Optimal Designs for Kriging Models with Multiple Responses

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Abstract

Exact optimal designs for efficient prediction in simple and ordinary bivariate kriging models with one dimensional inputs are determined in this article. Two families of stationary covariance structures, namely the generalized Markov type and proportional covariances are investigated. These designs are found by minimizing the integrated and maximum prediction variance. For simple cokriging models with known covariance parameters, the equispaced design is shown to be optimal for both criterion functions. The more realistic scenario of unknown covariance parameters is addressed by assuming prior distributions on the parameter vector. The prior information is incorporated into both criterion functions by integrating it over the prior distribution, thus adopting a pseudo-Bayesian approach to the design problem. The equispaced design is proved to be optimal in the pseudo Bayesian sense for both criterion functions. For ordinary bivariate kriging models, it is shown theoretically that the equispaced design minimizes the maximum prediction variance, irrespective of known or unknown covariance parameters. The proposed work is motivated by a water quality study from a river in South India, where the interest is in designing an optimal river monitoring system. To the best of knowledge of the authors, these are the first explicit results on exact optimal designs for bivariate kriging models.

Keywords: Cokriging, Gaussian Processes, Exponential Covariance, Cross-covariance

1 Introduction

Kriging is a method for estimating a variable of interest, known as the primary variable, at unknown input sites. When multiple responses are collected, multivariate kriging also known as cokriging, is a related method for estimating a variable of interest at a specific location using measurements of this variable at other input sites and measurements of auxilliary/secondary
variables, which may provide useful information about the primary variable (Myers, 1983, 1991; Chiles and Delfiner, 2009; Wackernagel, 2003). For example, consider a water quality study in which a geologist is interested in estimating pH levels (primary response) at several unsampled locations along a river, but auxiliary information such as phosphate concentration or amount of dissolved oxygen may facilitate in giving more accurate estimates of pH levels. We may also consider a computer experiment, where the engineering code produces the primary response and its partial derivatives, and the derivatives (secondary variables) provide valuable information about the response (Santner et al., 2010). This scenario is typical when the responses measured are correlated, both nonspatially (at the same input sites) and spatially (over different sites, particularly those close to each other). The key difficulty in using such multivariate models is specifying the cross-covariance between the different random processes. Unlike direct covariance matrices, cross covariance matrices need not be symmetric; indeed, these matrices must be chosen in such a way that the second-order structure always yields a nonnegative definite covariance matrix (Genton and Kleiber, 2015).

In this article we find exact optimal designs for efficient prediction in simple and ordinary kriging models with bivariate responses. We consider two stationary and isotropic random functions, $Z_1$ and $Z_2$, where $Z_1$ is the primary variable while $Z_2$ the secondary/auxiliary variable. Our main interest is in prediction of $Z_1$, at a single location, say $x_0$, in the region of interest. For defining covariance matrices for our bivariate responses, we use two families of stationary covariance structures, namely the generalized Markov type and the proportional type. The assumed covariance structures are proved to be valid. We consider the average and the maximum kriging variance of $Z_1(x_0)$ as our two design criterion functions. The kriging variance of $Z_1(x_0)$ for both simple and ordinary cokriging models depend on the covariance parameters. For known covariance parameters in simple and ordinary models, we prove that the equispaced design minimizes the maximum prediction variance, i.e., is G-optimal. Also, for simple cokriging models, the equispaced design is found to be the I-optimal design i.e., it minimizes the average prediction variance, However, in real life, the covariance parameters are most likely unknown. To address the dependency of the design selection criterion on the unknown covariance parameters, we assume prior distributions on the parameter vector and instead determine pseudo Bayesian optimal designs. The equispaced design is again shown to be the Bayesian I- and G-optimal design. For illustration purpose we use a pilot data set based on a river water quality monitoring experiment from South India. The relative efficiency of the monitoring design with respect to the equispaced design is computed for various scenarios.

The original contributions of this article include (i) finding I- and G-optimal exact designs for simple bivariate cokriging models with proportional or Markov type cross-covariance functions when covariance parameters are assumed to be known, (ii) finding Bayesian I- and G-
optimal exact designs for simple bivariate cokriging models with proportional or Markov type covariance functions when priors are assumed for covariance parameters, and (iii) determining exact G-optimal designs for ordinary cokriging models with known covariance parameters and also when priors are assumed for both covariance types.

In contrast to optimal design of experiments for uncorrelated responses, where numerous results are available, literature on designs for dependent observations is still very sparse. Determining optimal designs for correlated error structures is far more complicated, with usually the design criterion depending on the error structures and model parameters. Exact optimal designs for the location scale model were considered by Boltze and Näther (1982), Näther (1985a, chap. 4), Pázman and Müller (2001), Müller and Pázman (2003) and Zimmerman (2006). For Ornstein-Uhlenbeck processes with single responses and one dimensional inputs, Zagoraiou and Antognini (2009); Antognini and Zagoraiou (2010) proved that equispaced designs are optimal for trend parameter estimation with respect to average prediction error minimization and the D-optimality criterion. Zimmerman (2006) studied designs for universal kriging models and showed how the optimal design differs depending on whether covariance parameters are known or estimated using numerical simulations on a two-dimensional grid. Diggle and Lophaven (2006) proposed Bayesian geostatistical designs focusing on efficient spatial prediction while allowing the parameters to be unknown. Exact optimal designs for universal kriging models with one dimensional inputs and error structure of the autoregressive of order one form were determined by Dette et al. (2008). This work was further extended by Dette et al. (2013) to a broader class of covariance kernels, also the arcsine distribution was shown to be universally optimal for the polynomial regression model with correlation structure defined by the logarithmic potential. Baran and Stehlík (2015) investigated optimal designs for parameters of shifted Ornstein-Uhlenbeck sheets for two input variables. However, in their work the inputs were assumed to be independent with a separable covariance structure.

For multivariate geostatistical models, optimal designs based on numerical simulations have been proposed by Li and Zimmerman (2015), Bueso et al. (1999), Le and Zidek (1994) and Caselton and Zidek (1984). Design criteria considered were either minimization of the integrated or maximum mean squared error or the entropy function. Designs in the presence of unknown covariance parameters were studied by Li and Zimmerman (2015). Most of the literature on design of experiments in a multivariate setting Li and Zimmerman (2015), Bueso et al. (1999), Le and Zidek (1994) and Caselton and Zidek (1984) propose optimal designs using numerical methods. To the best of our knowledge, this is the first article which determines theoretical exact optimal designs for bivariate cokriging models.

In Section 2 we introduce bivariate cokriging models discuss and derive the two covariance structures. The design criterion functions and optimal designs for cokriging models with
known parameters are discussed in Section 3. In Section 4 we address Bayesian optimal
designs for simple cokriging processes. An illustration using a water quality data set is shown
in Section 5. Section 6 contains derivations of optimal designs for ordinary cokriging models.
Concluding remarks are given in Section 7.

2 Multi-response kriging/Cokriging Models and Covari-
ance Structures

In this section we define kriging models for multiple responses, including the underlying
covariance and cross-covariance structures. Our focus is on bivariate processes. Consider
two simultaneous random functions $Z_1(\cdot)$ and $Z_2(\cdot)$, where $Z_1(\cdot)$ is the primary response
and $Z_2(\cdot)$ the secondary response. We assume both responses are observed over the re-
gion $D \subseteq \mathbb{R}$. In multivariate studies usually the set at which different random functions
are observed might not coincide, but in case it does, we say the design to be completely
collocated or simply collocated (Li and Zimmerman, 2015). In this paper we work with a
completely collocated design and consider that $Z_1(\cdot)$ and $Z_2(\cdot)$ are both sampled at the same
set of points $S = \{x_1, x_2, ..., x_n\}$, where $S \subseteq D \subseteq \mathbb{R}$. We consider $Z_i$ to be the
$n \times 1$ vector of all observations for the random function $Z_i(\cdot)$ for $i = 1, 2$. The underlying linear model is
given by:

$$
\begin{pmatrix}
Z_1 \\
Z_2
\end{pmatrix}
= \begin{pmatrix}
F_1 & 0 \\
0 & F_2
\end{pmatrix}
\begin{pmatrix}
\pi_1 \\
\pi_2
\end{pmatrix}
+ \begin{pmatrix}
\epsilon_1 \\
\epsilon_2
\end{pmatrix},
$$

(1)

Where, $F_i$ is the $n \times p_i$ matrix, such that its $k^{th}$ row is given by $f_i(x_k)$, $f_i(x_k)^T$ is the $p_i \times 1$
vector of known basis drift functions $f_i^l(\cdot)$ $l = 0, ..., p_i$. So, $f_i(x_k)$ is the vector of basis drift
functions evaluated at the $k^{th}$ sampling point of $Z_i(\cdot)$, for $k = 1, \ldots, n$, $i = 1, 2$, and $\pi_i$ is
the $p_i \times 1$ vector of parameters. So, $E[Z_i(x)] = m_i(x) = f_i(x)\pi_i$ for $i = 1, 2$ and $x \in D$. We take $\epsilon_i$ to be zero mean $n \times 1$ column vector corresponding to the random variation of $Z_i$, and
$Cov(\epsilon_i(x), \epsilon_j(x')) = Cov(Z_i(x), Z_j(x')) = C_{ij}(x, x')$, for $x, x' \in D$ and $i, j = 1, 2$.
Using the notations, $Z = (Z_1^T, Z_2^T)^T$, where $Z$ is a $2n \times 1$ vector, $\epsilon = (\epsilon_1^T, \epsilon_2^T)^T$, $\pi = (\pi_1^T, \pi_2^T)^T$ and $F = \begin{pmatrix}
F_1 & 0 \\
0 & F_2
\end{pmatrix}$ the model in (1) can be rewritten as:

$$
Z = F\pi + \epsilon.
$$

(2)
We are interested in predicting the value of the primary random function \( Z_1(\cdot) \) at \( x_0 \in \mathcal{D} \), using the best linear unbiased predictor (BLUP). The true value of \( Z_1(x_0) \) is denoted by \( Z_0 \), that is, \( Z_1(x_0) = Z_0 \). We consider the cokriging estimator of \( Z_0 \), as suggested by Chiles and Delfiner (2009, chap. 5), an affine function of all available information on \( Z_1(\cdot) \) and \( Z_2(\cdot) \) at the \( n \) sample points, given by:

\[
Z^{**} = \sum_{i=1}^{n} \sum_{j=1}^{n} \lambda_{ij} Z_i(x_j) = \sum_{i=1}^{2} \lambda_i^T Z_i,
\]

where \( \lambda_i = (\lambda_{i1}, \lambda_{i2}, \ldots, \lambda_{in})^T \) is an \( n \times 1 \) vector of weights. This cokriging estimator can be shown to be the BLUP of \( Z_0 \) (see Ver Hoef and Cressie (1993) for details).

Some of the notations that we would use throughout the paper are: \( \sigma_{i0} = Cov(Z_i, Z_0) \) for \( i = 1, 2 \), \( \sigma_0 = (\sigma_{10}^T, \sigma_{20}^T) \) and \( \sigma_{00} = Var(Z_0, Z_0) \). Covariance matrix \( Cov(Z_i, Z_j) = C_{ij} \) for \( i, j = 1, 2 \) and covariance of the entire vector \( Z \) will be denoted by \( \Sigma = \begin{bmatrix} C_{11} & C_{12} \\ C_{21} & C_{22} \end{bmatrix} \). Note \( \Sigma \) is a \( 2n \times 2n \) matrix.

### 2.1 Simple Cokriging Estimation

In a simple cokriging model, the means \( m_i(x) \) are taken to be constant and known. Thus, without loss of generality we may assume in such cases that the \( Z_i \)'s are zero mean processes for \( i = 1, 2 \). For known covariance parameters (Chiles and Delfiner, 2009, Chapter 5) the BLUP of \( Z_0 \) is given by \( Z^{**} = \sigma_0^T \Sigma^{-1} Z \) and the cokriging variance, denoted by \( \sigma_{SK}^2(x_0) \), which is also the mean squared prediction error (MSPE) at \( x_0 \), is given by:

\[
\sigma_{SK}(x_0) = \sigma_{00} - \sigma_0^T \Sigma^{-1} \sigma_0.
\]  \( \hspace{1cm} (3) \)

### 2.2 Ordinary Cokriging Estimation

Another popular model known as ordinary kriging arises when the means are assumed to be constant but unknown, that is, \( m_i(x) = \mu_i, i = 1, 2 \). In this case (Ver Hoef and Cressie (1993), Chiles and Delfiner (2009, Chapter 5)) the BLUP of \( Z_0 \) is \( Z^{**} = \sigma_0^T \Sigma^{-1} Z + (f_0^T - \sigma_0^T \Sigma^{-1} F)(F^T \Sigma^{-1} F)^{-1} F^T \Sigma^{-1} Z. \) The MSPE at \( x_0 \), \( \sigma_{OK}(x_0) \) is given by

\[
\sigma_{OK}(x_0) = \sigma_{00} - \sigma_0^T \Sigma^{-1} \sigma_0 + (f_0 - F^T \Sigma^{-1} \sigma_0)^T (F^T \Sigma^{-1} F)^{-1} (f_0 - F^T \Sigma^{-1} \sigma_0),
\]  \( \hspace{1cm} (4) \)

where \( f_0 = (f_1, 0_{p_2}^T)^T \) is a \( (p_1 + p_2) \times 1 \) vector, \( f_1 \) is the \( p_1 \times 1 \) vector of basis drift functions of \( Z_1(\cdot) \) evaluated at \( x_0 \) and \( 0_{p_2} \) is a \( p_2 \times 1 \) zero vector.
Considering,$$
A = \begin{bmatrix} 0 & F^T \\ F & \Sigma \end{bmatrix}, \quad B = \begin{bmatrix} f_0 \\ \sigma_0 \end{bmatrix}
$$
we could write $\sigma_{OK}^2(x_0)$ in (4) in a more compact form given by:
$$\sigma_{OK}^2(x_0) = \sigma_{00} - B^TA^{-1}B.$$

Throughout this paper we use the notations, $1_n = (1, 1, \ldots, 1)^T_{n \times 1}$, $0_n = (0, 0, \ldots, 0)^T_{n \times 1}$. So, in the case of a bivariate ordinary cokriging model $F$ is a block diagonal matrix given by:
$$F = \begin{bmatrix} 1_n & 0_n \\ 0_n & 1_n \end{bmatrix} \quad \text{and} \quad f_0 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}.$$

### 2.3 Covariance Functions

In this paper two families of covariance structures: a generalized Markov type covariance and a proportional covariance model are studied for obtaining the optimal designs. We assume the covariance structures to be isotropic, that is, $C_{ij}(x, x') = C_{ij}(|x - x'|)$ for $x, x' \in D$. Details of these covariance structures and conditions required for their validity are discussed next.

A Markov type covariance structure is defined for both primary and secondary variables with unit variance in [Chiles and Delfiner (2009), Chapter 5]. In this paper we derive and use generalized version of the Markov type structure. Suppose the two random functions $Z_1(\cdot)$ and $Z_2(\cdot)$ have respective variances $\sigma_{11}$ and $\sigma_{22}$, where $\sigma_{11}, \sigma_{22} > 0$ and correlation coefficient $\rho$, $|\rho| < 1$. In the generalized Markov type structure, the cross-covariance function $C_{12}(\cdot)$ is considered to be proportional to $C_{11}(\cdot)$, that is, $C_{12}(h) = \rho C_{11}(h)$, and $C_{22}(h) = \rho^2 C_{11}(h) + (\sigma_{22} - \rho^2 \sigma_{11}) C_R(h)$ for some valid correlogram $C_R(\cdot)$ and $h \in \mathbb{R}$. Thus, the covariance matrix for the bivariate vector $\mathbf{Z}$ under the Markov structure is of the form:
$$\Sigma = \begin{bmatrix} M_1 & \rho M_1 \\ \rho M_1 & \rho^2 M_1 + (\sigma_{22} - \rho^2 \sigma_{11}) M_R \end{bmatrix},$$

where $(M_1)_{ij} = C_{11}(|x_i - x_j|)$ and $(M_R)_{ij} = C_R(|x_i - x_j|)$ for $i, j = 1, \ldots, n$. In the next result we state the conditions for the validity of the generalized Markov type covariance structure.

**Result 2.1.** Consider two random functions $Z_1(\cdot)$ and $Z_2(\cdot)$ with respective covariance functions $C_{ii}(\cdot)$ and spectral densities $s_i(\cdot)$ for $i = 1, 2$. Consider another valid correlation function $C_R(\cdot)$ with spectral density $s_R(\cdot)$. Then $\Sigma$ as defined in (8) is a valid covariance matrix if and only if $(\sigma_{22} - \rho^2 \sigma_{11}) \geq 0$. 


Proof. The cross-spectral density matrix $S_p(u)$ is,

$$S_p(u) = \begin{bmatrix} s_1(u) & \rho s_1(u) \\ \rho s_1(u) & \rho^2 s_1(u) + (\sigma_{22} - \rho^2 \sigma_{11}) s_R(u) \end{bmatrix}, u \in \mathbb{R}$$

with determinant $f_1(u)(\sigma_{22} - \rho^2 \sigma_{11}) f_R(u)$. Note, that the matrix $S_p(u)$ is positive definite whenever $(\sigma_{22} - \rho^2 \sigma_{11}) \geq 0$, as $s_1(\cdot)$ and $s_R(\cdot)$ correspond to the inverse Fourier transforms of the covariance functions $C_{11}(\cdot)$ and $C_R(\cdot)$. Using the criterion of [Cramér 1940], $\Sigma$ is then a valid covariance matrix if and only if $(\sigma_{22} - \rho^2 \sigma_{11}) \geq 0$.

The second covariance structure that we use is the proportional covariance. In this case the covariance and cross-covariances of the random functions $Z_1(\cdot)$ and $Z_2(\cdot)$ are proportional to a single underlying covariance structure, say $C_P(\cdot)$; that is, $C_{ij}(h) = \sigma_{ij} C_P(h)$ for $i, j = 1, 2$. [Chiles and Delfiner 2009] states that $\Sigma$ is a valid covariance matrix if $\begin{bmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{21} & \sigma_{22} \end{bmatrix}$ is a positive definite matrix. Thus, under the proportional model,

$$\Sigma = \begin{bmatrix} \sigma_{11} P & \sigma_{12} P \\ \sigma_{21} P & \sigma_{22} P \end{bmatrix}, \text{ where } (P)_{ij} = C_P(|x_i - x_j|). \quad (9)$$

We further assumed the covariance structure of $Z_1(\cdot)$ to be exponential with parameter $\theta > 0$. Hence, $C_{11}(h) = \sigma_{11} e^{-\theta |h|}$ in (8) and $C_P(h) = e^{-\theta |h|}$ in (9) for $h \in \mathbb{R}$.

In the next section two optimality criteria based on minimizing cokriging estimation errors for comparing designs are defined.

3 Optimal Designs

The design criterion that we use in this article is based on minimizing the cokriging prediction error. In the context of finding a design, we are essentially interested in choosing a set of distinct points $\{x_1, \ldots, x_n\}$ which maximizes the prediction accuracy of the primary response $Z_1(\cdot)$. To choose such a design an integrated version of MSPE denoted by IMSPE, where,

$$\text{IMSPE} = \int_{x_0 \in D} \text{MSPE}(x_0) dx_0, \quad (10)$$

or alternatively, the supremum of MSPE denoted as SMSPE, where,

$$\text{SMSPE} = \sup_{x_0 \in D} \text{MSPE}(x_0), \quad (11)$$
is used.

We consider the set $\mathcal{D}$ to be a connected subset of $\mathbb{R}$ on which the two random functions $Z_1(\cdot)$ and $Z_2(\cdot)$ are observed. As $\mathcal{D} \subseteq \mathbb{R}$ is connected, we may equivalently consider $\mathcal{D} = [0, 1]$, a similar approach is taken in Antognini and Zagoraiou (2010). Also, the set on which the two random functions are sampled is denoted by $\mathcal{S} = \{x_1, x_2, \ldots, x_n\}$, where $\mathcal{S} \subset \mathcal{D}$. Since replications are not allowed, we assume the points to be ordered, that is, $x_i < x_j$ for $i < j$.

The distance between two consecutive points is denoted by $d_i = x_{i+1} - x_i$, for $i = 1, \ldots, n - 1$, so $d_i \in [0, 1]$ for $i = 1, \ldots, n - 1$ with $\sum_{i=1}^{n-1} d_i = 1$. We equivalently denote the design by the vector $\xi = (d_1, d_2, \ldots, d_{n-1})$ in terms of the vector of distances.

In the upcoming section we will find the optimal design, in terms of the values of $d_i$’s for which IMSPE or SMSPE is minimized.

### 3.1 Optimal designs for a simple cokriging model with known parameters

In this section we determine optimal designs for a simple cokriging model. Lemma 3.1 and 3.2 show that the MSPE at any point $x_0$ depends on the characteristics of the primary random function $Z_1(\cdot)$. In the following Theorem 3.1 we will derive the optimal design. We begin by assuming that the parameters $\sigma_{ij}$, $(i, j = 1, 2)$, $\theta$ and $\rho$ are known.

**Lemma 3.1.** Consider a bivariate simple cokriging model with isotropic random functions $Z_1(\cdot)$ and $Z_2(\cdot)$, respective variances $\sigma_{11}$, $\sigma_{22}$ and correlation coefficient $\rho$. The primary variable $Z_1(\cdot)$ is assumed to have a isotropic exponential covariance structure with parameter $\theta > 0$. The covariance matrix $\Sigma$ is considered to have a generalized Markov type structure as in (8). Then, the MSPE at point $x_0 \in \mathcal{D}$, depends only on the characteristics of the primary variable $Z_1(\cdot)$ and is given by $\text{MSPE}(x_0) = \sigma_{11}(1 - \sigma_{p0}^T P^{-1} \sigma_{p0})$ where, $(\sigma_{p0})_i = e^{-\theta|z_i - x_0|}$ and $(P)_{ij} = e^{-\theta|x_i - x_j|}$ for all $i, j = 1, \ldots, n$.

**Proof.** From (8) we have,

$$
\Sigma = \begin{bmatrix}
M_1 & \rho M_1 \\
\rho M_1 & \rho^2 M_1 + (\sigma_{22} - \rho^2 \sigma_{11}) M_R
\end{bmatrix}.
$$

Thus,

$$
\Sigma^{-1} = \begin{bmatrix}
M_1^{-1} & 0 \\
0 & 0
\end{bmatrix} + \frac{1}{\sigma_{22} - \rho^2 \sigma_{11}} \begin{bmatrix}
\rho^2 M_R^{-1} & -\rho M_R^{-1} \\
-\rho M_R^{-1} & M_R^{-1}
\end{bmatrix}.
$$

(12)
Also,

\[
\sigma_0 = \begin{bmatrix} \sigma_{10} \\ \sigma_{20} \end{bmatrix} = \begin{bmatrix} \sigma_{10} \\ \rho \sigma_{10} \end{bmatrix}.
\] (13)

Putting \( \Sigma^{-1} \) and \( \sigma_0 \) in (3) we get \( \text{MSPE}(x_0) \) as:

\[
\text{MSPE}(x_0) = \sigma_{11} - \sigma_0^T \Sigma^{-1} \sigma_0
= \sigma_{11} - \begin{bmatrix} \sigma_{10}^T & \sigma_{20}^T \end{bmatrix} \Sigma^{-1} \begin{bmatrix} \sigma_{10} \\ \sigma_{20} \end{bmatrix}
= \sigma_{11} - \begin{bmatrix} \sigma_{10}^T & \rho \sigma_{10}^T \end{bmatrix} \begin{bmatrix} M_1^{-1} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \sigma_{10} \\ \rho \sigma_{10} \end{bmatrix}
- \frac{1}{\sigma_{22} - \rho^2 \sigma_{11}} \begin{bmatrix} \sigma_{10}^T & \rho \sigma_{10}^T \end{bmatrix} \begin{bmatrix} \rho^2 M_1^{-1} & -\rho M_1^{-1} \\ -\rho M_1^{-1} & M_1^{-1} \end{bmatrix} \begin{bmatrix} \sigma_{10} \\ \rho \sigma_{10} \end{bmatrix}
= \sigma_{11} - \sigma_{10}^T M_1^{-1} \sigma_{10}.
\]

Under the assumption that \( Z_1(\cdot) \) has an exponential covariance structure with parameter \( \theta > 0 \) and variance \( \sigma_{11} \), we can say \( M_1 = \sigma_{11} P \) and \( \sigma_{10} = \sigma_{11} \sigma_{p0} \). Hence, \( \text{MSPE}(x_0) \) can be rewritten as:

\[
\text{MSPE}(x_0) = \sigma_{11} (1 - \sigma_{p0}^T P^{-1} \sigma_{p0}),
\] (14)

which indicates \( \text{MSPE}(x_0) \) depends only on \( P, \sigma_{p0} \) and \( \sigma_{11} \), that is, the parameters corresponding to the primary variable \( Z_1(\cdot) \).

\textbf{Lemma 3.2.} Consider a bivariate simple cokriging model with isotropic random functions \( Z_1(\cdot) \) and \( Z_2(\cdot) \), with \( Z_1(\cdot) \) being the primary variable. The covariance matrix \( \Sigma \) is assumed to have a proportional covariance structure as in (9), with \( C_P(h) = e^{-|h| \theta}, \theta > 0 \). Then the MSPE at point \( x_0 \in D \), depends only on the characteristics of the primary variable \( Z_1(\cdot) \) and is given by \( \text{MSPE}(x_0) = \sigma_{11} (1 - \sigma_{p0}^T P^{-1} \sigma_{p0}) \) where, \( P \) and \( \sigma_{p0} \) are same as in Lemma 3.1.

\textit{Proof.} From (9) we have,

\[
\Sigma = \begin{bmatrix} \sigma_{11} P & \sigma_{12} P \\ \sigma_{21} P & \sigma_{22} P \end{bmatrix}.
\]
Thus,

\[
\Sigma^{-1} = \frac{1}{\sigma_{11}} \begin{bmatrix} P^{-1} & 0 \\ 0 & 0 \end{bmatrix} + \frac{1}{|P|} \begin{bmatrix} \sigma_{12}\sigma_{21}P^{-1} & -\sigma_{12}P^{-1} \\ \sigma_{11} & -\sigma_{21}P^{-1} \end{bmatrix}.
\]  \tag{15}

Also,

\[
\sigma_0 = \begin{bmatrix} \sigma_{11}\sigma_{p0} \\ \sigma_{12}\sigma_{p0} \end{bmatrix}.
\]  \tag{16}

In this case we have \(\sigma_{12} = \sigma_{21}\) due to isotropy of the covariance function. Using the above expression of \(\Sigma^{-1}\) and \(\sigma_0\) in (3) we get \(\text{MSPE}(x_0)\) as:

\[
\text{MSPE}(x_0) = \sigma_{11} - \sigma_0^T \Sigma^{-1} \sigma_0,
\]

\[
= \sigma_{11} - \frac{1}{\sigma_{11}} \left[ \sigma_{11}\sigma_{p0}^T \sigma_{12}\sigma_{p0}^T \right] \begin{bmatrix} P^{-1} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \sigma_{11}\sigma_{p0}^T \\ \sigma_{12}\sigma_{p0}^T \end{bmatrix} - \frac{1}{|P|} \left[ \sigma_{11}\sigma_{p0}^T \sigma_{12}\sigma_{p0}^T \right] \begin{bmatrix} \sigma_{12}^2P^{-1} & -\sigma_{12}P^{-1} \\ -\sigma_{12}P^{-1} & \sigma_{11}P^{-1} \end{bmatrix} \begin{bmatrix} \sigma_{11}\sigma_{p0}^T \\ \sigma_{12}\sigma_{p0}^T \end{bmatrix}
\]

\[
= \sigma_{11}(1 - \sigma_{p0}^T P^{-1} \sigma_{p0}),
\]  \tag{17}

which indicates \(\text{MSPE}(x_0)\) depends only on \(P, \sigma_{p0}\) and \(\sigma_{11}\), that is, the parameters corresponding to the primary variable \(Z_1(\cdot)\).

**Corollary 3.1.** For simple cokriging models, the \(\text{IMSPE} = \sigma_{11} \left(1 - \int_{[0,1]} \sigma_{p0}^T \sigma_{p0} d(x_0) \right)\)

and the \(\text{SMSPE} = \sigma_{11} \sup_{x_0 \in [0,1]} \left(1 - \sigma_{p0}^T P^{-1} \sigma_{p0} \right)\) depends only on the characteristics of the primary random function \(Z_1(\cdot)\) and is identical for both generalized Markov type and proportional covariance structures.

**Theorem 3.1.** For the bivariate simple cokriging model considered in Lemma 3.1 and Lemma 3.2 an **equispaced** design minimizes the \(\text{IMSPE}\).

**Proof.** From Corollary 3.1 we have,

\[
\text{IMSPE} = \sigma_{11} \left(1 - \int_{[0,1]} \sigma_{p0}^T P^{-1} \sigma_{p0} d(x_0) \right)
\]

\[
= \sigma_{11} \left\{1 - \frac{n - 1}{\theta} + 2 \Phi(\xi) \right\}
\]

(See [46] in Appendix B)
where, $\Phi(\xi) = \sum_{i=1}^{n-1} \phi(d_i)$ and $\phi(d) = \frac{d}{e^{2\theta d} - 1}$. To show that the equispaced design minimizes the IMSPE, we prove that the IMSPE is a Schur-convex function. First note, IMSPE is a symmetric function, that is, it is permutation invariant in the $d_i$'s. Next we show $\frac{\partial \text{IMSPE}}{\partial d_i}$ is an increasing function in $d_i$ for $i = 1, \ldots, n$. We have,

$$\frac{\partial \phi(d)}{\partial d} = \frac{e^{2\theta d} - 1 + 2\theta de^{2\theta d}}{(e^{2\theta d} - 1)^2}$$ which is an increasing function in $d \in (0, 1)$. \hspace{1cm} (18)

Since, $\frac{\partial^2 \phi(d)}{\partial d^2} = \frac{4e^{2\theta d}}{(e^{2\theta d} - 1)^3}(1 + \theta d + e^{2\theta d}(\theta d - 1))$

$$= \frac{4e^{2\theta d}}{(e^{2\theta d} - 1)^3} p(d, \theta) \geq 0, \text{ for } d \in (0, 1)$$

where, $p(d, \theta) = (1 + \theta d + e^{2\theta d}(\theta d - 1)) \geq 0$ and $\frac{\partial^2 \phi(d)}{\partial d^2}|_{d=0} = \frac{\partial^2 \phi(d)}{\partial d^2}|_{d=0} = 0$ and $\frac{\partial^2 \phi(d)}{\partial d^2} > 0$ for $d \in (0, 1]$.

As, $\frac{\partial \text{IMSPE}}{\partial d_i} = 2\sigma_{11} \frac{\partial \phi(d_i)}{\partial d_i}$ for $i = 1, \ldots, n - 1$, using (18) we can say:

$$\frac{\partial \text{IMSPE}}{\partial d_k} \leq \frac{\partial \text{IMSPE}}{\partial d_l} \quad \text{for any } d_k \leq d_l. \hspace{1cm} (19)$$

Thus, using Theorem A.4 from Marshall et al. (1979), we can say that IMSPE is Schur-convex. Hence IMSPE is minimized for an equispaced design. That is, $d_i = \frac{1}{n-1}$ for all $i = 1, \ldots, n - 1$ minimizes the IMSPE.

**Theorem 3.2.** For the bivariate simple cokriging model considered in Lemmas 3.1 and 3.2 an equispaced design minimizes the SMSPE. Thus, the equispaced design is the G-optimal design.

**Proof.** From Lemma 3.1 and 3.2 we have that for $x_0 \in D$,

$$\text{MSPE}(x_0) = \sigma_{11}(1 - \sigma_{10}^T P^{-1} \sigma_{10}).$$

Consider the case when $x_0 \in [x_i, x_{i+1}]$, $i = 1, \ldots, n - 1$. Then from Appendix C (51) we have,

$$\text{MSPE}(x_0) = \sigma_{11} \frac{(1 - e^{-2\theta a})(1 - e^{-2\theta d_i})}{(1 - e^{-2\theta d_i})}, \quad \text{where } a = x_0 - x_i. \hspace{1cm} (20)$$
Since, \( x_0 \in [x_i, x_{i+1}] \), therefore \( a \in [0, d_i] \) for \( i = 1, \ldots, n - 1 \). Now, consider the function:

\[
W_i : [0, d_i] \rightarrow \mathbb{R}
\]

\[
a \mapsto (1 - e^{-2\theta a}) \left(1 - e^{-2\theta(d_i-a)}\right)
\]

We have,

\[
\frac{dW_i(a)}{da} = \frac{2\theta (e^{-2\theta a} - e^{-2\theta(d_i-a)})}{(1 - e^{-2\theta d_i})},
\]

where,

\[
\left. \frac{dW_i(a)}{da} \right|_{a = d_i/2} = 0,
\]

and

\[
\frac{d^2W_i(a)}{da^2} = -4\theta^2 \frac{(e^{-2\theta a} + e^{-2\theta(d_i-a)})}{(1 - e^{-2\theta d_i})} < 0.
\]

From (21) and (22), for \( x_0 \in [x_i, x_{i+1}] \) the MSPE\( (x_0) \) is seen to be maximized at \( x_0 = x_i + \frac{d_i}{2} \), which is the mid-point of the interval \([x_i, x_{i+1}]\). Hence,

\[
\sup_{x_0 \in [x_i, x_{i+1}]} \text{MSPE}(x_0) = \sigma_{11} \frac{1 - e^{-\theta d_i}}{1 + e^{-\theta d_i}}.
\]

Consider, \( W_{\text{sup}}(\cdot) \) to be a function defined on \([0, 1]\) such that \( W_{\text{sup}}(d) = \frac{1 - e^{-\theta d}}{1 + e^{-\theta d}} \), then \( W_{\text{sup}}(d) \) is an increasing function, as \( W'_{\text{sup}}(d) = \frac{2\theta e^{-\theta d}}{1 + e^{-\theta d}} > 0 \). Hence,

\[
\text{SMPSE} = \sup_{x_0 \in [0,1]} \text{MSPE}(x_0) = \max_{i=1,\ldots,n-1} W_{\text{sup}}(d_i) \quad \text{(from (23))}
\]

\[
= \sigma_{11} \max_{i=1,\ldots,n-1} \frac{1 - e^{-\theta d_i}}{1 + e^{-\theta d_i}}
\]

\[
= \sigma_{11} W_{\text{sup}}(\max_i d_i)
\]
From (24), for known $\theta$ and $\sigma_{11}$, the SMSPE is a function of $\max_i d_i$. Since $W_{sup}(d)$ is an increasing function, therefore SMSPE is minimized when $\max_i d_i$ is minimized, which occurs for an equispaced partition.

4 Optimal Designs for Simple Cokriging Models when Parameters are Unknown

In real life, when designing an experiment, the exponential covariance parameters $\theta$ and $\sigma_{11}$, are usually unknown with very little prior information. In this section we discuss optimal design for simple cokriging models similar to those considered in Lemma 3.1 and 3.2 when the parameters are unknown, but prior distributions on these parameters are assumed to be known. The prior distributions on the covariance parameters are incorporated into the optimisation criteria by integrating over these distributions. This approach is known as the pseudo-Bayesian approach to optimal designs and has been used previously by Chaloner and Larntz (1989), Dette and Sperlich (1996), Woods and van de Ven (2011), Mylona et al. (2014), Singh and Mukhopadhyay (2016) and Singh and Mukhopadhyay (2019). We start by assuming $\theta$ and $\sigma_{11}$ are independent and their respective distributions are $r(\cdot)$ and $t(\cdot)$. A very high value of $\theta$ would mean that the covariance matrix for $Z_1(\cdot)$ is approximately an identity matrix, implying zero dependence among neighbouring. Since this is not reasonable for such correlated data, we assume, $0 < \theta_1 < \theta < \theta_2 < \infty$.

Using a pseudo-Bayesian approach as in Chaloner and Larntz (1989) we define risk functions corresponding to each design criterion,

$$R_1(\xi) = E[IMSP\E\theta, \sigma_{11}, \xi)],$$

$$R_2(\xi) = E[SMSP\E\theta, \sigma_{11}, \xi)].$$

Our objective is to select the designs that minimize these risks.

**Theorem 4.1.** Consider the bivariate cokriging models as in Theorem 3.1. The parameters $\theta$ and $\sigma_{11}$ are assumed to be independent with prior probability density functions $r(\cdot)$ and $t(\cdot)$ respectively, where the support of $r(\cdot)$ is $(\theta_1, \theta_2)$ for $\theta_1, \theta_2 > 0$. Then an equispaced design is optimal with respect to the risk function $R_1(\xi)$.

**Proof.** Consider $R_1 : \mathcal{I}^{n-1} \rightarrow \mathbb{R}$, where $\mathcal{I} = [0, 1]$. $R_1(\cdot)$ is symmetric on $\mathcal{I}^{n-1}$ as IMSPE is symmetric on $\mathcal{I}^{n-1}$, that is $R_1$ is permutation invariant in $d_i$. If we can show $\frac{\partial R_1(\xi)}{\partial d_k} \geq 0$, for any $d_l \geq d_k$, where $k, l = 1, \ldots, n - 1$, then as before in Theorem 3.1 using the Schur-convexity of $R_1$ we will prove the equispaced design is optimal.
Let \( q_1(\theta, \xi) = \{1 - \frac{n - 1}{\theta} + 2\Phi(\xi)\} \), then \( R_1(\xi) = \int_0^\infty \int_{\theta_1}^{\theta_2} \sigma_{11} q_1(\theta, \xi) \ r(\theta) \ t(\sigma_{11}) \ d(\sigma_{11}) \ d(\theta). \)

Consider,

\[
\Delta = \frac{\partial R_1(\xi)}{\partial d_l} - \frac{\partial R_1(\xi)}{\partial d_k}
\]

\[
= \frac{\partial}{\partial d_l} \int_0^\infty \int_{\theta_1}^{\theta_2} \sigma_{11} q_1(\theta, \xi) \ r(\theta) \ t(\sigma_{11}) \ d(\sigma_{11}) \ d(\theta)
\]

\[
- \frac{\partial}{\partial d_k} \int_0^\infty \int_{\theta_1}^{\theta_2} \sigma_{11} q_1(\theta, \xi) \ r(\theta) \ t(\sigma_{11}) \ d(\sigma_{11}) \ d(\theta)
\]

\[
= \int_0^\infty \sigma_{11} \ t(\sigma_{11}) \ d(\sigma_{11}) \left[ \int_{\theta_1}^{\theta_2} \left( \frac{\partial q_1(\theta, \xi)}{\partial d_l} - \frac{\partial q_1(\theta, \xi)}{\partial d_k} \right) r(\theta) \ d(\theta) \right]
\]

(Using Leibniz’s Rule (Protter et al., 2012, chapter 8))

\[
= E_t[\sigma_{11}] \left( 2 \int_{\theta_1}^{\theta_2} \left( \frac{\partial \Phi(\xi)}{\partial d_l} - \frac{\partial \Phi(\xi)}{\partial d_k} \right) r(\theta) \ d(\theta) \right)
\]

\[
= E_t[\sigma_{11}] \left( 2 \int_{\theta_1}^{\theta_2} \left( \frac{\partial \phi(d_l)}{\partial d_l} - \frac{\partial \phi(d_k)}{\partial d_k} \right) \ r(\theta) \ d(\theta) \right).
\]

For \( d_l \geq d_k \), the quantity \( \Delta \) in (27) is positive, since from (18) we have \( \frac{\partial \phi(d_l)}{\partial d_l} - \frac{\partial \phi(d_k)}{\partial d_k} > 0 \) for any \( d_l > d_k \). Thus, \( R_1(\xi) \) is Schur-convex and is minimized for an equispaced design. \( \square \)

**Theorem 4.2.** Consider the bivariate cokriging models as in Theorem 3.2. The parameters \( \theta \) and \( \sigma_{11} \) are assumed to be independent with prior probability density functions \( r(\cdot) \) and \( t(\cdot) \) respectively, with the support of \( r(\cdot) \) of the form \( (\theta_1, \theta_2) \), for \( \theta_1, \theta_2 > 0 \), then an equispaced design is optimal with respect to the risk function \( R_2(\xi) \).

**Proof.** From (24) we can write,

\[
SMPSE = \sigma_{11} W_{\sup}(\max_i d_i).
\]

Thus,

\[
R_2(\xi) = \int_0^\infty \int_{\theta_1}^{\theta_2} \sigma_{11} W_{\sup}(\theta, \max_i d_i) \ r(\theta) \ t(\sigma_{11}) \ d(\sigma_{11}) \ d(\theta)
\]

\[
= \int_0^\infty \sigma_{11} \ t(\sigma_{11})d(\sigma_{11}) \int_{\theta_1}^{\theta_2} W_{\sup}(\theta, \max_i d_i) \ r(\theta) \ d(\theta)
\]

\[
= E_t[\sigma_{11}] \int_{\theta_1}^{\theta_2} W_{\sup}(\theta, \max_i d_i) \ r(\theta) \ d(\theta). \quad (28)
\]
As $W_{sup}(\theta, d)$ is an increasing function of $d$, (28) shows $R_2$ is minimized for an equispaced design, since $\max_i d_i$ is minimized for an equispaced design.

Thus, we have proved the equispaced design is the I-optimal and G-optimal for simple cokriging models for parameters known or unknown.

5 Case Study

In this section, we are interested in designing a river monitoring network for efficient prediction of water quality. A pilot data set of water quality data from river Neyyar in southern India is used to obtain preliminary information about parameters. We will illustrate how the theory that we developed in Section 3 and 4 is applied to this problem. The image of the river is shown in Figure 1 where the monitoring stations on the river basin are marked in red. We will compare the performance of the equispace design with the given design of stations.

The location of each monitoring station is specified by its geographical coordinates, that is, latitude and longitude. At each of these stations, measurements are taken for two variables: pH and phosphate which are used to measure the quality of water. For carrying out the analysis, that is, gathering information on the covariance and cross covariance structures and

![Neyyar River Basin showing sampling stations](image)

Figure 1: Monitoring station postions on the Neyyar river basin. We use the station locations and data within the green area.
parameters of the two responses, we use data from a single branch of the river with 17 stations (see the region encircled in green in Figure 1). We denote this branch of the river by $D_2 (\subseteq \mathbb{R}^2)$ and denote the set of sampling points on this river branch by $S_2 = \{y_1, \ldots, y_n\} (\subseteq D_2)$, where each $y_i = (\text{latitude}_i, \text{longitude}_i), i = 1, \ldots, n$ for $n=17$. Let $y_1$ and $y_n$ respectively be the starting (station 6) and the end point (station 26) of the river branch, and suppose we assume $y_i$ is upstream of $y_j$ if $i < j$ for all $i, j = 1, \ldots, 17$.

The results that we obtained for determining optimal designs in earlier sections were based on one-dimensional inputs, that is, where the region of interest was denoted by $D \subset \mathbb{R}$. In fact, without loss of generality we had assumed $D = [0, 1]$. So, we first use a transformation on our two dimensional input sets $S_2$ and $D_2$ given by:

$$\varphi : D_2 \longrightarrow [0, 1]$$

$$y \mapsto \frac{|| y - y_1 ||}{|| y_n - y_1 ||},$$

where $|| u - v ||$ is the geodesic stream distance between the two points $u$ and $v$ along the river and $u, v \in D_2$. The geodesic distance could be used to calculate distance on earth surface and is discussed in Banerjee et al. (2014) in details. The stream distance, is the shortest distance between two locations on a stream, where the distance is computed along the stream Ver Hoef et al. (2006). In this case it was not possible to calculate the exact stream distance using solely the coordinates of monitoring points. So, the stream distance between two adjacent points was approximated by the geodesic distance between the two points.

The transformed region of interest $\varphi(D_2) = D_1 = [0, 1]$ and the set of sampling points $\varphi(S_2) = S_1$ are one dimensional. We had to constrain ourselves to a single branch of river as, a single branch of river is connected and hence can be considered to be a one dimensional object.

For example, consider stations 10, 18 and 23 which are very close to the main branch, but if included then this transformation could not be applied to transform the set of sampling points to a one dimensional set. The transformed set of observation points is given by $D_1 = \{x_1, x_2, \ldots, x_n\}$ where $\varphi(y_i) = x_i$ for all $i = 1, \ldots, n$ and $n = 17$. Also, by definition $x_1 = 0, x_n = 1$ and $x_i < x_j$ for $i < j$. We define $d_i = x_{i+1} - x_i$ for $i = 1, \ldots, 16$.

We consider the pH level (a scalar with no units) as the primary variable $Z_1(\cdot)$, and phosphate concentration (measured in mg/l) as the secondary variable $Z_2(\cdot)$, with both the variables centered and scaled. See the plots of the centered and scaled values of pH and Phosphate (in Figure 2) versus distance.

We tried to fit a linear regression model for both the responses. We considered the linear model with pH as the response and distance as covariate. However, we found that the p-value for intercept and slope of variable pH to be much higher than 0.5. We saw a similar trend in the phosphate model. Hence, we assume the mean responses are not functions of
Figure 2: Plots of standardized values of PH and Phosphate versus distance

distances from the plots in Figure 2. We discern no clear pattern so, we safely conclude that
using the assumption of constant mean (simple kriging) would be reasonable for both variables.
To investigate the covariance structure and corresponding parameters we conducted a model
fit by likelihood maximization, separately for each variable. Table 1 shows the results, and
suggests that an exponential variance structure is a reasonable choice for both variables. The
likfit function from the geoR package (R-3.6.0 software) was used in our computations. We
took the nugget effect here to be zero. Using the information from the univariate analysis of
pH and phosphate we next try to set up the appropriate bivariate simple cokriging model.

The results from Table 1 for pH and phosphate indicate a large difference between
$\hat{\theta}_1$ and $\hat{\theta}_2$; thus it seems more appropriate to assume a generalized Markov type bivariate
covariance structure rather than a proportional covariance structure in the bivariate cokriging
model. Based on the assumption of normal errors , the log-likelihood function is:

$$l = -\frac{n}{2} \log(2\pi) - \frac{1}{2} \log[det(\Sigma)] - \frac{1}{2} Z^T \Sigma^{-1} Z,$$

where $Z = (Z_1, Z_2)^T$, $\Sigma = \begin{bmatrix} M_1 & \rho M_1 \\ \rho M_1 & \rho^2 M_1 + (\sigma_{22} - \rho^2 \sigma_{22}) M_2 \end{bmatrix}$, and $M_2$ is chosen to be the
identity matrix.

Using the optim function in (R-3.6.0 software) we find the MLEs to be $\hat{\theta}_1 = 17.12$, $\sigma_{11} = 0.85$, $\sigma_{22} = 0.94$, $\hat{\rho} = .25$ and $l = -27.74$.

Illustration 5.1. Relative efficiency when parameter values are known
| Covariance Model | $C(h) = \sigma^2 \rho(h)$ | Log-Likelihood | Variance | Parameter $(\theta, \kappa)$ |
|------------------|--------------------------|----------------|----------|---------------------------|
| Exponential      | $\sigma^2 \exp(-\theta|h|)$ | -20.28         | 0.85     | 16.95                     |
| Gaussian         | $\sigma^2 \exp(-(\theta|h|)^2)$ | No Convergence | NA       | NA                        |
| Spherical        | $\sigma^2 \left\{ \begin{array}{ll} 1 - 1.5h\theta + 0.5(\theta\theta)^3, & \text{if } h < \frac{1}{\theta} \\ 0, & \text{otherwise} \end{array} \right.$ | -20.74   | 0.96     | 7.90                      |
| Matern           | $\sigma^2 \frac{1}{2(\kappa-1)\Gamma(\kappa)}(h\theta)^\kappa K_\kappa(h\theta)$ | -20.15   | 0.83     | (11.09, 0.35)             |

| Covariance Model | $C(h) = \sigma^2 \rho(h)$ | Log-Likelihood | Variance | Parameter $(\theta, \kappa)$ |
|------------------|--------------------------|----------------|----------|---------------------------|
| Exponential      | $\sigma^2 \exp(-\theta|h|)$ | -23.19         | 0.97     | 38.35                     |
| Gaussian         | $\sigma^2 \exp(-(\theta|h|)^2)$ | No Convergence | NA       | NA                        |
| Spherical        | $\sigma^2 \left\{ \begin{array}{ll} 1 - 1.5h\theta + 0.5(\theta\theta)^3, & \text{if } h < \frac{1}{\theta} \\ 0, & \text{otherwise} \end{array} \right.$ | -23.09   | 0.95     | 19.02                     |
| Matern           | $\sigma^2 \frac{1}{2(\kappa-1)\Gamma(\kappa)}(h\theta)^\kappa K_\kappa(h\theta)$ | -23.85   | 0.97     | (0.01, 0.003)             |

Table 1: Results of Likelihood Analysis of pH and Phosphate for Different Covariance Models

The design given for the pilot monitoring network is denoted by $\xi_0$, which is obtained by considering the 17 points on the river and applying the transformation $\varphi(\cdot)$. We computed $\xi_0 = \{0.04, 0.02, 0.04, 0.09, 0.2, 0.06, 0.12, 0.13, 0.04, 0.04, 0.02, 0.05, 0.04, 0.07, 0.02, 0.02\}$. We also denote the equispaced design by $\xi^*$, where $\xi^*_i = \frac{1}{n - 1}$ for all $i = 1, \ldots, n$ and $n = 17$. Relative efficiency based on IMSPE of design $\xi_0$ with respect to the optimal design $\xi^*$ is defined as the ratio, $\frac{\text{IMSPE}(\xi^*)}{\text{IMSPE}(\xi_0)}$. For known parameters, using the expression of IMSPE in Theorem 3.1, the relative efficiency of the river network (or design) used is found to be 0.797. Similarly, for the SMSPE criterion we define the ratio as $\frac{\text{SMSPE}(\xi^*)}{\text{SMSPE}(\xi_0)}$. For the SMSPE criterion, using Theorem 3.2, the relative efficiency of the river network is 0.524. Note, that relative efficiency values (< 1) in both cases indicate an increase in prediction accuracy when using equispaced designs.

**Illustration 5.2. Relative efficiency for unknown parameters**

Consider, $\theta \sim \text{Unif}(\theta_1, \theta_2)$ and $\sigma_{11} \sim t(\cdot)$ for some density function $t(\cdot)$. The risks are then,

$$\mathcal{R}_1(\xi) = E_\sigma \left[ 1 - \frac{n - 1}{\theta_2 - \theta_1} \ln \frac{\theta_2}{\theta_1} + \frac{1}{\theta_2 - \theta_1} \sum_{i=1}^{n-1} \ln \left( \frac{e^{2\theta_2 d_i} - 1}{e^{2\theta_1 d_i} - 1} \right) \right]$$
and,

\[ R_2(\xi) = E_{\sigma} \frac{1}{\theta_2 - \theta_1} \frac{1}{d_{\text{max}}} \left[ 2 \ln \frac{1 + e^{-\theta_2 d_{\text{max}}}}{1 + e^{-\theta_1 d_{\text{max}}}} + d_{\text{max}}(\theta_2 - \theta_1) \right]. \]

where \( d_{\text{max}} \) is written as \( d_{\text{max}} \) and \( E_{\sigma} = E_t[\sigma_{11}] \). The relative efficiency is then \( \frac{R_i(\xi^*)}{R_i(\xi_0)} \), \( i = 1, 2 \).

Using \( \hat{\theta} = 17.12 \), we choose \( \theta_1 \) and \( \theta_2 \) such that the mean of the interval is \( \hat{\theta} \). Varying the range of values for \( \theta_1 \) and \( \theta_2 \), the relative risks are shown in the following table. From Table 2

| \( \theta_1 \) | \( \theta_2 \) | \( \frac{R_1(\xi^*)}{E_{\sigma}} \) | \( \frac{R_1(\xi_0)}{E_{\sigma}} \) | \( \frac{R_1(\xi^*)}{R_1(\xi_0)} \) | \( \frac{R_2(\xi^*)}{E_{\sigma}} \) | \( \frac{R_2(\xi_0)}{E_{\sigma}} \) | \( \frac{R_2(\xi^*)}{R_2(\xi_0)} \) |
|---|---|---|---|---|---|---|---|
| 16.62 | 17.62 | 0.332 | 0.434 | 0.766 | 0.489 | 0.933 | 0.524 |
| 16.12 | 18.12 | 0.332 | 0.433 | 0.766 | 0.489 | 0.933 | 0.524 |
| 15.12 | 19.12 | 0.332 | 0.433 | 0.766 | 0.489 | 0.932 | 0.525 |
| 12.12 | 22.12 | 0.330 | 0.430 | 0.768 | 0.486 | 0.923 | 0.527 |

Table 2: Relative risk of given design - IMSPE and SMSPE criterion

we note small change in the relative efficiency for changes in \( \theta_1 \) and \( \theta_2 \), suggests that the criterion is robust to the changes in the prior information. This robustness persists when we change the values of \( \hat{\theta} \). We checked the values of relative efficiency for \( \hat{\theta} = 7.12, 27.12 \) and \( 47.12 \), however the results are not shown here.

6 Optimal Designs for Ordinary Cokriging Models

In this section we discuss optimal designs for bivariate ordinary cokriging models with generalized Markov type and proportional covariance structures. In case of ordinary cokriging the mean of the two random functions \( Z_1(\cdot) \) and \( Z_2(\cdot) \) are assumed to be unknown and constant (for details see Section 2.2). Taking a similar approach as before, we start by showing, in Lemmas 6.1 and 6.2 that the MSPE at \( x_0 \) depends only on the characteristics of the primary variable for both covariance structures. Further in this section we prove in Theorems 6.1 and 6.2 that the equispaced design is the optimal G-optimal design, irrespective of the covariance parameters being known or unknown. Numerical simulations are used, to show that equispaced design is I-optimal in Proposition 6.1.

**Lemma 6.1.** Consider a bivariate ordinary cokriging model for isotropic random functions \( Z_1(\cdot) \) and \( Z_2(\cdot) \) with respective variances \( \sigma_{11}, \sigma_{22} \) and correlation coefficient \( \rho \). The primary variable \( Z_1(\cdot) \) is assumed to have a isotropic exponential covariance structure with parameter
\( \theta > 0. \) The cross covariance structure is assumed to be of the generalized Markov type. Then the MSPE at point \( x_0 \in \mathcal{D} \) depends only on the characteristics of the primary variable \( Z_1(\cdot) \).

**Proof.** From (6) we have,

\[
\text{MSPE}(x_0) = \sigma_{11} - B^T A^{-1} B
\]

\[
= \sigma_{11} - tr(B^T A^{-1} B)
\]

\[
= \sigma_{11} - tr(BB^T A^{-1}).
\]

Let,

\[
g_1 = M_1^{-1} 1_n, \quad m_1 = 1_n^T M_1^{-1} 1_n, \quad g_p = P^{-1} 1_n, \quad F(\xi) = 1_n^T P^{-1} 1_n.
\]

From (54) in Appendix D we have:

\[
\text{MSPE}(x_0) = \sigma_{11} + \frac{1}{m_1} - \frac{2}{m_1} tr(g_1^T \sigma_{10}) - tr(M_1^{-1} \sigma_{10} \sigma_{10}^T) + \frac{1}{m_1} tr(g_p^T \sigma_{p0} \sigma_{p0}^T)
\]

where, \( M_1 = \sigma_{11} P \) and \( \sigma_{10} = \sigma_{11} \sigma_{p0} \) as in Lemma 3.1 Then,

\[
\text{MSPE}(x_0) = \sigma_{11} \left(1 + \frac{1}{F(\xi)} - \frac{2}{F(\xi)} tr(g_1^T \sigma_{p0}) + \frac{1}{F(\xi)} tr(g_p^T g_p^T \sigma_{p0} \sigma_{p0}^T) - tr(P^{-1} \sigma_{p0} \sigma_{p0}^T)\right),
\]

which shows, MSPE\((x_0)\) depends only on the covariance parameters of \( Z_1(\cdot) \). \(\square\)

**Lemma 6.2.** Consider a bivariate ordinary cokriging model with isotropic random functions \( Z_1(\cdot) \) and \( Z_2(\cdot) \), and \( Z_1(\cdot) \) as the primary variable. The covariance matrix \( \Sigma \) is assumed to have a proportional covariance structure as in (9), with \( C_P(h) = e^{-\theta|h|}, \theta > 0 \). Then, the MSPE at point \( x_0 \) depends only on the characteristics of primary variable \( Z_1(\cdot) \).

**Proof.** Taking the matrix \( P \) as \( P_{ij} = e^{-\theta|x_i-x_j|} \) for all \( i, j = 1, \ldots, n \), from (6) and (57) in Appendix D, we have:

\[
\text{MSPE}(x_0) = \sigma_{11} - B^T A^{-1} B
\]

\[
= \sigma_{11} - tr(A^{-1} BB^T)
\]

\[
= \sigma_{11} \left(1 + \frac{1}{F(\xi)} - \frac{2}{F(\xi)} tr(g_1^T \sigma_{p0}) + \frac{1}{F(\xi)} tr(g_p^T g_p^T \sigma_{p0} \sigma_{p0}^T) - tr(P^{-1} \sigma_{p0} \sigma_{p0}^T)\right).
\]

Thus, for the proportional covariance also, the MSPE\((x_0)\) depends on the covariance parameters of \( Z_1(\cdot) \). \(\square\)
Define, we will first show that

Consider that

For ordinary cokriging models also, the

and the

depends only on the characteristics of the primary random function \(Z_1(\cdot)\) and is identical for both generalized Markov type and proportional covariance structures.

In the following Theorem 6.1 we prove that the equispaced design is an optimal G-optimal design.

**Theorem 6.1.** For the bivariate ordinary cokriging model specified in Lemmas 6.1 and 6.2, an equispaced design is optimal with respect to the SMSPE criterion.

**Proof.** From Lemmas 6.1 and 6.2 we have:

\[
MSPE(x_0) = \sigma_{11} \left( 1 + \frac{1}{F(\xi)} - \frac{2\text{tr}(g_p^T \sigma_p)}{F(\xi)} + \frac{\text{tr}(g_p g_p^T \sigma_p \sigma_p^T)}{F(\xi)} - \text{tr}(P^{-1} \sigma_p \sigma_p^T) \right)
\]

\[
= \sigma_{11} \left( 1 - \sigma_p^T P^{-1} \sigma_p + \frac{1}{F(\xi)} \left( 1 - 2 g_p^T \sigma_p + \text{tr}(g_p g_p^T \sigma_p \sigma_p^T) \right) \right)
\]

\[
= \sigma_{11} \left( 1 - \sigma_p^T P^{-1} \sigma_p + \frac{1}{F(\xi)} \left( 1 - 2 1_n^T P^{-1} \sigma_p + \sigma_p^T P^{-1} 1_n 1_n^T P^{-1} \sigma_p \right) \right)
\]

\[
= \sigma_{11} \left( 1 - \sigma_p^T P^{-1} \sigma_p + \frac{1}{F(\xi)} \left( 1 - 1_n^T P^{-1} \sigma_p \right)^2 \right).
\]

We want to find \(\sup_{x_0 \in [0,1]} MSPE(x_0)\) and minimize it with respect to \(\xi\). We use the fact that,

\[
\sup_{x_0 \in [0,1]} MSPE(x_0) = \max_{i=1} \sup_{x_0 \in [x_i,x_{i+1}]} MSPE(x_0)
\]

\[
= \sigma_{11} \max_{i=1} \sup_{x_0 \in [x_i,x_{i+1}]} \left( 1 - \sigma_p^T P^{-1} \sigma_p + \frac{1}{F(\xi)} \left( 1 - 1_n^T P^{-1} \sigma_p \right)^2 \right).
\]

Consider that \(x_0 \in [x_i,x_{i+1}]\) for some \(i = 1, \ldots, n-1\).

We will first show that \(\sup_{x_0 \in [x_i,x_{i+1}]} \left( 1 - 1_n^T P^{-1} \sigma_p \right)^2\) is attained at \(x_0 = x_i + \frac{d_i}{2}\).

Define, \(a = x_0 - x_i\), then \(a \in [0,d_i]\) and from (52) in Appendix C we have,

\[
1_n^T P^{-1} \sigma_p = \frac{e^{-\theta a} + e^{-\theta(d_i-a)}}{1 + e^{-\theta d_i}}.
\]
Define the function,
\[
U_i : [0, d_i] \to \mathbb{R}
\]
\[
a \mapsto \left( 1 - \frac{e^{-\theta a} + e^{-\theta(d_i-a)}}{1 + e^{-\theta d_i}} \right)^2.
\]

Then,
\[
\frac{dU_i(a)}{da} = -2\theta \begin{bmatrix}
Term I \\
Term II
\end{bmatrix}
\]

where,
\[
\left. \frac{dU_i(a)}{da} \right|_{a = d_i/2} = 0
\]

and
\[
\frac{d^2U_i(a)}{da^2} = -4\theta^2 \left( \frac{1 - e^{-\theta d_i/2}}{1 + e^{-\theta d_i}} \right)^2 e^{-\theta d_i} < 0.
\]

From (30) and (31) we see \(U_i(\cdot)\) attains a local maxima at \(a = \frac{d_i}{2}\) and \(U_i(\frac{d_i}{2}) = \left( 1 - \frac{2e^{-\theta d_i/2}}{1 + e^{-\theta d_i}} \right)^2 > 0\). To find the point of maxima \(a = d_i/2\) we set Term II in (29) equal to zero. Any other point \(a_1\) at which \(U'(a_1) = 0\) is obtained by setting Term I equal to zero, however, those points could not be the maxima as \(U_i(a_1)\) is zero.

Hence, we have shown that \(\sup_{a \in [0, d_i]} U_i(a) = \sup_{x_0 \in [x_i, x_{i+1}]} \left( 1 - \frac{1^T P^{-1} \sigma_0}{n} \right)^2\) is attained at \(a = \frac{d_i}{2}\) or \(x_0 = x_i + \frac{d_i}{2}\) for some \(i = 1, \ldots, n - 1\), which is the mid-point of the interval \([x_i, x_{i+1}]\).

Since, for any \(i = 1, \ldots, n - 1\),
\[
\sup_{x_0 \in [x_i, x_{i+1}]} \left( 1 - \frac{1^T P^{-1} \sigma_0}{n} \right)^2 = U_i(\frac{d_i}{2})
\]
\[
= \left( 1 - \frac{2e^{-\theta d_i/2}}{1 + e^{-\theta d_i}} \right)^2
\]

Define \(U_{\text{sup}}(\cdot)\) on \([0, 1]\) such that \(U_{\text{sup}}(d) = \left( 1 - \frac{2e^{-\theta d/2}}{1 + e^{-\theta d}} \right)^2\), and \(U_{\text{sup}}(\cdot)\) is an increasing func-
tion in $d$ as $U'_{\text{sup}}(d) = 2\theta e^{-\theta d/2} \frac{(1 - e^{-\theta d/2})(1 - e^{-\theta d})}{(1 + e^{-\theta d})^3} > 0$.

Usually, supremum are not additive. However, if two functions $f_1, f_2 : \mathcal{D}_1 \mapsto \mathcal{D}_2$, where $\mathcal{D}_1, \mathcal{D}_2 \subseteq \mathbb{R}$ both attain supremum at the same point $x_1 \in \mathcal{D}_1$, then we have $\sup_{x \in \mathcal{D}_1} f_1(x) + f_2(x) = \sup_{x \in \mathcal{D}_1} f_1(x) + \sup_{x \in \mathcal{D}_1} f_2(x)$. We proved above that $\sup_{x_0 \in [x_i, x_{i+1}]} \left( 1 - \frac{1}{n} \mathbf{P}^{-1} \mathbf{\sigma}_{\mathbf{p}_0} \right)^2$ is attained at $x_0 = x_i + \frac{d_i}{2}$ and is equal to $U_{\text{sup}}(d_i)$. From the proof of Theorem 3.2 we have already seen $\sup_{x_0 \in [x_i, x_{i+1}]} \left( 1 - \mathbf{\sigma}_{\mathbf{p}_0}^T \mathbf{P}^{-1} \mathbf{\sigma}_{\mathbf{p}_0} \right)$ is attained at $x_0 = x_i + \frac{d_i}{2}$. Thus,

$$\sup_{x_0 \in [x_i, x_{i+1}]} \text{MSEP}(x_0) = \sigma_{11} \sup_{x_0 \in [x_i, x_{i+1}]} \left( 1 - \mathbf{\sigma}_{\mathbf{p}_0}^T \mathbf{P}^{-1} \mathbf{\sigma}_{\mathbf{p}_0} + \frac{1}{F(\mathbf{\xi})} \left( 1 - \frac{1}{n} \mathbf{P}^{-1} \mathbf{\sigma}_{\mathbf{p}_0} \right)^2 \right)$$

$$= \sigma_{11} \left( \sup_{x_0 \in [x_i, x_{i+1}]} \left( 1 - \mathbf{\sigma}_{\mathbf{p}_0}^T \mathbf{P}^{-1} \mathbf{\sigma}_{\mathbf{p}_0} \right) + \frac{1}{F(\mathbf{\xi})} \sup_{x_0 \in [x_i, x_{i+1}]} \left( 1 - \frac{1}{n} \mathbf{P}^{-1} \mathbf{\sigma}_{\mathbf{p}_0} \right)^2 \right)$$

$$= \sigma_{11} \left( W_{\text{sup}}(d_i) + \frac{U_{\text{sup}}(d_i)}{F(\mathbf{\xi})} \right).$$ (32)

Hence,

$$\text{SMSPE} = \sigma_{11} \max_{i=1}^{n-1} \left( W_{\text{sup}}(d_i) + \frac{U_{\text{sup}}(d_i)}{F(\mathbf{\xi})} \right)$$

$$= \sigma_{11} \left( W_{\text{sup}}(\max_i d_i) + \frac{U_{\text{sup}}(\max_i d_i)}{F(\mathbf{\xi})} \right)$$ (as, $F(\mathbf{\xi})$ permutation invariant). (33)

Since, $U_{\text{sup}}(\cdot)$ is an increasing function, so, $\max_{i=1}^{n-1} U_{\text{sup}}(d_i) = U_{\text{sup}}(\max_{i=1}^{n-1} d_i)$ and, $\max_{i=1}^{n-1} d_i$ is minimized for an equispaced partition. From Theorem 3.2, we already have $\max_{i=1}^{n-1} W_{\text{sup}}(d_i)$ is minimized for an equispaced partition. Further, from Appendix A $\frac{1}{F(\mathbf{\xi})}$ is seen to be minimized for an equispaced partition. So, the SMSPE in this case for known $\theta$ and $\sigma_{11}$ is minimized for an equispaced design. \qed

In Proposition 6.1 we find an expression for IMSPE for ordinary cokriging. Due to the presence of non-convex terms in the expression we take a different technique to find the optimal solution. We use the Lagrange multiplier method for constrained optimization as given in [Bertsekas 2014, chapter 1]. We first prove that an equispaced design is a regular point for the Lagrangian function $\mathcal{L}(\cdot, \cdot)$, which means this design could potentially be an optimal design. However, due to complexity of the Hessian matrix of $\mathcal{L}$ we could not proceed further in our mathematical investigation and used numerical simulations. The simulations
results suggest that an equispaced design is I-optimal.

**Proposition 6.1.** For a bivariate ordinary cokriging model as specified in Lemmas 6.1 and 6.2 an equispaced design is optimal with respect to the IMSPE criterion.

**Proof.** We first obtain the expression for IMSPE using MSPE\(x_0\) calculated as in Lemmas 6.1 and 6.2.

\[
\text{IMSPE} = \int_{[0,1]} \text{MSPE}(x_0) \, dx_0 \\
= \sigma_{11} \left( 1 + \frac{1}{F(\xi)} - \frac{2}{F(\xi)} \int_0^1 \text{tr}(g_p g_p^T \sigma_{p0} \sigma_{p0}) \, dx_0 \\
+ \frac{1}{F(\xi)} \int_0^1 \text{tr}(g_p g_p^T \sigma_{p0} \sigma_{p0}) \, dx_0 - \int_0^1 \text{tr}(P^{-1} \sigma_{p0} \sigma_{p0}^T) \, dx_0 \right). \tag{34}
\]

From (46), (48) and (47) in Appendix B we have,

\[
\int_0^1 \text{tr}(g_p g_p^T \sigma_{p0}) \, dx_0 = \frac{2}{\theta} \left( F(\xi) - 1 \right),
\]

\[
\int_0^1 \text{tr}(P^{-1} \sigma_{p0} \sigma_{p0}^T) \, dx_0 = \frac{n-1}{\theta} - 2\Phi(\xi) \text{ and}
\]

\[
\int_0^1 \text{tr}(g_p g_p^T \sigma_{p0} \sigma_{p0}) \, dx_0 = \frac{F(\xi) - 1}{\theta} + 2 \sum_{i=1}^{n-1} \frac{d_i e^{\theta d_i}}{(1 + e^{\theta d_i})^2}.
\]

Putting the above expressions in (34) we get,

\[
\text{IMSPE} = \sigma_{11} \left( 1 - \frac{n + 2}{\theta} + 2\Phi(\xi) + \frac{G(\xi)}{F(\xi)} \right), \tag{35}
\]
where,

\[ \Phi(\xi) = \sum_{i=1}^{n-1} \phi(d_i), \quad \phi(d) = \frac{d}{e^{2\theta d} - 1}, \]

\[ G(\xi) = \sum_{i=1}^{n-1} g(d_i), \quad g(d) = d + \frac{3d}{\theta} + \frac{2de^{\theta d}}{(1 + e^{\theta d})^2}, \]

\[ F(\xi) = \sum_{i=1}^{n-1} f(d_i), \quad f(d) = d + \frac{e^{\theta d} - 1}{e^{\theta d} + 1}. \]

The terms \( \frac{G(\xi)}{F(\xi)} \) are non-convex in nature, use a Lagrange multiplier approach rather than Schur-convexity. We define scalar valued functions \( IMSPE_{OK}(\cdot) \), which is the IMSPE for ordinary cokriging as in (35) and \( h_{ok}(\cdot) \) corresponding to the constrain \( \sum_{i=1}^{n-1} d_i = 1 \) over the set \( \mathbb{R}^{n-1} \).

\[ IMSPE_{OK}(d_1, d_2, \ldots, d_{n-1}) = \left( 1 - \frac{n+2}{\theta} + 2\Phi(\xi) + \frac{G(\xi)}{F(\xi)} \right) \]

\[ h_{ok}(d_1, d_2, \ldots, d_{n-1}) = \sum_{i=1}^{n-1} d_i - 1. \]

Let \( \lambda \in \mathbb{R} \) is the lagrange multiplier and \( \xi^* \) be the equispaced design. Then, the Lagrangian function is defined as:

\[ L(\xi, \lambda) = IMSPE_{OK}(\xi) + \lambda h_{ok}(\xi). \]

We obtain \( \lambda^* = -\left( \frac{2 \partial \phi(d_1)}{\partial d_1} + \frac{1}{F(\xi)} \frac{\partial g(d_1)}{\partial d_1} - \frac{G(\xi)}{F^2(\xi)} \frac{\partial f(d_1)}{\partial d_1} \right) \) by setting the derivative of \( L(\xi, \lambda) \) with respect to \( d_1 \) equal to zero and evaluating at \( \xi^* \). (There is nothing special about taking the derivative with respect to \( d_1 \). As, \( IMSPE_{OK}(\cdot) \) is a symmetric function in \( d_i \)’s, derivative with respect to any \( d_i, i = 1, \ldots, n - 1 \) gives same value for \( \lambda^* \).) We can check, \( L(\xi^*, \lambda^*) = 0 \) and \( \xi^* \) is a regular point. To show this regular point is a point of minima (Proposition 1.12 [Bertsekas, 2014]) we need to show further Hessian matrix of \( L(\cdot, \cdot) \) is positive definite. However, we were not able to do that due to the complexity of second order derivatives present in the matrix.

Hence, we carried out numerical simulations to investigate the nature of the optimal design. Observe that the optimal partition that minimizes the \( IMSPE \) depends only on the exponential parameter of primary variable, that is, \( \theta \) and not the variance \( \sigma_{11} \). So, for different
values of $\theta$ we numerically minimized the $IMSPE$ using the function $fmincon$ in MATLAB to determine the optimal partition. Following is the table which shows some of the results:

| Partition Size | $\theta$               | Optimal Partition         |
|----------------|-------------------------|----------------------------|
| 5              | 0.8, 15, 20,7,45,0.2    | [0.25 0.25 0.25 0.25]     |
| 7              | 4 , 5,9, 2.5 , 40       | [0.16667 0.16667 0.16667 0.16667 0.16667 0.16667] |
| 17             | .5,5, 17,12, 20,12,40,55 | equispaced design        |
| 4              | 40,20,10,5,2.5          | [0.33 0.33 0.33 ]        |

Table 3: Optimal designs for ordinary cokriging - IMSPE criterion

We conducted many more simulations for different values of $\theta$ and partition size (not reported here) to understand the nature of the I-optimal solutions. In each case we found that an equispaced design minimizes the $IMSPE$, which suggests that an equispaced design is I-optimal.

Theorem 6.1 and Proposition 6.1 both deals with the scenario where the parameters are known. To address the situation of unknown covariance parameters we take a similar approach as in Section 4. We only discuss the case of SMSPE criterion, the IMSPE criterion is not discussed as we were not able to find a theoretical solution in case of known parameter. The prior distributions of $\theta$ and $\sigma_{11}$ are assumed to be known. We minimize the expected value of SMSPE of ordinary cokriging denoted by:

$$R_3(\xi) = E[SMSE(\theta, \sigma_{11}, \xi)].$$

(36)

**Theorem 6.2.** Consider the bivariate cokriging model as in Theorem 6.1. The parameters $\theta$ and $\sigma_{11}$ are assumed to be independent and their probability density functions are $r(\cdot)$ and $t(\cdot)$ respectively, where support of $r(\cdot)$ is $(\theta_1, \theta_2)$, where $\theta_1, \theta_2 > 0$ then, an equispaced design is optimal with respect to the risk function $R_3(\xi)$.

**Proof.** Denoting max$_i d_i = d_{\text{max}}$ we have:

$$SMSE = \sigma_{11} \left( W_{\text{sup}}(d_{\text{max}}) + \frac{U_{\text{sup}}(d_{\text{max}})}{F(\xi)} \right) \text{ from (33)}. $$

(37)

Let, $q_3(\theta, \xi) = W_{\text{sup}}(d_{\text{max}}) + \frac{U_{\text{sup}}(d_{\text{max}})}{F(\xi)}$. Then,

$$R_3(\xi) = \int_{0}^{\infty} \int_{\theta_1}^{\theta_2} \sigma_{11} q_3(\theta, \xi) r(\theta) t(\sigma_{11}) d(\sigma_{11}) d(\theta).$$

26
Note that $R_3(\xi)$ is permutation invariant of $d_i$'s. Consider,

$$
\Delta = \frac{\partial R_3(\xi)}{\partial d_l} - \frac{\partial R_3(\xi)}{\partial d_k}
$$

(38)

$$
= \frac{\partial}{\partial d_l} \int_{d_l}^{\theta_2} \sigma_{11} q_3(\theta, \xi) r(\theta) t(\sigma_{11}) \, d(\sigma_{11}) \, d(\theta)
- \frac{\partial}{\partial d_k} \int_{d_k}^{\theta_2} \sigma_{11} q_3(\theta, \xi) r(\theta) t(\sigma_{11}) \, d(\sigma_{11}) \, d(\theta)
$$

$$
= \int_{0}^{\infty} \sigma_{11} t(\sigma_{11}) \, d(\sigma_{11}) \left[ \int_{\theta_1}^{\theta_2} \left( \frac{\partial q_3(\theta, \xi)}{\partial d_l} - \frac{\partial q_3(\theta, \xi)}{\partial d_k} \right) r(\theta) \, d(\theta) \right]
$$

(Using Leibniz’s Rule Protter et al. [2012])

$$
= E_l(\sigma_{11}) \left[ \int_{\theta_1}^{\theta_2} \left( \frac{\partial q_3(\theta, \xi)}{\partial d_l} - \frac{\partial q_3(\theta, \xi)}{\partial d_k} \right) r(\theta) \, d(\theta) \right].
$$

Note that, for $d_i \neq d_{\text{max}}$,

$$
\frac{\partial q_3(\theta, \xi)}{\partial d_i} = -\frac{U_{\text{sup}}(d_{\text{max}})}{(F(\xi))^2} \frac{\partial f(d_i)}{\partial d_i}
$$

and, if $d_i = d_{\text{max}}$,

$$
\frac{\partial q_3(\theta, \xi)}{\partial d_i} = W_{\text{sup}}(d_{\text{max}}) + \frac{U_{\text{sup}}(d_{\text{max}})}{F(\xi)} - \frac{U_{\text{sup}}(d_{\text{max}})}{(F(\xi))^2} \frac{\partial f(d_{\text{max}})}{\partial d_{\text{max}}}.
$$

Thus,

$$
\frac{\partial q_3(\theta, \xi)}{\partial d_l} - \frac{\partial q_3(\theta, \xi)}{\partial d_k} = \begin{cases} 
\frac{U_{\text{sup}}(d_{\text{max}})}{(F(\xi))^2} \left( \frac{\partial f(d_k)}{\partial d_k} - \frac{\partial f(d_l)}{\partial d_l} \right) & \text{for } d_k, d_l \neq d_{\text{max}} \\
W_{\text{sup}}(d_{\text{max}}) + \frac{U_{\text{sup}}(d_{\text{max}})}{F(\xi)} + \frac{U_{\text{sup}}(d_{\text{max}})}{(F(\xi))^2} \left( \frac{\partial f(d_k)}{\partial d_k} - \frac{\partial f(d_{\text{max}})}{\partial d_{\text{max}}} \right) & \text{for } d_k \neq d_l = d_{\text{max}}
\end{cases}
$$

(39)

Note that for $d_l > d_k$, the terms in (39) $> 0$, as from (42) we have $\left( \frac{\partial f(d_k)}{\partial d_k} - \frac{\partial f(d_l)}{\partial d_l} \right) > 0$, also we have from Theorem 3.2 and 6.1 that $W_{\text{sup}}(.) > 0$ and $U_{\text{sup}}(.) > 0$.

So, from (38) we get $\frac{\partial R_3(\xi)}{\partial d_l} - \frac{\partial R_3(\xi)}{\partial d_k} > 0$ for $d_l > d_k$, which implies $R_3(\xi)$ is Schur-convex and is minimized for an equispaced design.
7 Concluding Remarks

Multivariate kriging models are of particular practical interest in computer experiments, spatial and spatio-temporal applications. Very often, two or more correlated responses may be observed, and prediction from cokriging may improve prediction quality over that possible by kriging each variable separately. In this article, we address the designing of such multivariate simple and ordinary kriging models. Since the designs are dependent on the covariance parameters, Bayesian designs are proposed.

The main results obtained are summarized below:

- Equispaced design minimizes
  - the IMSPE and SMSPE for simple cokriging models with generalized Markov type and proportional covariance structure, when covariance parameters are assumed to be known and also when prior distributions are assumed on them.
  - the SMSPE for ordinary cokriging models with both covariance structures when parameters are assumed to be known and also when prior distributions are assumed on them.
  - the IMSPE numerically for an ordinary cokriging model when parameters are known.

8 Appendix

We list down some of the key matrices, vectors and their decompositions required for proving results in Theorems 3.1, 3.2, 6.1 and 6.1. In this paper we have used an exponential covariance matrix $P$. Some of it’s properties are given below:

$$P = \begin{bmatrix} 1 & e^{-\theta|x_1-x_2|} & \ldots & e^{-\theta|x_1-x_n|} \\ e^{-\theta|x_2-x_1|} & 1 & \ldots & e^{-\theta|x_2-x_n|} \\ . & . & \ddots & . \\ . & . & \ddots & . \\ e^{-\theta|x_n-x_1|} & e^{-\theta|x_n-x_2|} & \ldots & 1 \end{bmatrix}.$$
Then,

\[
\mathbf{P}^{-1} = \begin{bmatrix}
1 & -e^{\theta d_1} & 0 & 0 & \cdots & 0 \\
1-e^{-2\theta d_1} & 1 & -e^{\theta d_1} & 0 & \cdots & 0 \\
1-e^{-2\theta d_1} & 1-e^{-2\theta d_2} & \ddots & \ddots & \ddots & \ddots \\
0 & 1-e^{-2\theta d_{n-2}} & \ddots & \ddots & \ddots & \ddots \\
0 & 0 & \cdots & \cdots & 1 & -e^{\theta d_{n-1}} \\
\end{bmatrix}
\]

For matrices,

\[
\mathbf{L} = \begin{bmatrix}
1 & 0 & 0 & \cdots & 0 \\
e^{-\theta d_1} & 1 & 0 & \cdots & 0 \\
e^{-\theta \Sigma_{i=1}^{2} d_i} & e^{-\theta d_2} & 1 & \cdots & 0 \\
\vdots & \ddots & \ddots & \ddots & \ddots \\
e^{-\theta \Sigma_{i=1}^{n} d_i} & e^{-\theta \Sigma_{i=2}^{n-1} d_i} & e^{-\theta \Sigma_{i=3}^{n-1} d_i} & \cdots & 1 \\
\end{bmatrix}
\]

\[
\mathbf{D} = \text{diag}(1, 1-e^{-2\theta d_1}, \ldots, 1-e^{-2\theta d_{n-1}})
\]

It can be checked that,

\[
\mathbf{P} = \mathbf{L} \mathbf{D} \mathbf{L}^T,
\]

so,

\[
\mathbf{P}^{-1} = (\mathbf{D}^{-1/2} \mathbf{L}^{-1})^T (\mathbf{D}^{-1/2} \mathbf{L}^{-1})
\]

\[ (40) \]

9 Appendix A

We evaluate \(F(\xi) = \mathbf{1}_n^T \mathbf{P}^{-1} \mathbf{1}_n\) and show \(\frac{1}{F(\xi)}\) is a Schur-convex function minimized for an equispaced partition.

\[
\mathbf{1}_n^T \mathbf{P}^{-1} \mathbf{1}_n = (\mathbf{D}^{-1/2} \mathbf{L}^{-1} \mathbf{1}_n)^T (\mathbf{D}^{-1/2} \mathbf{L}^{-1} \mathbf{1}_n) = \gamma^T \gamma,
\]

Where,

\[
\gamma^T = (\mathbf{D}^{-1/2} \mathbf{L}^{-1} \mathbf{1}_n)^T = \left(1, \frac{1-e^{-\theta d_1}}{\sqrt{(1-e^{-2\theta d_1})}}, \ldots, \frac{1-e^{-\theta d_{n-1}}}{\sqrt{(1-e^{-2\theta d_{n-1}})}}\right).
\]
Hence,

\[ 1^T_n P^{-1} 1_n = 1 + \sum_{i=1}^{n} \frac{1 - e^{-\theta d_i}}{1 + e^{-\theta d_i}} = \sum_{i=1}^{n} d_i + \frac{1 - e^{-\theta d_i}}{1 + e^{-\theta d_i}}. \]

So,

\[ F(\xi) = \sum_{i=1}^{n} f(d_i), \text{ where, } f(d) = d + \frac{1 - e^{-\theta d}}{1 + e^{-\theta d}}. \quad (41) \]

Now we have,

\[ \frac{\partial f(\xi)}{\partial d_i} = 1 + \frac{2\theta e^{\theta d_i}}{(1 + e^{\theta d_i})^2}, \]

\[ \frac{\partial^2 f(\xi)}{\partial d_i^2} = \frac{2\theta^2 e^{\theta d_i}(1 - e^{\theta d_i})}{(1 + e^{\theta d_i})^3} < 0. \quad (42) \]

Hence, for

\[ Q(\xi) = \frac{1}{F(\xi)}, \]

\[ \frac{\partial Q(\xi)}{\partial d_l} - \frac{\partial Q(\xi)}{\partial d_k} = \frac{1}{(F(\xi))^2} \left[ \frac{\partial f(d_k)}{\partial d_k} - \frac{\partial f(d_l)}{\partial d_l} \right] \text{ for } k, l = 1, \ldots, n - 1. \quad (43) \]

Note, that \( Q(\cdot) \) is permutation invariant of \( d_i \)'s. Also, \( \frac{\partial Q(\xi)}{\partial d_i} > \frac{\partial Q(\xi)}{\partial d_k} \) for \( d_i > d_k \) for \( k, l = 1, \ldots, n - 1 \) (from (42) and (43)). So, we can say that \( Q(\cdot) \) is a Schur-convex function (from Theorem A.4 in [Marshall et al. (1979)](Marshall et al. 1979)) and hence it is minimized for an equispaced design that is \( d_i = \frac{1}{n - 1} \) for all \( i \).

10 Appendix B

In this section we calculate mainly the terms in Theorems 3.1 and 6.1. We take a similar approach as in [Antognini and Zagoraiou (2010)](Antognini and Zagoraiou 2010). Consider the following matrix which will be
used in this section:

\[
\Lambda = \begin{bmatrix}
0 & 0 & \ldots & 0 \\
d_1 e^{-\theta d_1} & 0 & \ldots & 0 \\
(d_1 + d_2) e^{-\theta (d_1 + d_2)} & d_2 e^{-\theta d_2} & \ldots & 0 \\
(d_1 + d_2 + d_3) e^{-\theta (d_1 + d_2 + d_3)} & (d_2 + d_3) e^{-\theta (d_2 + d_3)} & \ldots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
(\sum_{i=1}^{n-1} d_i) e^{-\theta \sum_{i=1}^{n-1} d_i} & (\sum_{i=2}^{n-1} d_i) e^{-\theta \sum_{i=2}^{n-1} d_i} & \ldots & d_{n-1} e^{-\theta d_{n-1}}
\end{bmatrix}
\]

Define, \(\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_n)\) and \(\beta = (\beta_1, \beta_2, \ldots, \beta_n)\), such that \(\alpha_i = e^{-\theta x_i}, \beta_i = e^{-\theta (1-x_i)}\) for all \(i = 1, \ldots, n\). Also we have, \(\sigma_{p0} = (e^{-\theta |x_0-x_1|}, e^{-\theta |x_0-x_2|}, \ldots, e^{-\theta |x_0-x_n|})^T\). So we can check,

\[
\int_0^1 \sigma_{p0}^T d x_0 = \frac{1}{\theta} (2 \mathbf{1}_n - \alpha - \beta),
\]

\[
\int_0^1 \sigma_{p0}^T d(x_0) = \frac{1}{2\theta} \left[ 2P + 2\theta (\Lambda + \Lambda^T) - \alpha \alpha^T - \beta \beta^T \right].
\]

I) We will prove \(tr(P^{-1} \int_0^1 \sigma_{p0}^T d x_0) = \frac{n-1}{\theta} - 2 \Phi(\xi)\), where \(\Phi(\xi) = \sum_{i=1}^{n-1} \frac{d_i}{e^{2\theta d_i} - 1}\).

Using (40), we have

\[
tr(P^{-1} \Lambda) = tr((D^{-1/2} L^{-1})^T (D^{-1/2} L^{-1}) \Lambda)
\]

\[
= tr\left((D^{-1/2} L^{-1}) \Lambda (D^{-1/2} L^{-1})^T\right) = - \sum_{i=1}^{n-1} \frac{d_i}{e^{2\theta d_i} - 1} = -\Phi(\xi),
\]

\[
tr(P^{-1} \alpha \alpha^T) = tr((D^{-1/2} L^{-1}) \alpha (D^{-1/2} L^{-1})^T) = tr(aa^T) = 1,
\]

\[
tr(P^{-1} \beta \beta^T) = tr((D^{-1/2} L^{-1}) \beta (D^{-1/2} L^{-1})^T) = tr(bb^T) = 1,
\]

for,

\[
a^T = \left( e^{-\theta x_1}, \frac{e^{-\theta x_2} - e^{-\theta (d_1+x_1)}}{\sqrt{1 - e^{-2\theta d_1}}}, \ldots, \frac{e^{-\theta x_n} - e^{-\theta (d_{n-1}+x_{n-1})}}{\sqrt{1 - e^{-2\theta d_{n-1}}}} \right),
\]

\[
b^T = \left( e^{-\theta (1-x_1)}, e^{-\theta (1-x_2)} \sqrt{1 - e^{-2\theta d_1}}, \ldots, e^{-\theta (1-x_n)} \sqrt{1 - e^{-2\theta d_{n-1}}} \right).
\]

Since, \(d_i = x_{i+1} - x_i\) for all \(i = 1, \ldots, n-1\) and \(x_1 = 0, x_n = 1\), so \(a^T = (1, 0, \ldots, 0)\) and
a' a = 1 and b' b = 1. Using (45) we get,

\[
\int_{[0,1]} \sigma_{p0}^T P^{-1} \sigma_{p0} \, dx_0 = \int_0^1 tr(P^{-1} \sigma_{p0} \sigma_{p0}^T) \, dx_0 = tr(P^{-1} \int_0^1 \sigma_{p0} \sigma_{p0}^T) \\
= \frac{1}{2\theta} tr(2P^{-1}P + 2\theta P^{-1}(\Lambda + \Lambda^T) - P^{-1}a\alpha^T - P^{-1}b\beta^T) \\
= n - 1 - \frac{2\Phi(\xi)}{\theta},
\]  

(46)

where, \( \Phi(\xi) = \sum_{i=1}^{n-1} \frac{d_i}{e^{2\theta d_i} - 1} \).

II) Next we calculate \( \int_0^1 tr(g_p^T \sigma_{p0}) \) using (44).

\[
\int_0^1 tr(g_p^T \sigma_{p0}) = \int_0^1 tr(1_n^T P^{-1} \sigma_{p0}) \\
= \int_0^1 1_n^T P^{-1} \sigma_{p0} \, dx_0 \\
= \frac{1}{\theta} 1_n^T P^{-1} (21_n - \alpha - \beta).
\]

We have,

\[
1_n^T P^{-1} 1_n = F(\xi), \\
1_n^T P^{-1} \alpha = (D^{-1/2}L^{-1}1_n)^T(D^{-1/2}L^{-1} \alpha) = \gamma^T a = 1, \\
1_n^T P^{-1} \beta = (D^{-1/2}L^{-1}1_n)^T(D^{-1/2}L^{-1} \beta) = \gamma^T b = 1.
\]

Hence,

\[
\int_0^1 tr(g_p^T \sigma_{p0}) \, dx_0 = \frac{2}{\theta}(F(\xi) - 1).
\]  

(47)
III) Finally we calculate $\int_0^1 tr(g_p^T g_p T \sigma_p \sigma_p^T) \, dx_0$ using (45).

\begin{align*}
\int_0^1 tr(g_p^T g_p T \sigma_p \sigma_p^T) \, dx_0 &= \int_0^1 tr(P^{-1}1_n (P^{-1}1_n)^T \sigma_p \sigma_p^T) \, dx_0 \\
&= \int_0^1 tr(P^{-1}1_n 1_n^T \sigma_p \sigma_p^T) \, dx_0 \\
&= tr\left[P^{-1}1_n 1_n^T P^{-1} \int_0^1 \sigma_p \sigma_p^T \, dx_0\right] \\
&= \frac{1}{2\theta} tr\left[P^{-1}1_n 1_n^T P^{-1} [2P + 2\theta(\Lambda + \Lambda^T) - \alpha \alpha^T - \beta \beta^T]\right].
\end{align*}

After some calculations we get,

\begin{align*}
tr(P^{-1}1_n 1_n^T) &= tr(1_n^T P^{-1}1_n) = F(\xi), \\
tr(P^{-1}1_n 1_n^T P^{-1} \alpha \alpha^T) &= tr(1_n^T P^{-1} \alpha \alpha^T P^{-1}1_n) = (1_n^T P^{-1} \alpha) tr(\alpha^T P^{-1}1_n) = (1_n^T P^{-1} \alpha)^2 = 1, \\
tr(P^{-1}1_n 1_n^T P^{-1} \beta \beta^T) &= tr(1_n^T P^{-1} \beta \beta^T P^{-1}1_n) = (1_n^T P^{-1} \beta) tr(\beta^T P^{-1}1_n) = (1_n^T P^{-1} \beta)^2 = 1, \\
tr(P^{-1}1_n 1_n^T P^{-1}(\Lambda + \Lambda^T)) &= 2 tr(1_n^T P^{-1} \Lambda P^{-1}) = 2 \sum_{i=1}^{n-1} \frac{d_i e^{\theta d_i}}{(1 + e^{\theta d_i})^2}.
\end{align*}

Hence,

$$
\int_0^1 tr(g_p^T g_p T \sigma_p \sigma_p^T) \, dx_0 = \frac{F(\xi) - 1}{\theta} + 2 \sum_{i=1}^{n-1} \frac{d_i e^{\theta d_i}}{(1 + e^{\theta d_i})^2}. \tag{48}
$$

11 Appendix C

In this part we look at the matrix and vector decompositions which are used for proving results involving the SMSPE for simple and ordinary cokriging models. Consider, $x_0 \in [x_i, x_{i+1}]$ for
some $i = 1, ..., n - 1$. Define $a = x_0 - x_i$. Take $n \times 1$ vectors $u_1, u_2^T, v_1^T$ and $v_2^T$ defined as:

$$
u_1^T = \begin{pmatrix} e^{-\theta \sum_{i=1}^{n-1} d_i}, e^{-\theta \sum_{i=2}^{n-1} d_i}, ..., 1^{i\text{th} \ pos}, 0, 0, ..., 0 \end{pmatrix},$$

$$
u_2^T = \begin{pmatrix} 0, 0, ..., 0, 1^{(i+1)\text{th} \ pos}, e^{-\theta d_{i+1}}, ..., e^{-\theta \sum_{i=n}^{n} d_i} \end{pmatrix},$$

$$

v_1 = \begin{pmatrix} 0, 0, ..., 0(i-1)^{\text{th} \ pos}, 1 - e^{-\theta d_i}, 0, ..., 0 \end{pmatrix},

$$

$v_2^T = \begin{pmatrix} 0, 0, ..., 0(i-1)^{\text{th} \ pos}, 1 - e^{-\theta d_i}, 0, ..., 0 \end{pmatrix}.$

It could be checked that the following vectors could be decomposed as:

$$\sigma_{p0} = e^{-\theta a} u_1 + e^{-\theta (d_i - a)} u_2, \quad (49)$$

$$P^{-1} \sigma_{p0} = \frac{v_1 + e^{-\theta (d_i - a)} v_2}{1 - e^{-\theta d_i}}, \quad \text{and} \quad (50)$$

$$\sigma_{p0}^T P^{-1} \sigma_{p0} = \frac{e^{-2\theta a} - 2e^{-\theta d_i} + e^{-2\theta (d_i - a)} - e^{-\theta d_i}}{1 - e^{-2\theta d_i}}, \quad (51)$$

$$1_n^T P^{-1} \sigma_{p0} = \frac{e^{-\theta a} + e^{-\theta (d_i - a)}}{1 + e^{-\theta d_i}}. \quad (52)$$

12 Appendix D

In this section we show calculations required for proving Lemmas $6.1$ and $6.2$. Note that in both the cases we need to calculate $A^{-1}$. From $[5]$ and $[7]$ we have, $A = \begin{bmatrix} 0 & F^T \\ F & \Sigma \end{bmatrix}$, where $F = \begin{bmatrix} 1_n & 0 \\ 0 & 1_n \end{bmatrix}$. Also note that,

$$BB^T = \begin{bmatrix} 1 & 0 & \sigma_{10}^T & \sigma_{20}^T \\ 0 & 0 & 0_n^T & 0_n^T \\ \sigma_{10} & 0_n & \sigma_{10} \sigma_{10}^T & \sigma_{10} \sigma_{20}^T \\ \sigma_{20} & 0_n & \sigma_{20} \sigma_{10}^T & \sigma_{20} \sigma_{20}^T \end{bmatrix}$$

Defining some notations below,

$$g_1 = M^{-1}_i 1_n, \quad g_2 = M^{-1}_R 1_n, \quad g_p = P^{-1} 1_n,$$

$$m_1 = 1_n^T M^{-1}_i 1_n, \quad m_2 = 1_n^T M^{-1}_R 1_n, \quad F(\xi) = 1_n^T P^{-1} 1_n,$$

$$0_n = (0, 0, ..., 0)^T_{n \times 1}, \quad 0_n = [0]_{n \times n}.$$

Proof of Lemma $6.1$
In case of Lemma 6.1 we assume the covariance structure to be generalized Markov type. So, the covariance matrix \( \text{Cov}(Z, Z) \) is given by
\[
\Sigma = \begin{bmatrix}
M_1 & \rho M_1 \\
\rho M_1 & \rho^2 M_1 + (\sigma_{22} - \rho^2 \sigma_{11}) M_R
\end{bmatrix} \tag{53}
\]
from (3). Also,
\[
\Sigma^{-1} = \begin{bmatrix}
M_1^{-1} & 0 \\
0 & 0
\end{bmatrix} + \frac{1}{\sigma_{22} - \rho^2 \sigma_{11}} \begin{bmatrix}
\rho^2 M_R^{-1} - \rho M_R^{-1} & -\rho M_R^{-1} \\
-\rho M_R^{-1} & M_R^{-1}
\end{bmatrix}, \tag{54}
\]
(see (12)). In this case,
\[
A^{-1} = \begin{bmatrix}
E_1 & -\phi_1 \\
-\phi_1^T & \Sigma^{-1} + \psi_1 \phi_1
\end{bmatrix},
\]
where,
\[
E_1 = -\frac{1}{m_1} \begin{bmatrix}
\rho & 0 \\
\rho & \rho^2
\end{bmatrix} - \frac{1}{m_2} \begin{bmatrix}
\sigma_{22} - \rho^2 \sigma_{11} & 0 \\
0 & 0
\end{bmatrix}, \\
\phi_1 = -\frac{1}{m_1} \begin{bmatrix}
g_1^T & 0_n^T \\
\rho g_1^T & 0_n^T
\end{bmatrix} - \frac{1}{m_2} \begin{bmatrix}
0_n^T & 0_n^T \\
-\rho g_2^T & g_2^T
\end{bmatrix}, \\
\psi_1 = \begin{bmatrix}
g_1 & 0_n \\
0_n & 0_n
\end{bmatrix} + \frac{1}{\sigma_{22} - \rho^2 \sigma_{11}} \begin{bmatrix}
\rho^2 g_2 & -\rho g_2 \\
-\rho g_2 & g_2
\end{bmatrix} \text{ and } \\
\psi_1 \phi_1 = -\frac{1}{m_1} \begin{bmatrix}
g_1 g_1^T & 0_{n \times n} \\
0_{n \times n} & 0_{n \times n}
\end{bmatrix} - \frac{1}{m_2 (\sigma_{22} - \rho^2 \sigma_{11})} \begin{bmatrix}
\rho^2 g_2 g_1^T & -\rho g_2 g_1^T \\
-\rho g_2 g_1^T & g_2 g_1^T
\end{bmatrix}.
\]

Also,
\[
BB^T = \begin{bmatrix}
1 & 0 & \sigma_{10}^T & \rho \sigma_{10}^T \\
0 & 0 & 0 & 0 \\
0 & \sigma_{10} & 0 & \sigma_{10} \sigma_{10}^T \\
0 & \rho \sigma_{10} & 0 & \rho^2 \sigma_{10} \sigma_{10}^T
\end{bmatrix}.
\]

After some simple but tedious calculations we are able to show that the MSPE(\( x_0 \)) is:
\[
\text{MSPE}(x_0) = 1 - \text{tr}(BB^T A^{-1})
\]
\[
= 1 + \frac{1}{m_1} - \frac{2}{m_1} \text{tr}(g_1 \sigma_{10}) - \text{tr}(M_1^{-1} \sigma_{10} \sigma_{10}^T) + \frac{1}{m_1} \text{tr}(g_1 \sigma_{10} \sigma_{10}^T) \tag{54}
\]

Proof of Lemma 6.2

In case of Lemma 6.2 we assume the covariance structure to be stationary isotropic and of the proportional type. So, the covariance matrix \( \text{Cov}(Z, Z) \) is given by
\[
\Sigma = \begin{bmatrix}
\sigma_{11} P & \sigma_{12} P \\
\sigma_{21} P & \sigma_{22} P
\end{bmatrix}, \tag{55}
\]
see (9).
and in this case \( \sigma_{12} = \sigma_{21} \). Also, from (15) \( \Sigma^{-1} = \frac{1}{\sigma_{11}} \begin{bmatrix} P^{-1} & 0 \\ 0 & 0 \end{bmatrix} + \frac{1}{|P|} \begin{bmatrix} \sigma_{12} \sigma_{21} P^{-1} & -\sigma_{12} P^{-1} \\ -\sigma_{12} P^{-1} & \sigma_{11} P^{-1} \end{bmatrix} \). In this case we obtain,

\[
A^{-1} = \begin{bmatrix} E_2 & -\phi_2 \\ -\phi_2^T & \Sigma^{-1} + \psi_2 \phi_2 \end{bmatrix},
\]

where,

\[
E_2 = -\frac{1}{F(\xi)} \begin{bmatrix} \sigma_{11} & \sigma_{12} \\ \sigma_{12} & \sigma_{11} \end{bmatrix} - \frac{|P|}{\sigma_{11} F(\xi)} \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix},
\]

\[
\phi_2 = -\frac{1}{\sigma_{11} F(\xi)} \begin{bmatrix} \sigma_{11} g_p^T T & 0_n^T \\ \sigma_{12} g_p^T T & 0_n^T \end{bmatrix} - \frac{1}{\sigma_{11} F(\xi)} \begin{bmatrix} 0_n^T & 0_n^T \\ -\sigma_{12} g_p^T & \sigma_{11} g_p \end{bmatrix} \]

and

\[
\psi_2 = \frac{1}{\sigma_{11} T} \begin{bmatrix} g_p & 0_n \\ 0_n & 0_n \end{bmatrix} + \frac{1}{|P|} \begin{bmatrix} \sigma_{12}^2 \sigma_p & -\sigma_{12} \sigma_p \\ -\sigma_{12} \sigma_p & \sigma_{11} \sigma_p \end{bmatrix}
\]

and

\[
\psi_2 \phi_2 = -\frac{1}{\sigma_{11} T} \begin{bmatrix} g_p g_p^T & 0_{n \times n} \\ 0_{n \times n} & 0_{n \times n} \end{bmatrix} - \frac{1}{\sigma_{11} T |P| F(\xi)} \begin{bmatrix} \sigma_{12}^2 \sigma_p g_p^T & -\sigma_{11} \sigma_p \sigma_p g_p^T \\ -\sigma_{11} \sigma_p \sigma_p g_p^T & \sigma_{11}^2 \sigma_p \sigma_p \end{bmatrix}
\]

Also,

\[
BB^T = \begin{bmatrix}
1 & 0 & \sigma_{11} \sigma_p^T & \sigma_{12} \sigma_p^T \\
0 & 0 & \sigma_{12} \sigma_p^T & \sigma_{11} \sigma_p^T \\
\sigma_{11} \sigma_p & 0_n & \sigma_{11} \sigma_p \sigma_p^T & \sigma_{12} \sigma_p \sigma_p^T \\
\sigma_{12} \sigma_p & 0_n & \sigma_{11} \sigma_p \sigma_p^T & \sigma_{11} \sigma_p \sigma_p^T
\end{bmatrix}
\]

Then, MSPE(\(x_0\)) is given by the following expression:

\[
MSPE(x_0) = \sigma_{11} \left( 1 + \frac{1}{F(\xi)} - \frac{2}{F(\xi)} tr(g_p^T \sigma_p) + \frac{1}{F(\xi)} tr(g_p^T \sigma_p \sigma_p^T) - tr(P^{-1} \sigma_p \sigma_p^T) \right).
\]

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