Spatio-temporal statistics (MATH4341) Michaelmas term, 2023

Homework 2: Geostatistics (Kriging and MLE inference)

Lecturer: Georgios P. Karagiannis georgios.karagiannis@durham.ac.uk

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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).

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

(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

(e) What is the sampling distribution of $\hat{\beta}_{(\phi,\xi)}$? Specify the distribution family along with its parameters.

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

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

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)

Exercise 2. ($\star$) Let $(Z_s)_{s\in\mathcal{S}}$ be a specified statistical model. Assume that process $(Z_s)_{s\in\mathcal{S}}$ has known mean $\mu(s) = \mathrm{E}(Z(s))$ 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 $Z_{\mathrm{SK}}(s_0)$ of $Z(s_0)$ at an unseen spatial location s_0 as the BLUE (Best Linear Unbiased Estimator)

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

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

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

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

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

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

3. Derive the Kriging estimator of $Z\left(s_0\right)$ 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 $\left[\mu\left(s_{1:n}\right)\right]_i=\mu\left(s_i\right)$.

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