Problem class sheet 3

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Exercise 1. ($\star\star$)

> **Inventory of useful formulas.**
>
> [Normal distr. conditioning] Let $x_1 \in \mathbb{R}^{d_1}$, and $x_2 \in \mathbb{R}^{d_2}$. If
>
> $$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \sim \mathrm{N}_{d_1+d_2} \left(\begin{bmatrix} \mu_1 \\ \mu_2 \end{bmatrix}, \begin{bmatrix} \Sigma_1 & \Sigma_{21}^\top \\ \Sigma_{21} & \Sigma_2 \end{bmatrix} \right)$$
>
> then it is
>
> $$x_2|x_1 \sim \mathrm{N}_{d_2} \left(\mu_{2|1}, \Sigma_{2|1} \right)$$
>
> where
>
> $$\mu_{2|1} = \mu_2 + \Sigma_{21}\Sigma_1^{-1} (x_1 - \mu_1) \ \text{ and } \ \Sigma_{2|1} = \Sigma_2 - \Sigma_{21}\Sigma_1^{-1}\Sigma_{21}^\top$$

Consider the Bayesian Kriging from your lecture notes:

$$Z(s) = Y(s) + \varepsilon(s), \ \ s \in \mathcal{S}$$

where

$$\varepsilon(\cdot) \sim \mathrm{GP}(0, c_\varepsilon(\cdot, \cdot | \tau))$$

with $c_\varepsilon(s, s'|\tau) = \tau^2 1_{\{0\}}(\|s - s'\|)$ and

$$Y(\cdot)|\beta, \theta \sim \mathrm{GP}\left(\mu(\cdot|\beta), c_Y(\cdot, \cdot|\sigma^2, \phi)\right)$$

with mean function $\mu(\cdot|\beta)$ (to be specified later) labeled by unknown parameter β and covariance function $c_Y(\cdot, \cdot|\sigma^2, \phi)$.

Assume there is available a dataset $\{(s_i, Z_i)\}_{i=1}^n$ where $Z_i = Z(s_i)$ is a realization of a stochastic process (Z_s).

(1) Write the hierarchical spatial model $Z(\cdot)|Y(\cdot), \beta, \varphi$ and $Y(\cdot)|\beta, \varphi$ where $\varphi = (\sigma^2, \phi, \tau)^\top$.

(2) Write the marginal process $Z(\cdot)|\beta, \varphi$ where $\varphi = (\sigma^2, \phi, \tau)^\top$, its mean function denoted as $\mu(\cdot|\cdot)$, and its covariance function denoted as $c(\cdot|\cdot)$.

    Hint:: Let Y and X be independent random variables with $X \sim \mathrm{N}(\mu_X, \Sigma_X)$, $Y \sim \mathrm{N}(\mu_Y, \Sigma_Y)$. Let A and B be fixed matrices. Let c be a fixed vector. Then

$$AX + BY + c \sim \mathrm{N}\left(A\mu_X + B\mu_Y + c, A\Sigma_X A^\top + B\Sigma_Y B^\top\right)$$

(3) Compute the predictive process $Z(\cdot)|Z, \beta, \varphi$ as

$$Z(\cdot)|Z, \beta, \varphi \sim \mathrm{GP}\left(\mu_1\left(\cdot|\beta, \varphi\right), c_1\left(\cdot, \cdot|\varphi\right)\right)$$

with

$$c_1\left(s, s'|\varphi\right) = c\left(s, s|\varphi\right) + \left(C\left(S, s|\varphi\right)\right)^\top \left(C\left(S, S|\varphi\right)\right)^{-1} C\left(S, s'|\varphi\right)$$
$$\mu_1\left(s|\beta, \varphi\right) = \mu\left(s|\beta\right) - \left(C\left(S, s|\varphi\right)\right)^\top \left(C\left(S, S|\varphi\right)\right)^{-1} \left(\mu\left(S|\beta\right) - Z\right)$$

Hint: See the Conditional Normal formula above.

(4) Assume $\mu(s|\beta) = \psi(s)^\top \beta$. Consider a conjugate prior $\beta \sim \mathrm{N}(b, B)$ on β where $B > 0$.

(a) Write down the Bayesian statistical model involving layers $[Z|\beta, \varphi]$, and $[\beta|\varphi]$.

(b) Compute the posterior distribution as

$$\beta|Z, \varphi \sim \mathrm{N}\left(b_n\left(\varphi\right), B_n\left(\varphi\right)\right)$$

with

$$B_n\left(\varphi\right) = \left(B^{-1} + \Psi^\top \left(C\left(S, S|\varphi\right)\right)^{-1} \Psi\right)^{-1}$$
$$b_n\left(\varphi\right) = B_n\left(\varphi\right)\left(B^{-1}b + \Psi^\top \left(C\left(S, S|\varphi\right)\right)^{-1} Z\right)$$

where $C\left(S, S|\varphi\right)$ is a matrix with $\left[C\left(S, S|\varphi\right)\right]_{i,j} = c\left(s_i, s_j|\varphi\right)$.

Hint: Use the following identity

$$(y - \Phi\beta)^\top \Sigma^{-1}(y - \Phi\beta) + (\beta - \mu)^\top V^{-1}(\beta - \mu) = (\beta - \mu^*)^\top \left(V^*\right)^{-1}(\beta - \mu^*) + S^*;$$
$$V^* = \left(V^{-1} + \Phi^\top \Sigma^{-1}\Phi\right)^{-1}; \qquad \mu^* = V^*\left(V^{-1}\mu + \Phi^\top \Sigma^{-1}y\right)$$
$$S^* = \mu^\top V^{-1}\mu - \left(\mu^*\right)^\top \left(V^*\right)^{-1}\left(\mu^*\right) + y^\top \Sigma^{-1}y;$$

(c) Compute the (posterior) predictive process $Z(\cdot)|Z, \varphi$ given the data Z and given the parameters φ as

$$Z(\cdot)|Z, \varphi \sim \mathrm{GP}\left(\mu_2\left(\cdot|\varphi\right), c_2\left(\cdot, \cdot|\varphi\right)\right)$$

with

$$\mu_2\left(s|\varphi\right) = \left(\psi(s) - \Psi^\top C^{-1}C(s)\right)^\top \left(B^{-1} + \Psi^\top C^{-1}\Psi\right)^{-1} B^{-1}b$$
$$+ \left[\left(C(s)\right)^\top + \left(\psi(s) - \Psi^\top C^{-1}C(s)\right)^\top \left(B^{-1} + \Psi^\top C^{-1}\Psi\right)^{-1} \Psi\right] C^{-1}Z$$
$$c_2\left(s, s'|\varphi\right) = c\left(s, s'|\varphi\right) - \left(C(s)\right)^\top C^{-1}C(s')$$
$$+ \left(\psi(s) - \Psi^\top C^{-1}C(s)\right)^\top \left(B^{-1} + \Psi^\top C^{-1}\Psi\right)^{-1} \left(\psi(s') - \Psi^\top C^{-1}C(s')\right)$$

with column vector $C(s) := \left(c\left(s, s_1|\varphi\right), ..., c\left(s, s_n|\varphi\right)\right)^\top$, and matrix $C := C\left(S, S|\varphi\right)$.

(d) Compute the marginal likelihood $\Pr(Z|\varphi)$ in the form

$$\Pr\left(Z|\sigma^2, \varphi\right) = \mathrm{N}\left(Z|\Psi b, \left(C^{-1} - C^{-1}\Psi\left(B^{-1} + \Psi^\top B^{-1}\Psi\right)^{-1}\Psi^\top C^{-1}\right)^{-1}\right)$$

where Ψ is a matrix with $[\Psi]_{i,j} = \psi_j(s_i)$, and R is a matrix with $[C]_{i,j} = c(s_i, s_j|\varphi)$.

Hint-2:: It is

$$\int \mathrm{N}\left(Z|\Psi\beta, C\right) \mathrm{N}\left(\beta|b, B\right) \mathrm{d}\beta = \mathrm{N}\left(Z|\Psi b, C + \Psi B\Psi^\top\right)$$

Hint 3:: [Woodbury matrix identity]

$$(A + UCV)^{-1} = A^{-1} - A^{-1}U\left(C^{-1} + VA^{-1}U\right)^{-1}VA^{-1}$$

(5) Consider non-informative prior $\Pr(\beta) \propto 1$ for β by specifying $b \to 0$ and letting $B^{-1} \to 0$. Argue whether such a prior can be used. Recompute the (asymptotic) quantities $\Pr(Z|\varphi)$, $[Z(\cdot)|Z, \varphi]$ under this new prior in the limit.

Solution.

(1) The hierarchical model is

$$Z(\cdot)|Y(\cdot), \tau \sim \mathrm{GP}\left(Y(\cdot), c_\varepsilon\left(\cdot, \cdot|\sigma^2, \xi\right)\right)$$
$$Y(\cdot)|\beta, \sim \mathrm{GP}\left(\mu(\cdot|\beta), c_Y\left(\cdot, \cdot|\sigma^2, \phi\right)\right)$$

(2) We use the additive property of the Gaussian distribution (in Hint) it is

$$Z(\cdot)|\beta, \varphi \sim \mathrm{GP}\left(\mu(\cdot|\beta), c(\cdot, \cdot|\varphi)\right)$$

where

$$c(s, s'|\varphi) = c_Y\left(s, s'|\sigma^2, \phi\right) + c_\varepsilon\left(s, s'|\sigma^2, \xi\right)$$

(3) Assume a vector of "unseen" sites $S_* = (s_{*,1}, ..., s_{*,q})^\top$ for any $q \in \mathbb{N}_0$. Let convenient notation $Z := Z(S)$, and $Z_* := Z(S_*)$. The join marginal distribution of $(Z_*, Z)^\top$ given β, $\varphi = (\sigma^2, \phi, \tau)^\top$ is

$$\begin{pmatrix} Z_* \\ Z \end{pmatrix} |\beta, \varphi \sim \mathrm{N}\left(\begin{pmatrix} \mu(S_*; \beta) \\ \mu(S; \beta) \end{pmatrix}, \begin{pmatrix} C(S_*, S_*|\varphi) & (C(S_*, S|\varphi))^\top \\ C(S_*, S|\varphi) & C(S, S|\varphi) \end{pmatrix}\right)$$

by using convenient notation $[C(S_*, S|\varphi)]_{i,j} = s(s_{*,i}, s_j|\varphi)$ and $[\mu(S; \beta)]_i = \mu(s_i; \beta)$. By conditioning the Normal distribution (see Hint), I get

$$Z_*|Z, \beta, \varphi \sim \mathrm{N}\left(\mu_*\left(S_*|\beta, \varphi\right), C_*\left(S_*, S_*|\varphi\right)\right)$$

where

$$C_1 \left(S_*, S_* | \varphi \right) = C \left(S_*, S_* | \varphi \right) + \left(C \left(S, S_* | \varphi \right) \right)^\top \left(C \left(S, S | \varphi \right) \right)^{-1} C \left(S, S_* | \varphi \right)$$

$$\mu_1 \left(S_* | \beta, \varphi \right) = \mu \left(S_* | \beta \right) - \left(C \left(S, S_* | \varphi \right) \right)^\top \left(C \left(S, S | \varphi \right) \right)^{-1} \left(\mu \left(S | \beta \right) - Z \right)$$

As it is for any length of of any vector S_*, then it is a Gaussian process

$$Z \left(\cdot \right) | Z, \beta, \varphi \sim \mathrm{GP} \left(\mu_1 \left(\cdot | \beta, \varphi \right), c_1 \left(\cdot, \cdot | \varphi \right) \right)$$

with

$$c_1 \left(s, s' | \varphi \right) = c \left(s, s' | \varphi \right) + \left(C \left(S, s | \varphi \right) \right)^\top \left(C \left(S, S | \varphi \right) \right)^{-1} C \left(S, s' | \varphi \right)$$

$$\mu_1 \left(s | \beta, \varphi \right) = \mu \left(s | \beta \right) - \left(C \left(S, s | \varphi \right) \right)^\top \left(C \left(S, S | \varphi \right) \right)^{-1} \left(\mu \left(S | \beta \right) - Z \right)$$

(4)

(a) The Bayesian model is

(0.1)
$$\begin{cases} Z | \beta, \varphi \sim \mathrm{N} \left(\Psi \beta, C \left(S, S | \varphi \right) \right) \\ \beta \sim \mathrm{N} \left(b, B \right) \end{cases}$$

(b) Let $C := C \left(S, S | \varphi \right)$. The posterior distribution (by using Bayes theorem) is

$$\Pr \left(\beta | Z, \varphi \right) \propto \Pr \left(Z | \beta, \varphi \right) \Pr \left(\beta | \varphi \right)$$

$$= \mathrm{N} \left(Z | \Psi \beta, C \right) \mathrm{N} \left(\beta | b, B \right)$$

$$\propto \exp \left(-\frac{1}{2} \left(Z - \Psi \beta \right)^\top C^{-1} \left(Z - \Psi \beta \right) \right) \exp \left(-\frac{1}{2} \left(\beta - b \right)^\top B^{-1} \left(\beta - b \right) \right)$$

$$= \exp \left(-\frac{1}{2} \left[\left(Z - \Psi \beta \right)^\top C^{-1} \left(Z - \Psi \beta \right) + \left(\beta - b \right)^\top B^{-1} \left(\beta - b \right) \right] \right)$$

By using the Hint I have

$$\left(Z - \Psi \beta \right)^\top C^{-1} \left(Z - \Psi \beta \right) + \left(\beta - b \right)^\top B^{-1} \left(\beta - b \right) = \left(\beta - b_n \right)^\top \left(B_n \right)^{-1} \left(\beta - b_n \right) + R_n$$

where by denoting $B_n := B_n \left(\varphi \right)$, and $b_n := b_n \left(\varphi \right)$ I get

$$B_n = \left(B^{-1} + \Psi^\top C^{-1} \Psi \right)^{-1}$$

$$b_n = B_n \left(B^{-1} b + \Psi^\top C^{-1} Z \right)$$

and R_n is a "constant" quantity that does not contain any β. Hence

$$\Pr \left(\beta | Z, \varphi \right) \propto \exp \left(-\frac{1}{2} (\beta - b_n)^\top \left(B_n \right)^{-1} \left(\beta - b_n \right) - \frac{1}{2} R_n \right)$$

$$\propto \exp \left(-\frac{1}{2} (\beta - b_n)^\top \left(B_n \right)^{-1} \left(\beta - b_n \right) \right)$$

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Well, from the above, I recognize the kernel of the Multivariate Normal distribution, as
$$\beta | Z, \varphi \sim \mathrm{N} \left(b_n \left(\varphi \right), B_n \left(\varphi \right) \right)$$

(c) Assume a vector of "unseen" sites $S_* = \left(s_{*,1}, ..., s_{*,q} \right)^\top$ for any $q \in \mathbb{N} - \{0\}$. Let convenient notation $Z := Z \left(S \right)$, and $Z_* := Z \left(S_* \right)$. I have already computed

$$\mathrm{Pr} \left(Z_* | Z, \beta, \varphi \right) = \mathrm{N} \left(Z_* | \mu_1 \left(S_* | \beta, \varphi \right), C_1 \left(S_*, S_* | \varphi \right) \right)$$

from the previous part. It is

$$\mathrm{Pr} \left(Z_* | Z, \varphi \right) = \int \mathrm{Pr} \left(Z_* | Z, \beta, \varphi \right) \mathrm{Pr} \left(\beta | Z, \varphi \right) \mathrm{d}\beta$$

$$= \int \mathrm{N} \left(Z_* | \mu_1 \left(S_* | \beta, \varphi \right), C_1 \left(S_*, S_* | \varphi \right) \right) \mathrm{N} \left(\beta | b_n, B_n \right) \mathrm{d}\beta$$

Denote $\Psi_* = \Psi \left(S_* \right)$, $C_* = C \left(S_*, S | \varphi \right)$, and $C_{**} = C \left(S_*, S_* | \varphi \right)$. Notice that

$$\mu_1 \left(S_* \right) = \Psi_* \beta - C_* C^{-1} \left(\Psi \beta - Z \right)$$
$$= \left[\Psi_* - C_* C^{-1} \Psi \right] \beta + C_* C^{-1} Z$$

Hence, for given/fixed Z, φ, it is

$$Z_* = C_* C^{-1} Z + \left[\Psi_* - C_* C^{-1} \Psi \right] \beta + \zeta, \quad \zeta \sim \mathrm{N} \left(0, C_1 \left(S_*, S_* \right) \right)$$

Hence, because $\beta \sim \mathrm{N} \left(b_n, B_n \right)$, and because $Z_* | Z, \varphi$ is a linear combination of the Normally distributed random vector $\beta \sim \mathrm{N} \left(b_n, B_n \right)$, $Z_* | Z, \varphi$ follows a Normal distribution, with mean

$$\mu_2 \left(S_* \right) = \mathrm{E}_{\beta \sim \mathrm{N}(b_n, B_n)} \left(Z_* | \mu_1 \left(S_* \right), C_1 \left(S_*, S_* \right) \right)$$
$$= \left(\Psi_* - C_* C^{-1} \Psi \right) \mathrm{E}_{\beta \sim \mathrm{N}(b_n, B_n)} \left(\beta \right) + C_* C^{-1} Z$$
$$= \left(\Psi_* - C_* C^{-1} \Psi \right) b_n + C_* C^{-1} Z$$
$$= \left(\Psi_* - C_* C^{-1} \Psi \right) \left(B^{-1} + \Psi^\top C^{-1} \Psi \right)^{-1} \left(B^{-1} b + \Psi^\top C^{-1} Z \right) + C_* C^{-1} Z$$
$$= \left(\Psi_* - C_* C^{-1} \Psi \right) \left(B^{-1} + \Psi^\top C^{-1} \Psi \right)^{-1} B^{-1} b$$
$$\quad + \left[\left(\Psi_* - C_* C^{-1} \Psi \right) \left(B^{-1} + \Psi^\top C^{-1} \Psi \right)^{-1} \Psi^\top + C_* \right] C^{-1} Z$$

and with covariance matrix

$$
\begin{aligned}
C_2\left(S_*, S_*\right) =& \operatorname{Var}_{\beta \sim \mathrm{N}\left(b_n, B_n\right)}\left(Z_* | \mu_1\left(S_*\right), C_1\left(S_*, S_*\right)\right) \\
=& \operatorname{Var}_{\beta \sim \mathrm{N}\left(b_n, B_n\right)}\left(\left[\Psi_* - C_* C^{-1} \Psi\right] \beta\right) + \operatorname{Var}_{\zeta \sim \mathrm{N}\left(0, C_1\left(S_*, S_*\right)\right)}(\zeta) \\
=& \left[\Psi_* - C_* C^{-1} \Psi\right] B_n \left[\Psi_* - C_* C^{-1}\right]^\top + C_1\left(S_*, S_*\right) \\
=& \left[\Psi_* - C_* C^{-1} \Psi\right]\left(B^{-1} + \Psi^\top C^{-1} \Psi\right)^{-1}\left[\Psi_* - C_* C^{-1} \Psi\right]^\top \\
& + C_{**} + C_* C^{-1}\left(C_*\right)^\top
\end{aligned}
$$

Recall that $C\left(s\right) = \left(c\left(s_1, s | \varphi\right), ..., c\left(s_n, s | \varphi\right)\right)^\top$ is a column vector.
Since this is for any vector S_* of any length, then

$$
Z\left(\cdot\right) | Z, \varphi \sim \mathrm{GP}\left(\mu_2\left(\cdot | \varphi\right), c_2\left(\cdot, \cdot | \varphi\right)\right)
$$

with mean function at s

$$
\begin{aligned}
\mu_2\left(s | \varphi\right) =& \left(\psi\left(s\right) - \left(C\left(s\right)\right)^\top C^{-1} \Psi\right)\left(B^{-1} + \Psi^\top C^{-1} \Psi\right)^{-1} B^{-1} b \\
& + \left[\left(\psi\left(s\right) - \left(C\left(s\right)\right)^\top C^{-1} \Psi\right)\left(B^{-1} + \Psi^\top C^{-1} \Psi\right)^{-1} \Psi^\top + \left(C\left(s\right)\right)^\top\right] C^{-1} Z
\end{aligned}
$$

and covariance function as s, s'

$$
\begin{aligned}
c_2\left(s, s' | \varphi\right) =& \left[\psi\left(s\right) - \left(C\left(s\right)\right)^\top C^{-1} \Psi\right]\left(B^{-1} + \Psi^\top C^{-1} \Psi\right)^{-1}\left[\psi\left(s'\right) - \left(C\left(s'\right)\right)^\top C^{-1} \Psi\right]^\top \\
& + c\left(s, s' | \varphi\right) + \left(C\left(s\right)\right)^\top C^{-1} C\left(s'\right)
\end{aligned}
$$

Recall that $C\left(s\right) = \left(c\left(s_1, s | \varphi\right), ..., c\left(s_n, s | \varphi\right)\right)^\top$ is a column vector.

(d) It is, from Hint-2,

$$
\begin{aligned}
\operatorname{Pr}\left(Z | \varphi\right) =& \int \operatorname{Pr}\left(Z | \beta, \varphi\right) \operatorname{Pr}\left(\beta\right) \mathrm{d}\beta \\
=& \int \mathrm{N}\left(Z | \Psi \beta, C\left(S, S | \varphi\right)\right) \mathrm{N}\left(\beta | b, B\right) \mathrm{d}\beta \\
=& \int \mathrm{N}\left(Z | \Psi \beta, C\left(S, S | \varphi\right)\right) \mathrm{N}\left(\Psi \beta | \Psi b, \Psi B \Psi^\top\right) \mathrm{d}\beta \\
=& \mathrm{N}\left(Z | \Psi b, C\left(S, S | \varphi\right) + \Psi B \Psi^\top\right)
\end{aligned}
$$

By letting $C := C\left(S, S | \varphi\right)$ and using the Hint I get

$$
\left(\left(C + \Psi B \Psi^\top\right)^{-1}\right)^{-1} = \left(C^{-1} - C^{-1} \Psi\left(B^{-1} + \Psi^\top C^{-1} \Psi\right)^{-1} \Psi^\top C^{-1}\right)^{-1}
$$

(5) Denote $C = C(S, S|\varphi)$. It is

$$\lim_{\substack{B^{-1} \to 0 \\ b \to 0}} \Pr(Z|\varphi) = \lim_{\substack{B^{-1} \to 0 \\ b \to 0}} N\left(Z|\Psi b, C + \Psi B \Psi^\top\right)$$

$$\propto N\left(Z|0, \left(C^{-1} - C^{-1}\Psi\left(\Psi^\top C^{-1}\Psi\right)^{-1}\Psi^\top C^{-1}\right)^{-1}\right)$$

$$< \infty$$

namely the bottom part of the fraction of the posterior of $\beta|Z, \varphi$ is bounded (finite); this implies that the posterior is proper. The posterior of $\beta|Z, \varphi$ has density such as

$$\Pr(\beta|Z, \varphi) \propto \exp\left(-\frac{1}{2}(\beta - b_n)^\top B_n^{-1}(\beta - b_n)\right)$$

then by computing the limit

$$\lim_{\substack{B^{-1} \to 0 \\ b \to 0}} \exp\left(-\frac{1}{2}(\beta - b_n)^\top B_n^{-1}(\beta - b_n)\right) =$$

$$\exp\left(-\frac{1}{2}\left(\beta - \left(\Psi^\top C^{-1}\Psi\right)^{-1}\Psi^\top C^{-1}Z\right)^\top \left(\Psi^\top C^{-1}\Psi\right)\left(\beta - \left(\Psi^\top C^{-1}\Psi\right)^{-1}\Psi^\top C^{-1}Z\right)\right)$$

Hence the limiting case is

$$\beta|Z, \varphi \overset{\text{approx}}{\sim} N\left(\left(\Psi^\top C^{-1}\Psi\right)^{-1}\Psi^\top C^{-1}Z, \left(\Psi^\top C^{-1}\Psi\right)^{-1}\right)$$

Hence the predictive process becomes

$$Z(\cdot)|Z, \varphi \overset{\text{approx}}{\sim} \text{GP}\left(\mu_3(\cdot|\varphi), c_3(\cdot, \cdot|\varphi)\right)$$

$$\mu_3(s|\varphi) = \left[\left(\psi(s) - (C(s))^\top C^{-1}\Psi\right)\left(\Psi^\top C^{-1}\Psi\right)^{-1}\Psi^\top + (C(s))^\top\right]C^{-1}Z$$

$$c_3(s, s'|\varphi) = \left(\psi(s) - (C(s))^\top C^{-1}\Psi\right)\left(\Psi^\top C^{-1}\Psi\right)^{-1}\left(\psi(s') - (C(s'))^\top C^{-1}\Psi\right)^\top$$

$$+ c(s, s'|\varphi) + (C(s))^\top C^{-1}C(s')$$

Exercise 2. ($\star$) Show that the extension variance $\sigma_E^2(v, V)$ of a small volume v to a larger volume V is obtained by

$$\sigma_E^2(v, V) = 2\bar{\gamma}(v, V) - \bar{\gamma}(v, v) - \bar{\gamma}(V, V)$$

where

$$\bar{\gamma}(v, V) = \frac{1}{|v|\,|V|}\int_{s \in v}\int_{s \in V}\gamma(s - s')\,\mathrm{d}s\mathrm{d}s'$$

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Solution. Essentially I need to show that that

$$\mathrm{Var}\left(Z\left(A\right)-Z\left(B\right)\right)=\frac{1}{\left|A\right|\left|B\right|}\int_{x\in A}\int_{y\in B}\gamma\left(x-y\right)\mathrm{d}x\mathrm{d}y$$

$$-\frac{1}{\left|A\right|\left|A\right|}\int_{x\in A}\int_{y\in A}\gamma\left(x-y\right)\mathrm{d}x\mathrm{d}y$$

$$-\frac{1}{\left|B\right|\left|B\right|}\int_{x\in B}\int_{y\in B}\gamma\left(x-y\right)\mathrm{d}x\mathrm{d}y$$

where I use A,B instead of v,V and x,y instead of s,s' for clarity on notation.

It is

$$\mathrm{Var}\left(Z\left(A\right)-Z\left(B\right)\right)=\mathrm{Cov}\left(Z\left(A\right)-Z\left(B\right),Z\left(A\right)-Z\left(B\right)\right)$$

$$=\mathrm{Cov}\left(Z\left(A\right),Z\left(A\right)\right)+\mathrm{Cov}\left(Z\left(B\right),Z\left(B\right)\right)-2\mathrm{Cov}\left(Z\left(A\right),Z\left(B\right)\right)$$

$$=\frac{1}{\left|A\right|\left|A\right|}\int_{x\in A}\int_{y\in A}\mathrm{Cov}\left(Z\left(x\right),Z\left(y\right)\right)\mathrm{d}x\mathrm{d}y$$

$$+\frac{1}{\left|B\right|\left|B\right|}\int_{x\in B}\int_{y\in B}\mathrm{Cov}\left(Z\left(x\right),Z\left(y\right)\right)\mathrm{d}x\mathrm{d}y$$

$$-2\frac{1}{\left|A\right|\left|B\right|}\int_{x\in A}\int_{y\in B}\mathrm{Cov}\left(Z\left(x\right),Z\left(y\right)\right)\mathrm{d}x\mathrm{d}y$$

OK, now I need to write all these Cov as γ ; I know that

$$\gamma\left(x-y\right)=\frac{1}{2}\mathrm{Var}\left(Z\left(x\right)-Z\left(y\right)\right)$$

$$=\frac{1}{2}\mathrm{Var}\left(Z\left(x\right)\right)+\frac{1}{2}\mathrm{Var}\left(Z\left(y\right)\right)-\mathrm{Cov}\left(Z\left(x\right),Z\left(y\right)\right)$$

that is

$$\mathrm{Cov}\left(Z\left(x\right),Z\left(y\right)\right)=\frac{1}{2}\mathrm{Var}\left(Z\left(x\right)\right)+\frac{1}{2}\mathrm{Var}\left(Z\left(y\right)\right)-\gamma\left(x-y\right)$$

Now I 'll gonna put all these in the quantity of interest, one by one

$$\frac{1}{\left|A\right|\left|A\right|}\int_{x\in A}\int_{y\in A}\mathrm{Cov}\left(Z\left(x\right),Z\left(y\right)\right)\mathrm{d}x\mathrm{d}y=\frac{1}{\left|A\right|\left|A\right|}\int_{x\in A}\int_{y\in A}\frac{1}{2}\mathrm{Var}\left(Z\left(x\right)\right)\mathrm{d}x\mathrm{d}y$$

$$+\frac{1}{\left|A\right|\left|A\right|}\int_{x\in A}\int_{y\in A}\frac{1}{2}\mathrm{Var}\left(Z\left(y\right)\right)\mathrm{d}x\mathrm{d}y$$

$$-\frac{1}{\left|A\right|\left|A\right|}\int_{x\in A}\int_{y\in A}\gamma\left(x-y\right)\mathrm{d}x\mathrm{d}y$$

$$=\frac{1}{\left|A\right|}\int_{x\in A}\mathrm{Var}\left(Z\left(x\right)\right)\mathrm{d}x$$

$$-\frac{1}{\left|A\right|^{2}}\int_{x\in A}\int_{y\in A}\gamma\left(x-y\right)\mathrm{d}x\mathrm{d}y$$

and by symmetry

$$\frac{1}{|B||B|} \int_{x \in B} \int_{y \in B} \mathrm{Cov}\left(Z\left(x\right), Z\left(y\right)\right) \mathrm{d}x\mathrm{d}y = \frac{1}{|B|} \int_{x \in B} \mathrm{Var}\left(Z\left(x\right)\right) \mathrm{d}x$$
$$- \frac{1}{|B|^2} \int_{x \in B} \int_{y \in B} \gamma\left(x - y\right) \mathrm{d}x\mathrm{d}y$$

and finally,

$$\frac{1}{|A||B|} \int_{x \in A} \int_{y \in B} \mathrm{Cov}\left(Z\left(x\right), Z\left(y\right)\right) \mathrm{d}x\mathrm{d}y = \frac{1}{|A||B|} \int_{x \in A} \int_{y \in B} \frac{1}{2}\mathrm{Var}\left(Z\left(x\right)\right) \mathrm{d}x\mathrm{d}y$$
$$+ \frac{1}{|A||B|} \int_{x \in A} \int_{y \in B} \frac{1}{2}\mathrm{Var}\left(Z\left(y\right)\right) \mathrm{d}x\mathrm{d}y$$
$$- \frac{1}{|A||B|} \int_{x \in A} \int_{y \in B} \gamma\left(x - y\right) \mathrm{d}x\mathrm{d}y$$
$$= \frac{1}{2}\frac{1}{|A|} \int_{x \in A} \mathrm{Var}\left(Z\left(x\right)\right) \mathrm{d}x$$
$$+ \frac{1}{2}\frac{1}{|B|} \int_{x \in B} \mathrm{Var}\left(Z\left(x\right)\right) \mathrm{d}x$$
$$- \frac{1}{|A||B|} \int_{x \in A} \int_{y \in B} \gamma\left(x - y\right) \mathrm{d}x\mathrm{d}y$$

Putting all these together, we get the result.

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