

Homework 2: Geostatistics (Kriging and MLE inference)

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Exercise 1. (★) Consider we the geostatistical model $(Z_s)_{s \in \mathcal{S}}$ with

$$Z(s) = \mu(s) + w(s) + \varepsilon(s)$$

where $w(s)$ is a weakly stationary process with mean zero and covariogram $c_w(h; \sigma^2, \phi) = \sigma^2 \exp\left(-\frac{1}{\phi} \|h\|\right)$, $\mu(s; \beta)$ is a deterministic function

$$\mu(s; \beta) = \sum_{j=0}^p \psi_j(s) \beta_j = (\psi(s))^\top \beta$$

with unknown coefficients $\beta = (\beta_0, \dots, \beta_p)^\top$ and known basis functions $\psi(s) = (\psi_0(s), \dots, \psi_p(s))^\top$, $\varepsilon(s)$ is a nugget effect process whose covariogram has sill τ^2 , and assume that $w(s)$ and $\varepsilon(s)$ are independent Gaussian Processes.

- (1) Write down the formula of the covariogram $c(h; (\sigma^2, \phi, \tau))$ of (Z_s) .
- (2) Consider a re-parametrization $\theta = (\sigma^2, \phi, \xi)$ where $\xi^2 = \frac{\tau^2}{\sigma^2}$ is called signal to noise ratio. Assume there is available a dataset $\{(s_i, Z_i)\}_{i=1}^n$ where $Z_i := Z(s_i)$ is a realization of $(Z_s)_{s \in \mathcal{S}}$ at site s_i .
 - (a) Let Ψ be a matrix with $[\Psi]_{i,j} = \psi_j(s_i)$. Let D be a matrix such as $[D]_{i,j} = \|s_i - s_j\|$. Consider that you can use convenient notation such as $\exp(D)$ meaning $[\exp(D)]_{i,j} = \exp(D_{i,j})$. Write down the covariance matrix $C(\theta)$ of $Z = (Z_1, \dots, Z_n)^\top$ as a function of D and θ .
 - (b) Write down the log likelihood function $\log(L(Z; \theta))$ of $Z = (Z_1, \dots, Z_n)^\top$ given $\theta = (\sigma^2, \phi, \xi)$.
- (3) Let $r(\cdot)$ (called correlogram) such as $c(\cdot) = \sigma^2 r(\cdot)$. Assume that (ϕ, ξ) as known constants.
 - (a) Compute the likelihood equations¹ w.r.t. (β, σ^2) , and for given (ϕ, ξ) .
 - (b) Compute the MLE $\hat{\beta}_{(\phi, \xi)}$ of β as a function of (ϕ, ξ)
 - (c) Compute the MLE $\hat{\sigma}_{(\phi, \xi)}^2$ of σ^2 as a function of (ϕ, ξ) .
 - (d) Compute the unbiased estimator of $\tilde{\sigma}^2$ of σ^2 .

Hint: Consider the fitted values $e = (e_1, \dots, e_n)^\top$ as $e = [I - H]Z$ where $H = (\Psi^\top R^{-1} \Psi)^{-1} \Psi^\top R^{-1}$, and write $\hat{\sigma}_{(\phi, \xi)}^2$ w.r.t. e .

Hint: It is given that $E(Z^\top A Z) = E(Z)^\top A E(Z) + \text{tr}(A \text{Var}(Z))$ when $Z \sim \text{Normal}$

¹that is, the gradient of the log-likelihood

(4) Compute the so-called log “profiled likelihood” $\log (L (Z; (\phi, \xi)))$ resulting as

$$L (Z; (\phi, \xi)) = L \left(Z; \beta = \hat{\beta}_{(\phi, \xi)}, \sigma^2 = \hat{\sigma}_{(\hat{\beta}_{(\phi, \xi)}, \phi, \xi)}^2, \phi, \xi \right)$$

by replacing the β with $\hat{\beta}_{(\phi, \xi)}$ and σ^2 with $\hat{\sigma}_{(\hat{\beta}_{(\phi, \xi)}, \phi, \xi)}^2$ in the actual likelihood $L (Z; \beta, \theta = (\sigma^2, \phi, \xi))$.

Describe how you would compute suitable values $(\hat{\phi}, \hat{\xi})$ for the MLE of (ϕ, ξ)

Solution. It is

(1) It is

$$\begin{aligned} c (h; (\sigma^2, \phi, \tau)) &= c_\delta (h; \sigma^2, \phi) + c_\varepsilon (h; \tau) \\ &= \sigma^2 \exp \left(-\frac{1}{\phi} \|h\| \right) + \tau 1_{\{0\}} (h) \end{aligned}$$

(2) It is

(a)

$$C (\sigma^2, \phi, \xi) = \sigma^2 \exp \left(-\frac{1}{\phi} D \right) + \sigma^2 \xi^2 I$$

(b)

$$\begin{aligned} 2 \log (L (Z; \theta)) &= 2 \log (N (Z | \Psi \beta, C (\theta))) \\ &= -n \log (\sigma^2) - \log \left(\left| \exp \left(-\frac{1}{\phi} D \right) + \xi^2 I \right| \right) \\ &\quad - \frac{1}{\sigma^2} (Z - \Psi \beta)^\top \left(\exp \left(-\frac{1}{\phi} D \right) + \xi^2 I \right)^{-1} (Z - \Psi \beta) \end{aligned}$$

(3) It is

$$\begin{aligned} 2 \log (L (Z; \theta)) &= -n \log (\sigma^2) - \log \left(\left| \exp \left(-\frac{1}{\phi} D \right) + \xi^2 I \right| \right) \\ &= -\frac{1}{\sigma^2} (Z - \Psi \beta)^\top \left(\exp \left(-\frac{1}{\phi} D \right) + \xi^2 I \right)^{-1} (Z - \Psi \beta) \end{aligned}$$

Let $R_{(\phi, \xi)}$ matrix with $[R_{(\phi, \xi)}]_{i,j} = r (s_i - s_j | \phi, \xi)$

(a) So the likelihood equations are $0 = \nabla_{(\beta, \sigma^2)} \log (L (Z; \theta))$

$$\begin{cases} 0 = \Psi^\top (R_{(\phi, \xi)})^{-1} Z - \Psi^\top (R_{(\phi, \xi)})^{-1} \Psi \beta \\ 0 = \frac{n}{2} \frac{1}{\sigma^2} + \frac{1}{2(\sigma^2)^2} (Z - \Psi \beta)^\top (R_{(\phi, \xi)})^{-1} (Z - \Psi \beta) \end{cases}$$

(b) It is

$$\hat{\beta}_{(\phi, \xi)} = \left(\Psi^\top (R_{(\phi, \xi)})^{-1} \Psi \right)^{-1} \Psi^\top (R_{(\phi, \xi)})^{-1} Z$$

(c) It is

$$\hat{\sigma}_{(\beta, \phi, \xi)} = \frac{1}{n} (Z - \Psi \beta)^\top (R_{(\phi, \xi)})^{-1} (Z - \Psi \beta)$$

and by substituting I get

$$\begin{aligned}\hat{\sigma}_{(\phi, \xi)} &= \hat{\sigma}_{(\hat{\beta}_{(\phi, \xi)}, \phi, \xi)} = \frac{1}{n} \left(Z - \Psi \hat{\beta}_{(\phi, \xi)} \right)^\top (R_{(\phi, \xi)})^{-1} \left(Z - \Psi \hat{\beta}_{(\phi, \xi)} \right) \\ &= \frac{1}{n} \left(Z - \Psi \hat{\beta}_{(\phi, \xi)} \right)^\top (R_{(\phi, \xi)})^{-1} \left(Z - \Psi \hat{\beta}_{(\phi, \xi)} \right)\end{aligned}$$

(d) It is

$$e = Z - \Psi \hat{\beta}_{(\phi, \xi)} = (I - H) Z$$

So

$$\begin{aligned}n \hat{\sigma}_{(\phi, \xi)} &= Z^\top (I - H) (R_{(\phi, \xi)})^{-1} (I - H) Z \\ &= [(I - H) Z]^\top (R_{(\phi, \xi)})^{-1} [(I - H) Z] \\ &= e^\top R_{(\phi, \xi)} e\end{aligned}$$

where

$$\mathbb{E}[e] = 0$$

then

$$\begin{aligned}\mathbb{E}(n \hat{\sigma}_{(\phi, \xi)}) &= \mathbb{E} \left(Z^\top (I - H) (R_{(\phi, \xi)})^{-1} (I - H) Z \right) \\ &= \underbrace{(\mathbb{E}[e])^\top}_{=0} \underbrace{(R_{(\phi, \xi)})^{-1}}_{=0} \underbrace{\mathbb{E}[e]}_{=0} + \text{tr} \left((R_{(\phi, \xi)})^{-1} \text{Var}(e) \right) \\ &= \text{tr} \left((R_{(\phi, \xi)})^{-1} \text{Var}((I - H) Z) \right) \\ &= \text{tr} \left((R_{(\phi, \xi)})^{-1} (I - H) \sigma^2 R_{(\phi, \xi)} (I - H) \right) = \sigma^2 \text{tr} \left((R_{(\phi, \xi)})^{-1} (I - H) R_{(\phi, \xi)} (I - H) \right) \\ &= \text{tr}((I - H)) = \sigma^2 (n - p)\end{aligned}$$

So it is

$$\tilde{\sigma}(\beta, \phi, \xi) = \frac{1}{n - p} (Z - \Psi \beta)^\top (R_{(\phi, \xi)})^{-1} (Z - \Psi \beta)$$

because

$$\mathbb{E}(\tilde{\sigma}(\beta, \phi, \xi)) = \sigma^2$$

(e) It is

$$\hat{\beta}(\phi, \xi) = \left(\Psi^\top (R_{(\phi, \xi)})^{-1} \Psi \right)^{-1} \Psi^\top (R_{(\phi, \xi)})^{-1} Z$$

so it is Normal as a linear combination of normal random variables, with mean

$$\mathbb{E}(\hat{\beta}(\phi, \xi)) = \left(\Psi^\top (R_{(\phi, \xi)})^{-1} \Psi \right)^{-1} \Psi^\top (R_{(\phi, \xi)})^{-1} \mathbb{E}(Z) = \beta$$

and Variance

$$\begin{aligned}\text{Var}(\hat{\beta}_{(\phi, \xi)}) &= \left(\Psi^\top (R_{(\phi, \xi)})^{-1} \Psi \right)^{-1} \Psi^\top (R_{(\phi, \xi)})^{-1} \underbrace{\text{Var}(Z)}_{= \sigma^2 R_{(\phi, \xi)}} \\ &= \left(R_{(\phi, \xi)} \right)^{-1} \Psi \left(\Psi^\top (R_{(\phi, \xi)})^{-1} \Psi \right)^{-1} = \left(\Psi^\top (R_{(\phi, \xi)})^{-1} \Psi \right)^{-1}\end{aligned}$$

(4) It is

$$\begin{aligned} \log(L(Z; (\phi, \xi))) &= L\left(Z; \beta = \hat{\beta}_{(\phi, \xi)}, \sigma^2 = \hat{\sigma}_{(\hat{\beta}_{(\phi, \xi)}, \phi, \xi)}^2, \phi, \xi\right) \\ &\quad - \frac{n}{2} \log\left(\hat{\sigma}_{(\hat{\beta}_{(\phi, \xi)}, \phi, \xi)}^2\right) - \frac{1}{2} \log(|R_{(\phi, \xi)}|) \end{aligned}$$

where obviously

$$0 = \nabla_{(\phi, \xi)} \log(L(Z; (\phi, \xi)))|_{(\phi, \xi) = (\hat{\phi}, \hat{\xi})}$$

cannot be solved numerically. The Newton method or the gradient descent method can be used to maximize $\log(L(Z; (\phi, \xi)))$.

Exercise 2. (★) Let $(Z_s)_{s \in \mathcal{S}}$ be a specified statistical model. Assume that process $(Z_s)_{s \in \mathcal{S}}$ has known mean $\mu(s) = E(Z(s))$ and known covariance function $c(\cdot, \cdot)$. Assume there is available a dataset $\{(s_i, Z_i := Z(s_i))\}_{i=1}^n$. Assume that the matrix C such as $[C]_{i,j} = c(s_i, s_j)$ has an inverse. Consider the “Kriging” estimator $Z_{\text{SK}}(s_0)$ of $Z(s_0)$ at an unseen spatial location s_0 as the BLUE (Best Linear Unbiased Estimator)

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

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

- (1) Find sufficient conditions on $w = (w_1, \dots, w_n)^\top$ so that the Kriging estimator $Z_{\text{SK}}(s_0)$ to be unbiased.
- (2) Derive the MSE of $Z_{\text{SK}}(s_0)$ as

$$E(Z_{\text{SK}}(s_0) - Z(s_0))^2 = w^\top C w + c(s_0, s_0) - 2w^\top C_0$$

where C_0 is a vector such as $[C_0]_i = c(s_0, s_i)$.

- (3) Derive the Kriging estimator of $Z(s_0)$ as

$$Z_{\text{SK}}(s_0) = \mu(s_0) + C_0^\top C^{-1} [Z - \mu(s_{1:n})]$$

where $\mu(s_{1:n})$ is a vector such as $[\mu(s_{1:n})]_i = \mu(s_i)$.

- (4) Compute the Kriging standard error $\sigma_{\text{SK}} = \sqrt{E(Z_{\text{SK}}(s_0) - Z(s_0))^2}$.

Solution. The method is called Simple Kriging, and hence we denote it as SK.

- (1) It is

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

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

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

$$E(Z_{\text{SK}}(s_0) - Z(s_0)) = E\left(w_{n+1} + \sum_{i=1}^n w_i Z(s_i) - Z(s_0)\right) = w_{n+1} + \sum_{i=1}^n w_i \mu(s_i) - \mu(s_0)$$

which is satisfied given the assumption

$$w_{n+1} = \mu(s_0) - \sum_{i=1}^n w_i \mu(s_i) \iff w_{n+1} = \mu(s_0) - w^\top \mu(s_{1:n})$$

where $w = (w_1, \dots, w_n)^\top$.

(2) It is

$$\begin{aligned} \mathbb{E}(Z_{\text{SK}}(s_0) - Z(s_0))^2 &= \text{Var}(Z_{\text{SK}}(s_0) - Z(s_0)) = \text{Var}(w_{n+1} + w^\top Z - Z(s_0)) \\ &= \text{Var}(w_{n+1} + w^\top Z) + \text{Var}(Z(s_0)) - 2\text{Cov}(w_{n+1} + w^\top Z, Z(s_0)) \\ &= w^\top C w + c(s_0, s_0) - 2w^\top \text{Cov}(Z, Z(s_0)) \\ &= w^\top C w + c(s_0, s_0) - 2w^\top C_0 \end{aligned}$$

where $C_0 = \text{Cov}(Z, Z(s_0))$, i.e. $[C_0]_j = c(s_j, s_0)$.

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

$$w^{\text{SK}} = \arg \min_w \mathbb{E}(Z_{\text{SK}}(s_0) - Z(s_0))^2, \text{ subject to } w_{n+1} = \mu(s_0) - w^\top \mu(s_{1:n})$$

As $\mathbb{E}(\mu_{\text{SK}} - Z(s_0))^2$ does not depend on w_{n+1} we minimize

$$\begin{aligned} 0 &= \nabla_w \mathbb{E}(Z_{\text{SK}}(s_0) - Z(s_0))^2 = \nabla_w \text{Var}(Z_{\text{SK}}(s_0) - Z(s_0)) \\ &= 2Cw - 2C_0 \end{aligned}$$

So I get

$$w_{\text{SK}} = C^{-1}C_0$$

So

$$\begin{aligned} Z_{\text{SK}}(s_0) &= w_{n+1} + C^{-1}C_0 Z \\ &= \mu(s_0) - (C^{-1}C_0)^\top \mu(s_{1:n}) + (C^{-1}C_0)^\top Z \\ &= \mu(s_0) + C_0^\top C^{-1} [Z - \mu(s_{1:n})] \end{aligned}$$

(4) It is

$$\begin{aligned} \sigma_{\text{SK}} &= \sqrt{\mathbb{E}(Z_{\text{SK}}(s_0) - Z(s_0))^2} \\ &= \sqrt{w_{\text{SK}}^\top C w_{\text{SK}} + c(s_0, s_0) - 2w_{\text{SK}}^\top C_0} \\ &= \sqrt{c(s_0, s_0) - C_0^\top C^{-1}C_0} \end{aligned}$$