Approximated optimum condition of second order response surface model with correlated observations

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Abstract. In the present paper we establish an inference procedure for the eigenvalues of the model matrix of the second-order response surface model (RSM). In contrast to the classical treatment where the sample are assumed to be independently distributed, in this work we do not need such distributional simplification. The confidence region for the unknown vector of the eigenvalues is derived by means of delta method. The finite sample behavior of the convergence result is discussed by Monte Carlo Simulation. We get the approximated distribution of the pivotal quantity of the population eigenvalues as a chi-square distribution model. Next we attempt to apply the method to a real data provided by a mining industry. The data represents the percentage of cobalt (Co) observed over the exploration region.

1. Introduction
The problem of determining the optimum condition of a reproduction process is a common objective in the subject of response surface modelling. Optimum condition means a situation on the experimental region under which the reproduction process attains maximum or minimum yield, cf. Bisgaard and Ankenman [3], Carter, Chincilli and Campbell [5], Myers and Kuhri [10], Myers and Montgomery [11, 12] and Somayasa [17]. In the case of the second-order RSM such an optimum condition is represented by the eigenvalues of the so-called model matrix of the response variable. It can be inferred from the magnitude of the eigenvalues of the model matrix whether or not the process in a fixed stationary point achieves a maximum or a minimum value. This subject has found much attention in the literatures, see e.g. [3, 5, 10, 11, 12, 17].

We study throughout this paper a second-order response surface model on a p-dimensional compact space \( \mathbf{I}^p := \Pi_i=1^p [a_i, b_i], a_i \leq b_i \) with correlated observations defined as follows:

\[
Y_i = \beta_0 + \sum_{j=1}^p \beta_j x_{ij} + \sum_{j=1}^p \sum_{k=j}^p \beta_{jk} x_{ij} x_{ik} + \varepsilon_i, \quad i = 1, \ldots, n, \tag{1}
\]

where \( Y_i \) is the response variable (dependent variable), \( \mathbf{x}_i := (x_{i1, \ldots, x_{ip}})^\top \in \Pi_i=1^p [a_i, b_i] \) is the experimental condition (independent variable), \( \beta := (\beta_0, \beta_1, \ldots, \beta_p, \beta_{11}, \beta_{12}, \ldots, \beta_{pp})^\top \in \mathcal{R}^{(p+1)(p+2)/2} \) is the vector of unknown parameters, and \( \varepsilon_i \) is the stochastically dependent random error having mean zero and finite positive variance \( \sigma_{\varepsilon i}^2 \). Let us introduce a vector
b := (β_1, ..., β_p)^T ∈ R^p, and a p × p symmetric matrix B defined by

\[
B := \begin{pmatrix}
β_{11} & 1/2β_{12} & \cdots & 1/2β_{1p} \\
1/2β_{12} & β_{22} & \cdots & 1/2β_{2p} \\
\vdots & \vdots & \ddots & \vdots \\
1/2β_{1p} & 1/2β_{2p} & \cdots & β_{pp}
\end{pmatrix} ∈ R^{p×p}.
\]

Then Model 1 can be written in vector and matrix form which is more compact and useful for our interest, i.e.

\[
Y_i = β_0 + x_0^T b + x_i^T B x + ε_i, \quad i = 1, \ldots, n. \tag{2}
\]

Hence by using differential technique, the unknown stationary point of the model is given by \( x_0 = -1/2B^{-1} b \), see e.g. [8, 10, 11, 12] and the references cited therein. There are many methods and approaches that have been established for investigating the optimality of the point \( x_0 \). Among other are ridge and steepest ascent methods studied in the references mentioned above. The application of these methods seem to be limited in that the optimum point is subjected by considering the points lie in a sphere of radius \( r \). We refer interested reader to [8, 10, 11, 12] for a more complete discussion on these methods.

Response surface model with correlated observations are frequently found in spatial data analysis in which data is regarded as a realization of a spatial process \{Y(x) : x ∈ P\} such that for every \( x_i, x_j ∈ P \), \( Cov(Y(x_i), Y(x_j)) \) is represented as a function of \( (x_i - x_j) \), that is \( Cov(Y(x_i), Y(x_j)) = γ(x_i - x_j) \) for some function \( γ \). When the process is assumed to be isotropic, then the covariance function depends only on the distance of their position, see e.g. Cressie [6], pp. 32–68 for further discussion regarding stationary spatial process. Study regarding generalized linear model can be found in Arnold [1] and Stapleton [18].

It was investigated in [3, 5, 8, 11, 12] that upon transforming the model to its canonical form it can be seen that the characteristic of the response can be determined by observing the magnitude of the eigenvalues of \( B \). More precisely, if the eigenvalues of \( B \) are all positive, then the response variable attains minimum value at \( x_0 \). On the other hand if the eigenvalues of \( B \) are all negative, the stationary point \( x_0 \) represents a point in which the response attains maximum value. In the case where the eigenvalues differ in sign, the stationary point is a saddle point. Thus deriving an inference procedure for the eigenvalues of \( B \) is an essential task in response surface methodology. In this paper we construct the asymptotic confidence region as well as the confidence interval for the eigenvalues of the model matrix by applying the so-called delta method. Note that for our results we do not need to assume any specific distribution for the random errors.

The motivating idea in applying the delta method is that the vector of eigenvalues of \( B \) is a differentiable function of \( B \). If the parameter \( β \) is estimated by some unbiased estimator such as the least squares estimator \( \hat{β}_n \) then we get immediately the estimator of the eigenvalues. By adopting some result from Arnold [2] and Pruscha [14] the limiting distribution of the eigenvalues can be obtained.

The derivation of the asymptotic distribution of the estimator of the eigenvalues of \( B^{(n)} \) using delta method is discussed in Section 2. In Section 3 we extend the study to a second-order RSM with correlated responses. The finite distribution of the eigenvalue is investigated in Section 4 using Monte Carlo simulation. The result is then applied to construct the asymptotic confidence region and the confidence interval for the optimal condition of a data obtained from a mining industry, see Section 5. We close this paper in Section 6 with a discussion about several open problems and topics for future researches.
2. Delta method

The application of delta method in RSM was proposed in the work of [3] and [5] for response surface model with independent observations. Let us consider a triangular array of observation

\[ Y_{ni} = \beta_0^{(n)} + \sum_{j=1}^{p} \beta_j^{(n)} x_{ij} + \sum_{j=1}^{p} \sum_{k=j}^{p} \beta_{jk}^{(n)} x_{ij} x_{ik} + \varepsilon_{ni}, \quad i = 1, \ldots, n, \]

where \( \{ \varepsilon_{ni} | i = 1, \ldots, n, \ n \geq 1 \} \) is a sequence of triangular array of correlated random errors with \( \mathbb{E}(\varepsilon_{ni}) = 0 \) and \( \text{Cov}(\varepsilon_{ni}, \varepsilon_{nj}) = \sigma_{ij} \), for \( i, j = 1, \ldots, n \). We call this model throughout this paper the asymptotic second-order RSM. Let \( f_0, f_1, \ldots, f_p \) be linearly independent as functions in \( L_2(\lambda^p, \mathbb{P}) \) defined by \( f_0(x) = 1, f_1(x) = x_1, \ldots, f_p(x) = x_p \), for \( x = (x_1, \ldots, x_p)^\top \in \mathbb{P} \), where \( L_2(\lambda^p, \mathbb{P}) \) is the space of squared integrable function on \( \mathbb{P} \) with respect to the Lebesgue measure \( \lambda^p \). Let \( X_n \) be an \( n \times (p+1)(p+2)/2 \) design matrix defined by

\[
X_n = \begin{pmatrix}
 f_0(x_1) & f_1(x_1) & \cdots & f_p(x_1) & f_{11}(x_1) & f_{12}(x_1) & \cdots & f_{pp}(x_1) \\
 \vdots & \vdots & & \vdots & \vdots & \vdots & & \vdots \\
 f_0(x_n) & f_1(x_n) & \cdots & f_p(x_n) & f_{11}(x_n) & f_{12}(x_n) & \cdots & f_{pp}(x_n)
\end{pmatrix} \in \mathbb{R}^{n \times (p+1)(p+2)/2},
\]

where for \( i = 1, \ldots, n, x_i := (x_{i1}, \ldots, x_{ip})^\top \in \mathbb{P} \), and for \( k, \ell = 1, \ldots, p \) \( f_{kl}(x) := f_k(x)f_\ell(x) \), for \( x \in \mathbb{P} \). By referring to the work of Pruscha [14], pp. 115–117, there exist an \( n_0 \geq 1 \), such that \( \text{rank}(X_n) = (p+1)(p+2)/2 \) for all \( n \geq n_0 \). For our purpose we need to represent the model using vector and matrix notation. Let \( Y_{nm} := (Y_{n1}, \ldots, Y_{nn}) \), \( \varepsilon_{nm} := (\varepsilon_{n1}, \ldots, \varepsilon_{nn})^\top \) be the vector of observations and random errors, respectively. Then Model 3 can be equivalently written as \( Y_{nm} = X_n \beta + \varepsilon_{nm} \), where \( \mathbb{Cov}(\varepsilon_{nm}) = \Sigma := (\sigma_{ij})_{i=1,j=1}^{n,n} \) is an \( n \times n \) symmetric matrix. As an example Schabenberger and Gotway [15], pp. 320–321 studied a spatial regression model with correlated observations. They considered \( \Sigma = \sigma^2 \Psi = \sigma^2 (\psi_{ij})_{i=1,j=1}^{n,n} \), where \( \psi_{ij} = \exp(-|x_i - x_j|) \), for \( i, j = 1, \ldots, n \).

If the covariance matrix \( \Sigma \) is positive definite (\( \Sigma > 0 \)), then there exists \( \Sigma^{-1/2} \Sigma^{-1/2} = \Sigma^{-1} \). By using the linear transformation represented by \( \Sigma^{-1/2} \), the asymptotic model \( Y_{nn} = X_n \beta + \varepsilon_{nn} \) can be transformed to \( Y_{nn}^* = X_n^* \beta^* + \varepsilon_{nn}^* \), where \( Y_{nn}^* = \Sigma^{-1/2} Y_{nn}, \ X_n^* = \Sigma^{-1/2} X_n, \) and \( \varepsilon_{nn}^* = \Sigma^{-1/2} \varepsilon_{nn} \). The transformed model has the property \( \mathbb{E}(\varepsilon_{nn}^*) = \mathbb{E}(\Sigma^{-1/2} \varepsilon_{nn}) = 0 \) and \( \text{Cov}(\varepsilon_{nn}^*) = \text{Cov}(\Sigma^{-1/2} \varepsilon_{nn}) = I_n \). Hence the estimator for \( \beta \) is immediately obtained by applying the least squares principle (cf. [1, 2, 18]) which is given by

\[
\hat{\beta}^{(n)} = (X_n^* \Sigma^{-1} X_n^*)^{-1} X_n^* \Sigma^{-1} Y_{nn}.
\]

Moreover, by the plug-in principle we get the least squares estimator of matrix \( B^{(n)} \). That is

\[
\hat{B}^{(n)} := \begin{pmatrix}
\hat{\beta}_{11}^{(n)} & 1/2 \hat{\beta}_{12}^{(n)} & \cdots & 1/2 \hat{\beta}_{1p}^{(n)} \\
1/2 \hat{\beta}_{21}^{(n)} & \hat{\beta}_{22}^{(n)} & \cdots & 1/2 \hat{\beta}_{2p}^{(n)} \\
\vdots & \vdots & \ddots & \vdots \\
1/2 \hat{\beta}_{p1}^{(n)} & 1/2 \hat{\beta}_{p2}^{(n)} & \cdots & \hat{\beta}_{pp}^{(n)}
\end{pmatrix},
\]

where the entries of \( \hat{B}^{(n)} \) is obtained from the corresponding elements of \( \hat{\beta}^{(n)} \). Furthermore, by applying the result presented in Pruscha [14], pp. 115–117, we get the limit distribution of
Suppose that the components of \( \varepsilon_{nn}^* \) are independent then for \( n \to \infty \), it holds

\[
\sqrt{n}(Vech(\hat{B}^{(n)}) - Vech(B)) \Rightarrow N_{\frac{1}{2}(p+1)}(O, T_p G^{-1} T_p^\top),
\]

where \( G := \lim_{n \to \infty} X_n^\top X_n \) and \( T_p \) is the linear operator represented by a \( \frac{1}{2}p(p+1) \times \frac{1}{2}(p+2) \) matrix defined by

\[
T_p := \left( O|\text{diag}(a_{p1}^\top, a_{p-1}^\top, \ldots, a_1^\top) \right),
\]

where \( O \) is the \( \frac{1}{2}p(p+1) \times (p+1) \) zero matrix, and \( a_p := (1, 1/2, 1/2, \ldots, 1/2)^\top \in \mathcal{R}^p \). Here and throughout this paper “\( \Rightarrow \)” stand for the weak convergence or convergence in distribution (cf. Billingsley [4]).

To get the asymptotic distribution of the sequence of the vector of eigenvalues of \( \hat{B}^{(n)} \) we need further notations. It is worth mentioning that the Euclidean space \( \mathcal{R}^{p \times p} \) is furnished with an inner product denoted by \( \langle \cdot, \cdot \rangle_{\mathcal{R}^{p \times p}} \), defined by \( \langle A, C \rangle_{\mathcal{R}^{p \times p}} := \text{trace}(A^\top C) \), and the corresponding norm is denoted by \( \| A \|_{\mathcal{R}^{p \times p}} := \sqrt{\text{trace}(A^\top A)} \), for every \( A \) and \( C \) in \( \mathcal{R}^{p \times p} \). A closed ball in \( \mathcal{R}^{p \times p} \) with radius \( r > 0 \) and a center \( A \) is denoted by \( N_r(A) \), defined by \( N_r(A) := \{ X \in \mathcal{R}^{p \times p} : \| X - A \|_{\mathcal{R}^{p \times p}} \leq r \} \). Note that \( Vech^{(n)} \) denotes the well-known Vech operator defined in the literatures of matrix algebra, see e.g. Harville [7], pp. 340–343.

Now we are ready to state our main result giving the asymptotic distribution of the vector of the eigenvalues of \( \hat{B}^{(n)} \). See also [3, 5].

**Theorem 2.1. ([3, 5])** Suppose that the components of \( \Sigma^{-1/2} \varepsilon_{nn} \) are independent. Let \( \lambda_s \) be a simple eigenvalue of \( B \) with associated normalized eigenvector \( u_s := (u_{s1}, \ldots, u_{sp})^\top \). That is \( Bu_s = \lambda_s u_s \) and \( u_i^\top u_k = \delta_{jk} \), for \( s, i, j = 1, \ldots, p \), where \( \delta_{jk} \) is the Kronecker delta. Let \( \hat{\lambda}_s^{(n)} \) be the eigenvalue of \( \hat{B}^{(n)} \) with normalized eigenvector \( \hat{u}_s^{(n)} := (\hat{u}_{s1}, \ldots, \hat{u}_{sp})^\top \). That is \( \hat{B}^{(n)} \hat{u}_s^{(n)} = \hat{\lambda}_s^{(n)} \hat{u}_s^{(n)} \), for \( s = 1, \ldots, p \). Furthermore, let \( H \) be a \( \frac{1}{2}p(p+1) \times p \) real matrix (Hessian matrix) defined by

\[
H := \begin{pmatrix}
Vech^\top(u_1 u_1^\top - D_1)
Vech^\top(u_2 u_2^\top - D_2)
\vdots
Vech^\top(u_p u_p^\top - D_p)
\end{pmatrix}^\top \in \mathcal{R}_{\frac{1}{2}p(p+1) \times p},
\]

where for \( s = 1, \ldots, p \), \( D_s := \text{diag}(u_{s1}^2, \ldots, u_{sp}^2) \), and \( W_p := H^\top T_p G^{-1} T_p^\top H \). Then for \( n \to \infty \), it holds true

\[
\sqrt{n}(\hat{\lambda}_s^{(n)} - \lambda) \Rightarrow N_{\frac{1}{2}p(p+1)}(0, W_p).
\]

**Proof:** By Theorem 7 in Magnus and Neudecker [9], there exist continuously differentiable eigenvalue and eigenvector functions \( \lambda \) and \( u \) defined on the open ball \( N_r(B) \cap \text{Sym}(p) \) centered at the unknown parameter \( B \), such that for every \( X \in N_r(B) \cap \text{Sym}(p) \), it holds \( X u(X) = \lambda(X) u(X) \). In particular, we have \( B u(B) = \lambda(B) u(B) \) and \( \hat{B}^{(n)} \hat{u}^{(n)} = \hat{\lambda}^{(n)} \hat{u}^{(n)} \). Next for every \( t := (t_1, \ldots, t_p)^\top \in \mathcal{R}^p \), we define a function \( F_t \) on the open ball \( N_r(B) \cap \text{Sym}(p) \), such that for every \( X \in N_r(B) \cap \text{Sym}(p) \), \( F_t(X) := t^\top \lambda(X) \). By Taylor expansion, we have an approximation of \( F_t(X) \) for any \( X \) lies in the ball \( X \in N_r(B) \cap \text{Sym}(p) \). Especially we have

\[
\sqrt{n}(F_t(\hat{B}^{(n)}) - F_t(B)) = \sqrt{n} Vech^\top(\hat{B}^{(n)} - B) \frac{\partial F_t(B)}{\partial Vech(X)} + R_{\hat{B}^{(n)}},
\]

where
where $R_{\hat{B}^{(n)}} := \|\sqrt{n}Vech(\hat{B}^{(n)} - B)\| r(Vech(\hat{B}^{(n)} - B))$. We notice that $R_{\hat{B}^{(n)}}$ immediately converges to zero stochastically by the consistency of $\hat{B}^{(n)}$ to $B$. Next by substituting

$$\frac{\partial F_1(B)}{\partial Vech(X)} = Vech\left(\frac{\partial F_1(B)}{\partial X}\right) = Vech\left(\sum_{s=1}^{p} t_s \lambda_s\right)$$

$$= \sum_{s=1}^{p} t_s Vech(2u_s u_s^T - D_s)$$

to Equation 4 we finally get

$$\sqrt{n}(\hat{\lambda}^{(n)} - \lambda) = \sqrt{n}Vech^T(\hat{B}^{(n)} - B)\sum_{s=1}^{p} t_s Vech(2u_s u_s^T - D_s) + R_{\hat{B}^{(n)}}$$

Since $R_{\hat{B}^{(n)}}$ converges to zero, and $\sqrt{n}Vech(\hat{B}^{(n)} - B)$ converges to $N_{\frac{1}{2}p(p+1)}(0, T_p G^{-1} T_p^T)$, then by applying the Cramér-Wald technique, the assertion follows.

**Remark 2.1.** In the application the covariance matrix is estimated by a positive definite matrix

$$\hat{\Sigma}^{(n)} := \frac{1}{n}(I_n - X_n(X_n^T X_n)^{-1}X_n^T)Y_{nn}Y_{nn}^T(I_n - X_n(X_n^T X_n)^{-1}X_n^T),$$

where $I_n$ is the $n \times n$ identity matrix. The Hessian matrix is estimated by the following consistent estimator

$$\hat{H}^{(n)} := \left(\begin{array}{c}
Vech^T(\hat{u}_1^{(n)} - \hat{D}_1^{(n)}) \\
Vech^T(\hat{u}_2^{(n)} - \hat{D}_2^{(n)}) \\
\vdots \\
Vech^T(\hat{u}_p^{(n)} - \hat{D}_p^{(n)})
\end{array}\right)^T \in \mathbb{R}^{\frac{1}{2}p(p+1) \times p}.$$

Hence by the plug-in principle, $W_p$ is estimated by $\hat{W}_p^{(n)} := \hat{H}^{(n)^T} T_p G^{-1} T_p^T \hat{H}^{(n)}$.

**Remark 2.2.** In the case of the covariance structure $\Sigma = \sigma^2 \Psi$ defined in [15], a consistent estimator for $\sigma^2$ proposed in [1, 2] can be applied. That is

$$\hat{\sigma}_2^{(n)} := \frac{Y_{nn}^T (I_n - X_n^s(X_n^s)^{-1}X_n^s)^{-1}X_s^T) Y_{nn}^s}{n - \frac{1}{2}(p+1)(p+2)}.$$

As an immediate implication of the multivariate central limit theorem (Pruscha [14]) we have

$$\sqrt{n}(\hat{\lambda}^{(n)} - \lambda)^T (\hat{W}_p^{(n)})^{-1} \sqrt{n}(\hat{\lambda}^{(n)} - \lambda) \Rightarrow \chi^2(p), \text{ for } n \to \infty,$$

where $\chi^2(p)$ is the random variable having a chi-square distribution with $p$ degrees of freedom. Hence, the $(1 - \alpha) \times 100\%$ confidence region of $\lambda$ is given by

$$\mathcal{R}_{\lambda} := \left\{ \mathbf{x} \in \mathbb{R}^p : \sqrt{n}(\hat{\lambda}^{(n)} - \mathbf{x})^T (\hat{W}_p^{(n)})^{-1} \sqrt{n}(\hat{\lambda}^{(n)} - \mathbf{x}) \leq \chi^2_{1-\alpha}(p) \right\}, \quad (5)$$

where $\chi^2_{1-\alpha}(p)$ is the $(1 - \alpha)$ quantile of the chi-square distribution with $p$ degrees of freedom. One is interested not only on the simultaneous confidence region for the vector $\lambda$ but also on the
partial confidence interval for each component of \( \lambda \). For \( s = 1, \ldots, p \), let \( \mathbf{1}_s \) be the unit vector in \( \mathbb{R}^p \) whose \( s \)-th component is 1 and the remainder is 0. Then by Theorem 2.1 we get

\[
\sqrt{n} \mathbf{1}_s^\top (\hat{\lambda}^{(n)} - \lambda) \sqrt{1_s^\top \hat{\mathbf{W}}^{(n)}_p 1_s} \Rightarrow N(0, 1),
\]
giving us the partial \( (1 - \alpha) \times 100\% \) confidence interval for the component \( \lambda_s \) of \( \lambda \)

\[
\hat{\lambda}_s^{(n)} - z_{1-\alpha/2} \frac{1}{\sqrt{n}} \sqrt{1_s^\top \hat{\mathbf{W}}^{(n)}_p 1_s}, \quad \hat{\lambda}_s^{(n)} + z_{1-\alpha/2} \frac{1}{\sqrt{n}} \sqrt{1_s^\top \hat{\mathbf{W}}^{(n)}_p 1_s},
\]
where \( z_{1-\alpha} \) is the \( (1 - \alpha) \)-th quantile of the standard normal distribution.

Algorithm for constructing the confidence region or confidence interval for the eigenvalue of \( \mathbf{B} \) is presented below.

(i) Compute \( \hat{\Sigma}^{(n)} \);
(ii) Compute \( \hat{\beta}^{(n)} \);
(iii) Compute the estimated model matrix \( \hat{\mathbf{B}}^{(n)} \);
(iv) Compute the eigenvalue vector \( \hat{\lambda}^{(n)} \);
(v) Compute \( \hat{\mathbf{W}}^{(n)}_p \);
(vi) Construct the confidence region by using (5) and the confidence interval by using (6).

**Figure 1.** The empirical distribution functions of \( \hat{\beta}_0^{(n)} \), \( \hat{\beta}_1^{(n)} \), \( \hat{\beta}_2^{(n)} \), \( \hat{\beta}_{11}^{(n)} \), \( \hat{\beta}_{12}^{(n)} \) and \( \hat{\beta}_{22}^{(n)} \).
3. Simulation study

We develop simulations in investigating the behavior of the finite sample distribution of the pivotal quantities defined in the preceding section. The sample is generated from a second-order RSM with the experimental design given by\( n \times n \) regular lattice on the rectangle \([0, 1] \times [0, 1]\).

\[
Y_{\ell k} = \beta_0 + \beta_1 \ell/n + \beta_2 k/n + \beta_{11} (\ell/n)^2 + \beta_{12} \ell k/(n^2) + \beta_{22} (k/n)^2 + \varepsilon_{\ell k}, \quad 1 \leq \ell, k \leq n.
\]

We consider the case \( \Psi = I_{n^2 \times n^2} \). For our results we generated the error terms independently from the standard normal distribution. In the first simulation we investigate the weak convergence of the quantity

\[
\hat{\sigma}_n \sqrt{n} \left( \hat{\beta}_n - \beta \right)
\]

with the covariance \( G^{-1} \), where \( G \) is obtained as the limit

\[
G = \lim_{n \to \infty} \frac{1}{n^2} \mathbf{X}_n^\top \mathbf{X}_n = \begin{pmatrix}
1 & 1/2 & 1/2 & 1/3 & 1/4 & 1/3 \\
1/2 & 1/3 & 1/4 & 1/4 & 1/6 & 1/6 \\
1/2 & 1/4 & 1/3 & 1/6 & 1/6 & 1/4 \\
1/3 & 1/4 & 1/6 & 1/5 & 1/8 & 1/9 \\
1/4 & 1/6 & 1/6 & 1/8 & 1/9 & 1/8 \\
1/3 & 1/6 & 1/4 & 1/9 & 1/8 & 1/5
\end{pmatrix}.
\]

Figure 1 exhibits the graphs of the empirical distribution function of \( \hat{\beta}_0, \hat{\beta}_1, \hat{\beta}_2, \hat{\beta}_{11}, \hat{\beta}_{12} \) and \( \hat{\beta}_{22} \) indicated by dotted line, whereas the graph of the CDF of the standard normal distribution is represented as smooth line. In the second case we consider the finite sample distribution of the quantity \( \frac{\sqrt{n} \mathbf{1}_s^\top (\hat{\beta}_n - \lambda)}{\sigma(\mathbf{1}_s \mathbf{1}_s^\top)^{1/2}} \), for \( s = 1, 2 \), which is shown to converge to the standard normal distribution. The simulation result is presented in Figure 2. Next in Figure 3
we present the empirical distribution function os the quantity

$$V_n := \frac{1}{\sigma(n)} \sqrt{n} (\hat{\lambda}^{(n)} - \lambda)^\top (\hat{\Sigma}_P^{(n)})^{-1} \frac{1}{\sigma(n)} \sqrt{n} (\hat{\lambda}^{(n)} - \lambda).$$

The dotted line is the empirical distribution function of $V_n$, whereas the smooth line is the empirical distribution function of a chi-square distribution with 2 degrees of freedom.

Based on the simulation result it can be concluded that our approach gives us a reasonable way to approximate the confidence region of the eigenvalues of $\hat{\mathbf{B}}^{(n)}$.

![ECDF of Lambda](image)

**Figure 3.** The empirical distribution functions of $V_n$ (dotted line) for $n = 25$ and 35.

### 4. Application to a mining data

We consider a data obtained from a mining industry in Southeast Sulawesi. The data is the percentage of Co (Cobalt) recorded over 98 points of drilling bore with 14 equidistance columns running south to north and 7 equidistance rows running west to east. By performing model-check using the partial sums technique proposed in Somayasa and et. al. [16] a second-order polynomial model with isotropic observation is appropriate for representing the model.

We assume a covariance structure as in [15]. After transforming the experimental region to the unit rectangle $[0, 1] \times [0, 1]$, we get

$$\hat{\mathbf{B}}^{(n)} = (-0.847, 0.611)^\top, \hat{\mathbf{B}}^{(n)} = \begin{pmatrix} -1.146 & +4.949 \\ +4.949 & -5.579 \end{pmatrix}, \hat{\mathbf{x}}_0 = (0.047, 0.096)^\top.$$

The eigenvalue and the associated eigenvector of $\hat{\mathbf{B}}^{(n)}$ are given by

$$\hat{\lambda}^{(n)} = (2.060, -8.785)^\top, \hat{\mathbf{u}}_1^{(n)} = (-0.839, -0.544)^\top, \hat{\mathbf{u}}_2^{(n)} = (0.544, -0.839)^\top.$$

By the transformation
Table 1. Percentages of Co (Cobalt) observed over 96 points \((x, y)\) of bore.

| x     | y     | Co(%) | x     | y     | Co(%) | x     | y     | Co(%) |
|-------|-------|-------|-------|-------|-------|-------|-------|-------|
| -5825 | -6000 | 0.07  | -5825 | -5900 | 0.06  | -5750 | -5825 | 0.04  | -5675 | -5750 | 0.07  |
| -5800 | -6000 | 0.06  | -5800 | -5900 | 0.06  | -5725 | -5825 | 0.04  | -5825 | -5725 | 0.05  |
| -5775 | -6000 | 0.06  | -5775 | -5900 | 0.05  | -5700 | -5825 | 0.06  | -5800 | -5725 | 0.05  |
| -5750 | -6000 | 0.05  | -5750 | -5900 | 0.05  | -5675 | -5800 | 0.06  | -5725 | -5725 | 0.05  |
| -5725 | -6000 | 0.08  | -5725 | -5900 | 0.05  | -5825 | -5800 | 0.06  | -5750 | -5725 | 0.05  |
| -5700 | -6000 | 0.07  | -5700 | -5900 | 0.10  | -5800 | -5800 | 0.05  | -5725 | -5725 | 0.05  |
| -5675 | -6000 | 0.04  | -5675 | -5900 | 0.14  | -5775 | -5800 | 0.04  | -5700 | -5725 | 0.04  |
| -5825 | -5975 | 0.07  | -5825 | -5875 | 0.05  | -5750 | -5800 | 0.04  | -5675 | -5725 | 0.06  |
| -5800 | -5975 | 0.08  | -5800 | -5875 | 0.05  | -5725 | -5800 | 0.13  | -5825 | -5700 | 0.04  |
| -5775 | -5975 | 0.09  | -5775 | -5875 | 0.05  | -5700 | -5800 | 0.13  | -5800 | -5700 | 0.05  |
| -5750 | -5975 | 0.08  | -5750 | -5875 | 0.07  | -5675 | -5800 | 0.10  | -5775 | -5700 | 0.07  |
| -5725 | -5975 | 0.10  | -5725 | -5875 | 0.08  | -5825 | -5775 | 0.09  | -5750 | -5700 | 0.07  |
| -5700 | -5975 | 0.11  | -5700 | -5875 | 0.05  | -5800 | -5775 | 0.08  | -5725 | -5700 | 0.06  |
| -5675 | -5975 | 0.13  | -5675 | -5875 | 0.06  | -5775 | -5775 | 0.07  | -5700 | -5700 | 0.07  |
| -5825 | -5950 | 0.06  | -5825 | -5850 | 0.06  | -5750 | -5775 | 0.06  | -5675 | -5700 | 0.05  |
| -5800 | -5950 | 0.09  | -5800 | -5850 | 0.06  | -5725 | -5775 | 0.06  | -5825 | -5675 | 0.05  |
| -5775 | -5950 | 0.12  | -5775 | -5850 | 0.07  | -5700 | -5775 | 0.07  | -5800 | -5675 | 0.05  |
| -5750 | -5950 | 0.08  | -5750 | -5850 | 0.07  | -5675 | -5775 | 0.06  | -5775 | -5675 | 0.05  |
| -5725 | -5950 | 0.10  | -5725 | -5850 | 0.14  | -5825 | -5750 | 0.06  | -5750 | -5675 | 0.05  |
| -5700 | -5950 | 0.12  | -5700 | -5850 | 0.09  | -5800 | -5750 | 0.05  | -5725 | -5675 | 0.06  |
| -5675 | -5950 | 0.08  | -5675 | -5850 | 0.05  | -5775 | -5750 | 0.04  | -5700 | -5675 | 0.05  |
| -5825 | -5925 | 0.05  | -5825 | -5825 | 0.05  | -5750 | -5750 | 0.05  | -5675 | -5675 | 0.05  |
| -5800 | -5925 | 0.05  | -5800 | -5825 | 0.04  | -5725 | -5750 | 0.05  | -5750 | -5925 | 0.06  |
| -5775 | -5925 | 0.07  | -5775 | -5825 | 0.05  | -5700 | -5750 | 0.06  | -5725 | -5925 | 0.06  |
| -5700 | -5925 | 0.07  | -5700 | -5925 | 0.07  |

Source of Data: PT. Aneka Tambang Tbk. Pomalaa, available in Tahir [19].

\[
\begin{pmatrix}
  w_1 \\
  w_2
\end{pmatrix} = \begin{pmatrix}
  -0.839 & -0.544 \\
  +0.544 & -0.839
\end{pmatrix} \begin{pmatrix}
  x_1 - 0.047 \\
  x_2 - 0.096
\end{pmatrix},
\]

we obtain the canonical form of the fitted model as \(\hat{\lambda}^{(n)} = 0.947 + 2.060 w_1^2 - 8.785 w_2^2\). Since the estimated eigenvalues have different signs, we can infer that the estimated stationary point \(\lambda_0\) seems to be a saddle point. We get the estimated Hessian matrix and the estimated covariance matrix of \(\lambda^{(n)}\) as

\[
\hat{H}^{(n)} = \begin{pmatrix}
  +0.704 & +0.913 & +0.296 \\
  +0.296 & -0.913 & +0.704
\end{pmatrix}, \quad \hat{\Sigma}^{(n)} = \begin{pmatrix}
  135.357 & 45.207 \\
  45.207 & 135.357
\end{pmatrix}.
\]

Hence the approximated \((1 - \alpha) \times 100\%\) confidence region for \(\lambda\) is given by

\[
\left\{ \begin{pmatrix}
  \lambda_1 \\
  \lambda_2
\end{pmatrix} \in \mathbb{R}^2 : \begin{pmatrix}
  +2.060 - \lambda_1 \\
  -8.785 - \lambda_2
\end{pmatrix}^\top \begin{pmatrix}
  +0.008 & -0.003 \\
  -0.003 & +0.008
\end{pmatrix} \begin{pmatrix}
  +2.060 - \lambda_1 \\
  -8.785 - \lambda_2
\end{pmatrix} \leq \frac{1}{1600} \lambda^{2-\alpha}(2) \right\}.
\]

The last region is actually an ellipsoid on two dimensional region. To see this let us define a
new coordinate system \((\lambda'_1, \lambda'_2)^\top\) according to the transformation formula
\[
\begin{pmatrix}
\lambda_1 \\
\lambda_2
\end{pmatrix}
= \begin{pmatrix}
-\frac{1}{2}\sqrt{2} & -\frac{1}{2}\sqrt{2} \\
\frac{1}{2}\sqrt{2} & -\frac{1}{2}\sqrt{2}
\end{pmatrix}
\begin{pmatrix}
\lambda'_1 \\
\lambda'_2
\end{pmatrix}
+ \begin{pmatrix}
+2.060 \\
-8.785
\end{pmatrix}.
\]
Then by substituting \(\lambda_1\) and \(\lambda_2\) then we get the new confidence region in term of \(\lambda'_1\) and \(\lambda'_2\):
\[
\left\{ \left( \begin{array}{c} \lambda'_1 \\ \lambda'_2 \end{array} \right) \in \mathbb{R}^2 : \left( \begin{array}{c} \frac{\lambda'_1}{\sqrt{\frac{1}{17}b \lambda'^2_1(2)}} \\ \frac{\lambda'_2}{\sqrt{\frac{8}{3} \lambda'^2_1(2)}} \end{array} \right) \leq 1 \right\}.
\]

The computation result gives us information that the stationary point of the process is set on the point \((0.047, 0.096)\) which lies on the experimental region. Unfortunately the stationary point associated to a saddle point. Therefore we can not determine whether on that point the process attains a maximum or a minimum value.

5. Conclusion

We have developed an asymptotic method for constructing the confidence region as well as confidence interval for the eigenvalues of the model matrix in normal second-order response surface model with spatially correlated observations. From the practical view point the computation of the derived formula is easily executed so that it seems to be very helpful for the practitioner. Given a data observed from a second-order RSM the optimum property of the stationary point can be immediately identified by conducting a computation according the algorithm presented at the end of Section 2. The stationary point of the percentage of Co data which lies on the point \((0.047, 0.096)\) is a saddle point.

Acknowledgement

The authors wishes to thank the Indonesian Ministry of Research and Technology and Higher Education for the financial support through the SAME 2015 program. A special thank is also dedicated to the Institut fuer Stochastik of Karlsruhe Institut fuer Technologie for hospitality.

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