Spatio-temporal statistics (MATH4341) Michaelmas term, 2023

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

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

which is satisfied given the assumption

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

(2) It is

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

$$
=\sum_{i=1}^{n}\sum_{j=1}^{n}w_iw_j\left(c\left(s_i-s_j\right)-\mu\right)=\sum_{i=1}^{n}\sum_{j=1}^{n}w_iw_jc\left(s_i-s_j\right)=w^{\top}Cw
$$

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

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

The Lagrange function is

$$
\begin{aligned}
\mathfrak{L}\left(w,\lambda\right)&=\sum_{i=1}^{n}\sum_{j=1}^{n}w_iw_jc\left(s_i-s_j\right)-2\lambda\left(\sum_{i=1}^{n}w_i-1\right)\\
&=w^{\top}Cw-2\lambda\left(1^{\top}w-1\right)
\end{aligned}
$$

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

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

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

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

$$
21^{\top}\cancelto{=I}{C^{-1}C}w-21^{\top}C^{-1}\lambda 1=0
$$

so

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

I substitute and I get

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

So

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

(4) It is

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

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

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

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

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

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

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

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

.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

By substitution I get

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

Hence

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

(4) It is

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

Note regarding the calculations in MSE:

$$
\begin{aligned}
\left(\sum_{i=1}^{n} w_i \left(Z\left(s_i\right)-Z\left(s_0\right)\right)\right)^2 &= \left(\sum_{i=1}^{n} w_i \left(Z_i - Z_0\right)\right)^2 \\
&= \sum_{i=1}^{n} w_i^2 \left(Z_i - Z_0\right)^2 + 2 \sum_{1<i<j<n} w_i \left(Z_i - Z_0\right) w_j \left(Z_j - Z_0\right) \\
&= \sum_{i=1}^{n} \sum_{j=1}^{n} w_i w_j \left(Z_i - Z_0\right)\left(Z_j - Z_0\right) \\
&= 2\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} w_i w_j \left(Z_i - Z_0\right)\left(Z_j - Z_0\right) \\
&\quad - \frac{1}{2} \sum_{i=1}^{n} w_i \left(Z_i - Z_0\right)^2 - \frac{1}{2} \sum_{j=1}^{n} w_j \left(Z_j - Z_0\right)^2 \\
&\quad + 2\frac{1}{2} \sum_{i=1}^{n} w_i \left(Z_i - Z_0\right)^2 \\
&= -\frac{1}{2} \left(\sum_{i=1}^{n} w_i \sum_{j=1}^{n} w_j \left[\left(Z_i - Z_0\right)^2 + \left(Z_j - Z_0\right)^2 - 2 w_i w_j \left(Z_i - Z_0\right)\left(Z_j - Z_0\right)\right]\right) \\
&\quad + 2\frac{1}{2} \sum_{i=1}^{n} w_i \left(Z_i - Z_0\right)^2 \\
&= -\frac{1}{2} \left(\sum_{i=1}^{n} w_i \sum_{j=1}^{n} w_j \left[\left(Z_i - Z_0\right) - \left(Z_j - Z_0\right)\right]^2\right) + 2\frac{1}{2} \sum_{i=1}^{n} w_i \left(Z_i - Z_0\right)^2 \\
&= -\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} w_i w_j \left(Z_i - Z_j\right)^2 + 2\frac{1}{2} \sum_{i=1}^{n} w_i \left(Z_i - Z_0\right)^2 \\
&= -\frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{n} w_i w_j \left(Z\left(s_i\right) - Z\left(s_j\right)\right)^2 + 2\frac{1}{2} \sum_{i=1}^{n} w_i \left(Z\left(s_i\right) - Z\left(s_0\right)\right)^2
\end{aligned}
$$
