Homework 2: Geostatistics (Kriging and MLE inference)

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Exercise 1. ($\star$) 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 $c_w\left(h; \sigma^2, \phi\right) = \sigma^2 \exp\left(-\frac{1}{\phi}\|h\|\right)$, $\mu(s; \beta)$ is a deterministic function

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

with unknown coefficients $\beta = (\beta_0, ..., \beta_p)^\top$ and known basis functions $\psi(s) = (\psi_0(s), ..., \psi_p(s))^\top$, $\varepsilon(s)$ 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 $c\left(h; \left(\sigma^2, \phi, \tau\right)\right)$ of (Z_s).

(2) Consider a re-parametrization $\theta = \left(\sigma^2, \phi, \xi\right)$ 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 $Z = (Z_1, ..., Z_n)^\top$ as a function of D and θ.

  (b) Write down the log likelihood function $\log(L(Z; \theta))$ of $Z = (Z_1, ..., Z_n)^\top$ given $\theta = \left(\sigma^2, \phi, \xi\right)$.

(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 equations[1] w.r.t. $\left(\beta, \sigma^2\right)$, 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 $\hat{\sigma}^2_{(\phi,\xi)}$ 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 $e = (e_1, ..., e_n)^\top$ as $e = [I - H] Z$ where $H = \left(\Psi^\top R^{-1} \Psi\right)^{-1} \Psi^\top R^{-1}$, and write $\hat{\sigma}^2_{(\phi,\xi)}$ w.r.t. e.

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

[1] that is, the gradient of the log-likelihood

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

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

by replacing the β with $\hat{\beta}_{(\phi,\xi)}$ and σ^2 with $\hat{\sigma}^{2}_{\left(\hat{\beta}_{(\phi,\xi)},\phi,\xi\right)}$ in the actual likelihood $L\left(Z;\beta,\theta=\left(\sigma^{2},\phi,\xi\right)\right)$. Describe how you would compute suitable values $\left(\hat{\phi},\hat{\xi}\right)$ for the MLE of (ϕ,ξ)

Solution.

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

$$Z_{\mathrm{SK}}\left(s_0\right)=w_{n+1}+\sum_{i=1}^{n}w_iZ\left(s_i\right)=w_{n+1}+w^{\top}Z,$$

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

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

(2) Derive the MSE of $Z_{\mathrm{SK}}\left(s_0\right)$ as

$$\mathrm{E}\left(Z_{\mathrm{SK}}\left(s_0\right)-Z\left(s_0\right)\right)^{2}=w^{\top}Cw+c\left(s_0,s_0\right)-2w^{\top}C_0$$

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

(3) Derive the Kriging estimator of $Z\left(s_0\right)$ as

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

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

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

Solution.