} \overset{=1}{\cancel{w_j \mu}}$$

$$= \sum_{i=1}^{n} \sum_{j=1}^{n} w_i w_j \left(c \left(s_i - s_j \right) - \mu \right) = \sum_{i=1}^{n} \sum_{j=1}^{n} w_i w_j c \left(s_i - s_j \right) = w^\top C w$$

(3) To learn the unknown weights $\{w_i\}$ we need to solve

$$w^{\text{KM}} = \arg\min_{w} E \left(\mu_{\text{KM}} - \mu \right)^2, \quad \text{subject to} \quad \sum_{i=1}^{n} w_i = 1$$

The Lagrange function is

$$\mathfrak{L} \left(w, \lambda \right) = \sum_{i=1}^{n} \sum_{j=1}^{n} w_i w_j c \left(s_i - s_j \right) - 2\lambda \left(\sum_{i=1}^{n} w_i - 1 \right)$$

$$= w^\top C w - 2\lambda \left(1^\top w - 1 \right)$$

The Kriging to mean equations are $0 = \nabla_{w,\lambda} \mathfrak{L} \left(w, \lambda \right)$ producing

$$\begin{cases} 0 = 2 \sum_{j=1}^{n} w_j^{\text{KM}} c \left(s_i - s_j \right) - 2\lambda & \forall i = 1, ..., n \\ 1 = \sum_{i=1}^{n} w_i^{\text{KM}} \end{cases}$$

$$\begin{cases} 2 C w^{\text{KM}} - 2\lambda 1 = 0 \\ 1^\top w^{\text{KM}} = 1 \end{cases}$$

Given that C^{-1} exists, I multiply by $1^\top C^{-1}$ and I get

$$2 1^\top \underbrace{C^{-1} C}_{= I} w - 2 1^\top C^{-1} \lambda 1 = 0$$

so

$$\lambda = \frac{1}{1^\top C^{-1} 1}$$

I substitute and I get

$$w^{\text{KM}} = \frac{C^{-1} 1}{1^\top C^{-1} 1}$$

So

$$\mu_{\text{KM}} = \left(\frac{C^{-1} 1}{1^\top C^{-1} 1} \right)^\top Z$$

(4) It is

$$\sigma_{\text{KM}} = \sqrt{E \left(\mu_{\text{KM}} - \mu \right)^2} = \sqrt{\left(\frac{C^{-1} 1}{1^\top C^{-1} 1} \right)^\top C \frac{C^{-1} 1}{1^\top C^{-1} 1}} = \frac{1}{\sqrt{1^\top C^{-1} 1}}$$

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Exercise 3. Let $(Z_s)_{s \in \mathcal{S}}$ be a specified statistical model. Assume that $(Z_s)_{s \in \mathcal{S}}$ is an intrinsic stationary process with unknown constant mean $\mu(s) = \mathrm{E}(Z(s))$ and known semi-variogram $\gamma(\cdot)$. Assume there is available a dataset $\{(s_i, Z_i := Z(s_i))\}_{i=1}^n$. Consider the "Kriging" estimator $Z_{\mathrm{OK}}(s_0)$ of $Z(s_0)$ at any unseen spatial location s_0 as the BLUE (Best Linear Unbiased Estimator)

$$Z_{\mathrm{OK}}(s_0) = w_{n+1} + \sum_{i=1}^n w_i Z(s_i) = w_{n+1} + w^\top Z$$

for some unknown $\{w_i\}$ that we need to learn, and $Z = (Z_1, ..., Z_n)^\top$. Let $w = (w_1, ..., w_n)^\top$.

    (1) Find sufficient conditions on $w = (w_1, ..., w_n)$ so that the Kriging estimator $Z_{\mathrm{OK}}(s_0)$ to be unbiased.

    (2) Derive the MSE of $Z_{\mathrm{OK}}(s_0)$ as

$$\mathrm{E}(Z_{\mathrm{OK}}(s_0) - Z(s_0))^2 = -w^\top \boldsymbol{\Gamma} w + 2 w^\top \boldsymbol{\gamma}_0$$

    where $\boldsymbol{\gamma}_0 = (\gamma(s_0 - s_i), ..., \gamma(s_0 - s_n))^\top$ and Γ with $[\boldsymbol{\Gamma}]_{i,j} = \gamma(s_i - s_j)$

    (3) Assume Γ is invertable matrix. Derive the Kriging estimator of $Z(s_0)$ as

$$Z_{\mathrm{OK}}(s_0) = \boldsymbol{\Gamma}^{-1}\left(\boldsymbol{\gamma}_0 + \frac{1 - 1^\top \boldsymbol{\Gamma}^{-1}\boldsymbol{\gamma}_0}{1^\top \boldsymbol{\Gamma}^{-1}1}1\right) Z$$

    (4) Derive the Kriging standard error of $Z_{\mathrm{OK}}(s_0)$ as

$$\sigma_{\mathrm{SK}} = \sqrt{\boldsymbol{\gamma}_0 \boldsymbol{\Gamma}^{-1} \boldsymbol{\gamma}_0 - \frac{\left(1 - 1^\top \boldsymbol{\Gamma}^{-1}\boldsymbol{\gamma}_0\right)^2}{1^\top \boldsymbol{\Gamma}^{-1}1}}$$

.

Solution. The method is called Ordinary Kriging, and hence we denote it as OK.

    (1) It is

$$Z_{\mathrm{OK}}(s_0) = w_{n+1} + \sum_{i=1}^n w_i Z(s_i) = w_{n+1} + w^\top Z,$$

    where $\{w_i\}$ is a set of unknown weights to be learned.

$$\mathrm{E}(Z_{\mathrm{OK}}(s_0)) = w_{n+1} + \sum_{i=1}^n w_i \mathrm{E}(Z(s_i)) \Leftrightarrow \mu = w_{n+1} + \mu \sum_{i=1}^n w_i$$

    Unbiasness is satisfied given the assumption $w_{n+1} = 0$, and

$$\sum_{i=1}^n w_i = 1 \Longleftrightarrow 1^\top w = 1 \quad \text{(ASSUMPTION)}$$

(2) The MSE of $Z_{\text{OK}}(s_0)$ is

$$\text{MSE}(Z_{\text{OK}}(s_0)) = \text{E}(Z_{\text{OK}}(s_0) - Z(s_0))^2 = \text{E}\left(\sum_{i=1}^{n} w_i Z(s_i) - \underbrace{\sum_{i=1}^{n} w_i}_{=1} Z(s_0)\right)^2$$

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

$$= -\text{E}\left(\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} w_i w_j (Z(s_i) - Z(s_j))^2 - 2\sum_{i=1}^{n}\frac{1}{2} w_i (Z(s_i) - Z(s_0))^2\right)$$

$$= -\sum_{i=1}^{n} w_i \sum_{j=1}^{n} w_j \frac{1}{2}\text{E}\left(Z(s_i) - Z(s_j)^2\right) + 2\sum_{i=1}^{n} w_i \frac{1}{2}\text{E}\left(Z(s_i) - Z(s_0)^2\right)$$

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

$$= -w^\top \mathbf{\Gamma} w + 2w^\top \boldsymbol{\gamma}_0$$

where $w = (w_1, ..., w_n)^\top$, $\boldsymbol{\gamma}_0 = (\gamma(s_0 - s_i), ..., \gamma(s_0 - s_n))^\top$, and $[\mathbf{\Gamma}]_{i,j} = \gamma(s_i - s_j)$.

(3) The Lagrange multiplier function to minimize the MSE under the assumption is

$$\mathfrak{L}(w, \lambda) = -\sum_{i=1}^{n} w_i w_j \gamma(s_i - s_j) + 2\sum_{i=1}^{n} w_i \gamma(s_0 - s_i) - \lambda\left(\sum_{i=1}^{n} w_i - 1\right)$$

$$= -w^\top \mathbf{\Gamma} w + 2w^\top \boldsymbol{\gamma}_0 - \lambda\left(1^\top w - 1\right)$$

The OK system of equations is $0 = \nabla_{(\{w_i\}, \lambda)} L(w, \lambda)\big|_{(w,\lambda)}$ producing

$$\begin{cases} 0 = -2\sum_{j=1}^{n} w_j^{\text{OK}} \gamma(s_i - s_j) + 2\gamma(s_0 - s_i) - \lambda, & i = 1, ..., n \\ 1 = \sum_{i=1}^{n} w_i^{\text{OK}} \end{cases} \iff$$

$$\begin{cases} 0 = -2\mathbf{\Gamma} w_{\text{OK}} + 2\boldsymbol{\gamma}_0 - \lambda_{\text{OK}} 1 \\ 1 = 1^\top w_{\text{OK}} \end{cases}$$

Assuming $\mathbf{\Gamma}$ is invertable and multiplying by $1^\top \mathbf{\Gamma}^{-1}$ it is

$$0 = -2\mathbf{\Gamma} w_{\text{OK}} + 2\boldsymbol{\gamma}_0 - \lambda_{\text{OK}} 1 \iff$$

$$0 = -2 1^\top \mathbf{\Gamma}^{-1} \overbrace{\mathbf{\Gamma} w_{\text{OK}}}^{=1} + 2 1^\top \mathbf{\Gamma}^{-1} \boldsymbol{\gamma}_0 - 1^\top \mathbf{\Gamma}^{-1} \lambda 1 \iff$$

$$\lambda_{\text{OK}} = 2\frac{1^\top \mathbf{\Gamma}^{-1} \boldsymbol{\gamma}_0 - 1}{1^\top \mathbf{\Gamma}^{-1} 1}$$

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By substitution I get

$$w_{\text{OK}} = \mathbf{\Gamma}^{-1}\left(\boldsymbol{\gamma}_0 + \frac{1 - 1^\top\mathbf{\Gamma}^{-1}\boldsymbol{\gamma}_0}{1^\top\mathbf{\Gamma}^{-1}1}1\right)$$

Hence

$$Z_{\text{OK}}(s_0) = w_{\text{OK}}Z = \mathbf{\Gamma}^{-1}\left(\boldsymbol{\gamma}_0 + \frac{1 - 1^\top\mathbf{\Gamma}^{-1}\boldsymbol{\gamma}_0}{1^\top\mathbf{\Gamma}^{-1}1}1\right)Z$$

(4) It is

$$\begin{aligned}
\sigma_{\text{OK}}(s_0) &= \sqrt{\text{MSE}(Z_{\text{OK}}(s_0))}\\
&= \sqrt{-w^\top\mathbf{\Gamma}w + w^\top\boldsymbol{\gamma}_0}\\
&= \sqrt{\boldsymbol{\gamma}_0\mathbf{\Gamma}^{-1}\boldsymbol{\gamma}_0 - \frac{\left(1 - 1^\top\mathbf{\Gamma}^{-1}\boldsymbol{\gamma}_0\right)^2}{1^\top\mathbf{\Gamma}^{-1}1}}
\end{aligned}$$

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Note regarding the calculations in MSE:

$$\left(\sum_{i=1}^{n} w_i \left(Z\left(s_i\right) - Z\left(s_0\right)\right)\right)^2 = \left(\sum_{i=1}^{n} w_i \left(Z_i - Z_0\right)\right)^2$$

$$= \sum_{i=1}^{n} w_i^2 \left(Z_i - Z_0\right)^2 + 2\sum_{1<i<j<n} w_i \left(Z_i - Z_0\right) w_j \left(Z_j - Z_0\right)$$

$$= \sum_{i=1}^{n}\sum_{j=1}^{n} w_i w_j \left(Z_i - Z_0\right)\left(Z_j - Z_0\right)$$

$$= 2\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} w_i w_j \left(Z_i - Z_0\right)\left(Z_j - Z_0\right)$$

$$- \frac{1}{2}\sum_{i=1}^{n} w_i \left(Z_i - Z_0\right)^2 - \frac{1}{2}\sum_{j=1}^{n} w_j \left(Z_j - Z_0\right)^2$$

$$+ 2\frac{1}{2}\sum_{i=1}^{n} w_i \left(Z_i - Z_0\right)^2$$

$$= -\frac{1}{2}\left(\sum_{i=1}^{n} w_i \sum_{j=1}^{n} w_j \left[\left(Z_i - Z_0\right)^2 + \left(Z_j - Z_0\right)^2 - 2w_i w_j \left(Z_i - Z_0\right)\left(Z_j - Z_0\right)\right]\right)$$

$$+ 2\frac{1}{2}\sum_{i=1}^{n} w_i \left(Z_i - Z_0\right)^2$$

$$= -\frac{1}{2}\left(\sum_{i=1}^{n} w_i \sum_{j=1}^{n} w_j \left[\left(Z_i - Z_0\right) - \left(Z_j - Z_0\right)\right]^2\right) + 2\frac{1}{2}\sum_{i=1}^{n} w_i \left(Z_i - Z_0\right)^2$$

$$= -\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} w_i w_j \left(Z_i - Z_j\right)^2 + 2\frac{1}{2}\sum_{i=1}^{n} w_i \left(Z_i - Z_0\right)^2$$

$$= -\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} w_i w_j \left(Z\left(s_i\right) - Z\left(s_j\right)\right)^2 + 2\frac{1}{2}\sum_{i=1}^{n} w_i \left(Z\left(s_i\right) - Z\left(s_0\right)\right)^2$$