

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.

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 μ_{SK} . 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.