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

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

(2) It is

$$
\begin{aligned}
\mathrm{E}\left(\mu_{\mathrm{KM}}-\mu\right)^2 = \mathrm{E}\left(\mu_{\mathrm{KM}}^2+\mu^2-2\mu_{\mathrm{KM}}\mu\right) &= \sum_{i=1}^{n}\sum_{j=1}^{n} w_i w_j \mathrm{E}\left(Z\left(s_i\right)Z\left(s_j\right)\right) - \overbrace{\cancel{\sum_{i=1}^{n} w_i}}^{=1}\overbrace{\cancel{\sum_{j=1}^{n} w_j}}^{=1}\mu \\
&= \sum_{i=1}^{n}\sum_{j=1}^{n} w_i w_j \left(c\left(s_i-s_j\right)-\mu\right) = \sum_{i=1}^{n}\sum_{j=1}^{n} w_i w_j c\left(s_i-s_j\right) = w^\top C w
\end{aligned}
$$

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

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

The Lagrange function is

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

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

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

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

$$\begin{aligned}\text{MSE}\left(Z_{\text{OK}}\left(s_0\right)\right) =& \text{E}\left(Z_{\text{OK}}\left(s_0\right)-Z\left(s_0\right)\right)^2 = \text{E}\left(\sum_{i=1}^{n} w_i Z\left(s_i\right) - \underbrace{\sum_{i=1}^{n} w_i}_{=1} Z\left(s_0\right)\right)^2 \\
&= \text{E}\left(\sum_{i=1}^{n} w_i\left(Z\left(s_i\right)-Z\left(s_0\right)\right)\right)^2 \\
=& - \text{E}\left(\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} w_i w_j\left(Z\left(s_i\right)-Z\left(s_j\right)\right)^2 - 2\sum_{i=1}^{n}\frac{1}{2} w_i\left(Z\left(s_i\right)-Z\left(s_0\right)\right)^2\right) \\
=& - \sum_{i=1}^{n} w_i \sum_{j=1}^{n} w_j \frac{1}{2}\text{E}\left(Z\left(s_i\right)-Z\left(s_j\right)^2\right) + 2\sum_{i=1}^{n} w_i \frac{1}{2}\text{E}\left(Z\left(s_i\right)-Z\left(s_0\right)^2\right) \\
=& - \sum_{i=1}^{n} w_i \sum_{j=1}^{n} w_j \gamma\left(s_i - s_j\right) + 2\sum_{i=1}^{n} w_i \gamma\left(s_i - s_0\right) \\
=& - w^\top \boldsymbol{\Gamma} w + 2 w^\top \boldsymbol{\gamma}_0\end{aligned}$$

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

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

$$\begin{aligned}\mathfrak{L}\left(w,\lambda\right) =& - \sum_{i=1}^{n} w_i w_j \gamma\left(s_i - s_j\right) + 2\sum_{i=1}^{n} w_i \gamma\left(s_0 - s_i\right) - \lambda\left(\sum_{i=1}^{n} w_i - 1\right) \\
=& - w^\top \boldsymbol{\Gamma} w + 2 w^\top \boldsymbol{\gamma}_0 - \lambda\left(1^\top w - 1\right)\end{aligned}$$

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

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

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

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

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

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

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

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:

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