

## 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  $\tau^2$ , 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  $\Psi$  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  $\theta$ .
  - (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  $(\phi, \xi)$  as known constants.
  - (a) Compute the likelihood equations<sup>1</sup> w.r.t.  $(\beta, \sigma^2)$ , and for given  $(\phi, \xi)$ .

<sup>1</sup>that is, the gradient of the log-likelihood

- (b) Compute the MLE  $\hat{\beta}_{(\phi, \xi)}$  of  $\beta$  as a function of  $(\phi, \xi)$
- (c) Compute the MLE  $\hat{\sigma}_{(\phi, \xi)}^2$  of  $\sigma^2$  as a function of  $(\phi, \xi)$ .
- (d) Compute the unbiased estimator of  $\tilde{\sigma}^2$  of  $\sigma^2$ .

**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  $Z \sim \text{Normal}$

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  $\beta$  with  $\hat{\beta}_{(\phi, \xi)}$  and  $\sigma^2$  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  $(\phi, \xi)$

**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  $\mu_{\text{SK}}$ . 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  $\sigma_{\text{SK}} = \sqrt{\text{E} (Z_{\text{SK}} (s_0) - Z (s_0))^2}$ .