

Asymptotic normality of the optimal solution in multiresponse surface methodology

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Abstract

In this work is obtained an explicit form for the perturbation effect on the matrix of regression coefficients on the optimal solution in multiresponse surface methodology. Then, the sensitivity analysis of the optimal solution is studied and the critical point characterisation of the convex program, associated with the optimum of a multiresponse surface, is also analysed. Finally, the asymptotic normality of the optimal solution is derived by standard methods.

2000 Mathematical Subject Classification: primary 62K20, 90C25, 90C31.

Key words: Asymptotic normality; multiresponse surface optimisation; sensitivity analysis; mathematical programming.

1 Introduction

The multiresponse surface methodology has been considered as a very useful tool in the study of designs, phenomena and experiments. Which enables us to propose a set of analytical relationship between responses and controlled variables through a process of continuous improvement and optimisation.

It is assumed that a researcher knows a system and a corresponding set of observable responses variables Y_1, \dots, Y_r which depends on some input variables, x_1, \dots, x_n . This also supposes that the input variables x_i 's can be controlled by the researcher with a minimum error.

Typically we have that

$$Y_k(\mathbf{x}) = \eta_k(x_1, \dots, x_n), \quad k = 1, \dots, r, \quad \text{and } \mathbf{x} = (x_1, \dots, x_n)', \quad (1.1)$$

where the form of the functions $\eta_k(\cdot)$'s are unknown and perhaps, very complex, and it is usually termed as the true response surface. The success of the response surfaces methodology depends on the approximation of $\eta_k(\cdot)$ for a polynomial of low degree in some region.

For purposes of this paper is assumed that $\eta_k(\cdot)$ can be soundly approximated by a polynomial of second order, that is

$$Y_k(\mathbf{x}) = \beta_{0k} + \sum_{i=1}^n \beta_{ik}x_i + \sum_{i=1}^n \beta_{iik}x_i^2 + \sum_{i=1}^n \sum_{j>i}^n \beta_{ijk}x_ix_j \quad (1.2)$$

where the unknown parameters β_j^s can be estimated via regression's techniques, as it will be described in next section.

Next, we are interested in obtaining the levels of the input variables x_i^s such that the response variables Y_1, \dots, Y_r are simultaneously minimal (optimal). This can be achieved if the following multiobjective mathematical program is solved

$$\begin{aligned} \min_{\mathbf{x}} \quad & \begin{pmatrix} Y_1(\mathbf{x}) \\ Y_2(\mathbf{x}) \\ \vdots \\ Y_r(\mathbf{x}) \end{pmatrix} \\ & \text{subject to} \\ & \mathbf{x} \in \mathfrak{X}, \end{aligned} \quad (1.3)$$

where \mathfrak{X} is certain operating region for the input variables x_i^s .

Now, two questions, closely related, can be observed:

1. When the estimations of (1.2) for $k = 1, \dots, r$ are considered into (1.3), the critical point \mathbf{x}^* obtained as solution shall be a function of the estimators $\widehat{\beta}_j^s$ of the β_j^s . Thus, given that $\widehat{\beta}_j^s$ are random variables, then $\mathbf{x}^* \equiv \mathbf{x}^*(\widehat{\beta}_j^s)$ is a random vector too. So, under the assumption that the distribution of $\widehat{\beta}$ is known, then, what is the distribution of $\mathbf{x}^*(\widehat{\beta}_j^s)$?
2. And, perhaps it is not sufficient to know only a point estimate of $\mathbf{x}^*(\widehat{\beta}_j^s)$, could be more convenient to know a estimated region or a estimated interval.

In particular, the distribution of the critical point in a univariate response surface model was studied by Díaz García and Ramos-Quiroga (2001, 2002), when $y(\mathbf{x})$ is defined as an hyperplane.

Now, in the context of the mathematical programming problems, the sensitivity analysis studies the effect of small perturbations in: (1) the parameters on the optimal objective function value and (2) the critical point. In general, these parameters shape the objective function and constraint the approach to the mathematical programming problem. In particular, Jagannathan (1977), Dupačová (1984) and Fiacco and Ghaemi (1982) have studied the sensitivity analysis of the mathematical programming, among many other authors. As an immediate consequence of the sensitivity analysis emerges the asymptotic normality study of the critical point, which can be performed by standard methods of mathematical statistics (see similar results for the case of maximum likelihood estimates Aitchison and Silvey (1958)). This last consequence makes the sensitivity analysis very appealing for researching from a statistical point of view. However, this approach must be fitted into the classical philosophy of the sensitivity analysis; i.e., we need to translate into the statistical language, the general sensitivity analysis methodology, which deals with a number of ways in

which the estimators of certain model are affected by omission of a particular set of variables or by the inclusion or omission of a particular observation or set of observations, see Chatterjee and Hadi (1988).

This papers pursues to important aims: the effect of perturbations of the matrix of regression parameters on the optimal solution of the multiresponse surface model and the asymptotic normality of the critical point. First, in Section 2 some notation is defined. Then, the multiresponse surface mathematical program is proposed in Section 3 as a multiobjective mathematical programming problem and a general solution is considered in terms of a functional. The characterisation of the critical point is given in Section 4 by stating the first-order and second-order Kuhn-Tucker conditions. Finally, the asymptotic normality of a critical point is established in Section 5 and for a particular form of the functional, the asymptotic normality of a critical point is also derived.

2 Notation

For convenience, the principal properties and usual notations are given here. A detailed discussion of the multiresponse surface methodology can be found in Khuri and Cornell (1987, Chap. 7) and Khuri and Conlon (1981).

Let N be the number of experimental runs and r be the number of response variables, which can be measured for each setting of a group of n coded variables x_1, x_2, \dots, x_n . It is assumed that the response variables can be modelled by a second order polynomial regression model in terms of $x_i, i = 1, \dots, n$. Hence, the k^{th} response model can be written as

$$\mathbf{Y}_k = \mathbf{X}_k \boldsymbol{\beta}_k + \boldsymbol{\varepsilon}_k, \quad k = 1, \dots, r, \quad (2.4)$$

where \mathbf{Y}_k is an $N \times 1$ vector of observations on the k^{th} response, \mathbf{X}_k is an $N \times p$ matrix of rank p termed the design or regression matrix, $p = 1 + n + n(n+1)/2$, $\boldsymbol{\beta}_k$ is a $p \times 1$ vector of unknown constant parameters, and $\boldsymbol{\varepsilon}_k$ is a random error vector associated with the k^{th} response. For purposes of this study is assumed that $\mathbf{X}_1 = \dots = \mathbf{X}_r = \mathbf{X}$. Therefore, (2.4) can be written as

$$\mathbf{Y} = \mathbf{X}\mathbb{B} + \mathbb{E} \quad (2.5)$$

where $\mathbf{Y} = \begin{bmatrix} \mathbf{Y}_1 \\ \mathbf{Y}_2 \\ \vdots \\ \mathbf{Y}_r \end{bmatrix}$, $\mathbb{B} = \begin{bmatrix} \boldsymbol{\beta}_1 \\ \boldsymbol{\beta}_2 \\ \vdots \\ \boldsymbol{\beta}_r \end{bmatrix}$, moreover

$$\boldsymbol{\beta}_k = (\beta_{0k}, \beta_{1k}, \dots, \beta_{nk}, \beta_{11k}, \dots, \beta_{nnk}, \beta_{12k}, \dots, \beta_{(n-1)nk})'$$

and $\mathbb{E} = \begin{bmatrix} \boldsymbol{\varepsilon}_1 \\ \boldsymbol{\varepsilon}_2 \\ \vdots \\ \boldsymbol{\varepsilon}_r \end{bmatrix}$, such that $\mathbb{E} \sim \mathcal{N}_{N \times r}(\mathbf{0}, \mathbf{I}_N \otimes \boldsymbol{\Sigma})$ i.e. \mathbb{E} has an $N \times r$ matrix multivariate normal distribution with $\mathbb{E}(\mathbb{E}) = \mathbf{0}$ and $\text{Cov}(\text{vec } \mathbb{E}') = \mathbf{I}_N \otimes \boldsymbol{\Sigma}$, where $\boldsymbol{\Sigma}$ is a $r \times r$ positive definite matrix. Now, if $\mathbf{A} = \begin{bmatrix} \mathbf{A}_1 \\ \mathbf{A}_2 \\ \vdots \\ \mathbf{A}_r \end{bmatrix}$, with $\mathbf{A}_j, j = 1, \dots, r$ the columns of \mathbf{A} ; then $\text{vec } \mathbf{A} = (\mathbf{A}'_1, \mathbf{A}'_2, \dots, \mathbf{A}'_r)'$ and \otimes denotes the direct (or Kronecker) product of matrices, see Muirhead (1982, Theorem 3.2.2, p. 79). In addition denote

- $\mathbf{x} = (x_1, x_2, \dots, x_n)'$: The vector of controllable variables or factors. Formally, an x_i variable is associated with each factor A, B, \dots

- $\widehat{\mathbb{B}} = \begin{bmatrix} \widehat{\boldsymbol{\beta}}_1 \\ \widehat{\boldsymbol{\beta}}_2 \\ \vdots \\ \widehat{\boldsymbol{\beta}}_r \end{bmatrix}$: The least squares estimator of \mathbb{B} given by $\widehat{\mathbb{B}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$, from where

$$\widehat{\boldsymbol{\beta}}_k = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}_k = (\widehat{\beta}_{0k}, \widehat{\beta}_{1k}, \dots, \widehat{\beta}_n, \widehat{\beta}_{11k}, \dots, \widehat{\beta}_{nnk}, \widehat{\beta}_{12k}, \dots, \widehat{\beta}_{(n-1)nk})'$$

- $k = 1, 2, \dots, r$. Moreover, under the assumption that $\mathbb{E} \sim \mathcal{N}_{N \times r}(\mathbf{0}, \mathbf{I}_N \otimes \boldsymbol{\Sigma})$, then $\widehat{\mathbb{B}} \sim \mathcal{N}_{p \times r}(\mathbb{B}, (\mathbf{X}'\mathbf{X})^{-1} \otimes \boldsymbol{\Sigma})$, with $\text{Cov}(\text{vec } \widehat{\mathbb{B}}') = (\mathbf{X}'\mathbf{X})^{-1} \otimes \boldsymbol{\Sigma}$.
- $\mathbf{z}(\mathbf{x}) = (1, x_1, x_2, \dots, x_n, x_1^2, x_2^2, \dots, x_n^2, x_1x_2, x_1x_3, \dots, x_{n-1}x_n)'$.
 - $\widehat{\boldsymbol{\beta}}_{1k} = (\widehat{\beta}_{1k}, \dots, \widehat{\beta}_{nk})'$ and

$$\widehat{\mathbf{B}}_k = \frac{1}{2} \begin{pmatrix} 2\widehat{\beta}_{11k} & \widehat{\beta}_{12k} & \cdots & \widehat{\beta}_{1nk} \\ \widehat{\beta}_{21k} & 2\widehat{\beta}_{22k} & \cdots & \widehat{\beta}_{2nk} \\ \vdots & \vdots & \ddots & \vdots \\ \widehat{\beta}_{n1k} & \widehat{\beta}_{n2k} & \cdots & 2\widehat{\beta}_{nnk} \end{pmatrix}$$

$$\begin{aligned} \widehat{Y}_k(\mathbf{x}) &= \mathbf{z}'(\mathbf{x})\widehat{\boldsymbol{\beta}}_k \\ &= \widehat{\beta}_{0k} + \sum_{i=1}^n \widehat{\beta}_{ik}x_i + \sum_{i=1}^n \widehat{\beta}_{iik}x_i^2 + \sum_{i=1}^n \sum_{j>i}^n \widehat{\beta}_{ijk}x_ix_j \\ &= \widehat{\boldsymbol{\beta}}_{0k} + \widehat{\boldsymbol{\beta}}_{1k}'\mathbf{x} + \mathbf{x}'\widehat{\mathbf{B}}_k\mathbf{x} : \end{aligned}$$

The response surface or predictor equation at the point \mathbf{x} for the k^{th} response variable.

- $\widehat{\mathbf{Y}}(\mathbf{x}) = (\widehat{Y}_1(\mathbf{x}), \widehat{Y}_2(\mathbf{x}), \dots, \widehat{Y}_r(\mathbf{x}))' = \widehat{\mathbb{B}}'\mathbf{z}(\mathbf{x})$: The multiresponse surface or predicted response vector at the point \mathbf{x} .
- $\widehat{\boldsymbol{\Sigma}} = \frac{\mathbf{Y}'(\mathbf{I}_N - \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}')\mathbf{Y}}{N-p}$: The estimator of the variance-covariance matrix $\boldsymbol{\Sigma}$ such that $(N-p)\widehat{\boldsymbol{\Sigma}}$ has a Wishart distribution with $(N-p)$ degrees of freedom and the parameter $\boldsymbol{\Sigma}$; this fact is denoted as $(N-p)\widehat{\boldsymbol{\Sigma}} \sim \mathcal{W}_r(N-p, \boldsymbol{\Sigma})$. Here, \mathbf{I}_m denotes an identity matrix of order m .
- Finally, note that

$$E(\widehat{\mathbf{Y}}(\mathbf{x})) = E(\widehat{\mathbb{B}}'\mathbf{z}(\mathbf{x})) = \mathbb{B}'\mathbf{z}(\mathbf{x}) \quad (2.6)$$

and

$$\text{Cov}(\widehat{\mathbf{Y}}(\mathbf{x})) = \mathbf{z}'(\mathbf{x})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{z}(\mathbf{x})\boldsymbol{\Sigma}. \quad (2.7)$$

An unbiased estimator of $\text{Cov}(\widehat{\mathbf{Y}}(\mathbf{x}))$ is given by

$$\widehat{\text{Cov}}(\widehat{\mathbf{Y}}(\mathbf{x})) = \mathbf{z}'(\mathbf{x})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{z}(\mathbf{x})\widehat{\boldsymbol{\Sigma}}. \quad (2.8)$$

3 Multiresponse surface mathematical programming

In the following sections, we make use of the multiresponse mathematical programming and multiobjective mathematical programming. For convenience, the concepts and notations required are listed below in terms of the estimated model of multiresponse surface mathematical programming. Definitions and detailed properties can be found in Khuri and Conlon (1981), Khuri and Cornell (1987), Ríos *et al.* (1989), Steuer (1986), and Miettinen (1999).

The multiresponse mathematical programming or multiresponse optimisation (MRO) problem is proposed, in general, as follows

$$\min_{\mathbf{x}} \widehat{\mathbf{Y}}(\mathbf{x}) = \min_{\mathbf{x}} \begin{pmatrix} \widehat{Y}_1(\mathbf{x}) \\ \widehat{Y}_2(\mathbf{x}) \\ \vdots \\ \widehat{Y}_r(\mathbf{x}) \end{pmatrix} \quad (3.9)$$

subject to
 $\mathbf{x} \in \mathfrak{X}$.

It is a nonlinear multiobjective mathematical programming problem, see Steuer (1986), Ríos *et al.* (1989) and Miettinen (1999); and \mathfrak{X} denotes the experimental region, usually taken as a hypercube

$$\mathfrak{X} = \{\mathbf{x} | l_i < x_i < u_i, \quad i = 1, 2, \dots, n\},$$

where $\mathbf{l} = (l_1, l_2, \dots, l_n)'$, defines the vector of lower bounds of factors and $\mathbf{u} = (u_1, u_2, \dots, u_n)'$, gives the vector of upper bounds of factors. Alternatively, the experimental region can taken as a hypersphere

$$\mathfrak{X} = \{\mathbf{x} | \mathbf{x}'\mathbf{x} \leq c^2, c \in \mathfrak{R}\},$$

where, c is set according to the experimental design model under consideration, see Khuri and Cornell (1987). Alternatively (3.9) can be written as

$$\min_{\mathbf{x} \in \mathfrak{X}} \widehat{\mathbf{Y}}(\mathbf{x}).$$

In the response surface methodology context, the multiobjective mathematical programs rarely contains a point \mathbf{x}^* which can be considered as an optimum, i.e. few cases satisfy the requirement that $\widehat{Y}_k(\mathbf{x})$ is minimum for all $k = 1, 2, \dots, r$. From the viewpoint of multiobjective mathematical programming, this justifies the following notion of the *Pareto point*:

We say that $\widehat{\mathbf{Y}}^(\mathbf{x})$ is a Pareto point of $\widehat{\mathbf{Y}}(\mathbf{x})$, if there is no other point $\widehat{\mathbf{Y}}^1(\mathbf{x})$ such that $\widehat{\mathbf{Y}}^1(\mathbf{x}) \leq \widehat{\mathbf{Y}}^*(\mathbf{x})$, i.e. for all k , $\widehat{Y}_k^1(\mathbf{x}) \leq \widehat{Y}_k^*(\mathbf{x})$ and $\widehat{\mathbf{Y}}^1(\mathbf{x}) \neq \widehat{\mathbf{Y}}^*(\mathbf{x})$.*

Steuer (1986), Ríos *et al.* (1989) and Miettinen (1999) established the existence criteria for Pareto points in a multiobjective mathematical programming problem and the extension of scalar mathematical programming (*Kuhn-Tucker's conditions*) to the vectorial case.

Methods for solving a multiobjective mathematical program are based on the existing information about a particular problem. There are three possible scenarios: when the investigator possesses either complete, partial or null information, see Ríos *et al.* (1989), Miettinen (1999) and Steuer (1986). In a response surface methodology context, complete information means that the investigator understands the population in such a way that it is possible to propose a *value function* reflecting the importance of each response variable. In partial information, the investigator knows the main response variable of the study very well and this is sufficient support for the research. Finally, under null information, the researcher only possesses information about the estimators of the response surface parameter, and with this elements an appropriate solution can be found too.

In general, an approach for solving a multiobjective mathematical program consist of proposing an equivalent nonlinear scalar mathematical program, i.e. as a solution of (3.9) is proposed the following problem

$$\begin{aligned} & \min_{\mathbf{x}} f\left(\widehat{\mathbf{Y}}(\mathbf{x})\right) \\ & \text{subject to} \\ & \mathbf{x} \in \mathfrak{X}, \end{aligned} \tag{3.10}$$

where $f(\cdot)$ defines a functional ($f(\cdot)$ is a function that takes functions as its argument, i.e. a function whose domain is a set of functions). Moreover, in the context of multiobjective mathematical programming, the functional $f(\cdot)$ is such that if $\mathfrak{M} \subset \mathfrak{R}^r$ denotes a set of multiresponse surface functions, then

The functional is a function $f : \mathfrak{M} \rightarrow \mathfrak{R}$ such that $\min \widehat{\mathbf{Y}}(\mathbf{x}^) < \min \widehat{\mathbf{Y}}(\mathbf{x}_1) \Leftrightarrow f(\widehat{\mathbf{Y}}(\mathbf{x}^*)) < f(\widehat{\mathbf{Y}}(\mathbf{x}_1))$, $\mathbf{x}^* \neq \mathbf{x}_1$.*

In order to consider a greater number of potential solutions of (3.9), usually studied in the multicriteria mathematical programming, the following alternative problem to (3.10) can be proposed

$$\begin{aligned} \min_{\mathbf{x}} f\left(\widehat{\mathbf{Y}}(\mathbf{x})\right) \\ \text{subject to} \\ \mathbf{x} \in \mathfrak{X} \cap \mathfrak{S}, \end{aligned} \quad (3.11)$$

where \mathfrak{S} is a subset generated by additional potential constraints, generally derived by a particular technique used for establishing the equivalent scalar mathematical program (3.10). In some particular cases of (3.10), a new fixed parameter may appear, a vector of response weights $\mathbf{w} = (w_1, w_2, \dots, w_r)'$, and/or a vector of target values for the response vector $\boldsymbol{\tau} = (\tau_1, \tau_2, \dots, \tau_r)'$. Particular examples of this equivalent univariate objective mathematical programming are the use of goal programming, see Kazemzadeh *et al.* (2008), and of the ϵ -constraint model, see Biles (1975), among many others. In particular, under the ϵ -constraint model, (3.11) is proposed as

$$\begin{aligned} \min_{\mathbf{x}} \widehat{Y}_j(\mathbf{x}) \\ \text{subject to} \\ \widehat{Y}_1(\mathbf{x}) \leq \tau_1 \\ \vdots \\ \widehat{Y}_{j-1}(\mathbf{x}) \leq \tau_{j-1} \\ \widehat{Y}_{j+1}(\mathbf{x}) \leq \tau_{j+1} \\ \vdots \\ \widehat{Y}_r(\mathbf{x}) \leq \tau_r \\ \mathbf{x} \in \mathfrak{X}. \end{aligned} \quad (3.12)$$

4 Characterisation of the critical point

In the rest of the paper we shall develop the theory of the problem (3.10); it is easy to see that this problem can be extended with minor modifications to the problem (3.11).

Let $\mathbf{x}^*(\widehat{\mathbb{B}}) \in \mathfrak{R}^n$ be the unique optimal solution of program (3.10) with the corresponding Lagrange multiplier $\lambda^*(\widehat{\mathbb{B}}) \in \mathfrak{R}$. The Lagrangian is defined by

$$L(\mathbf{x}, \lambda; \widehat{\mathbb{B}}) = f\left(\widehat{\mathbf{Y}}(\mathbf{x})\right) + \lambda(|\mathbf{x}|^2 - c^2). \quad (4.13)$$

Similarly, $\mathbf{x}^*(\mathbb{B}) \in \mathfrak{R}^n$ denotes the unique optimal solution of program (1.3) with the corresponding Lagrange multiplier $\lambda^*(\mathbb{B}) \in \mathfrak{R}$.

Now we establish the local Kuhn-Tucker conditions that guarantee that the Kuhn-Tucker point $\mathbf{r}^*(\widehat{\mathbb{B}}) = [\mathbf{x}^*(\widehat{\mathbb{B}}), \lambda^*(\widehat{\mathbb{B}})]' \in \mathfrak{R}^{n+1}$ is a unique global minimum of convex program (3.10).

First recall that for $f : \mathfrak{R}^n \rightarrow \mathfrak{R}$, $\frac{\partial f}{\partial \mathbf{x}} \equiv \nabla_{\mathbf{x}} f$ denotes the gradient of function f .

Theorem 4.1. *The necessary and sufficient conditions that a point $\mathbf{x}^*(\widehat{\mathbb{B}}) \in \mathfrak{R}^n$ for arbitrary fixed $\widehat{\mathbb{B}} \in \mathfrak{R}^p$, be a unique global minimum of the convex program (3.10) is that, $\mathbf{x}^*(\widehat{\mathbb{B}})$ and the corresponding Lagrange multiplier $\lambda^*(\widehat{\mathbb{B}}) \in \mathfrak{R}$, fulfill the Kuhn-Tucker first order conditions*

$$\nabla_{\mathbf{x}} L(\mathbf{x}, \lambda; \widehat{\mathbb{B}}) = \nabla_{\mathbf{x}} f\left(\widehat{\mathbf{Y}}(\mathbf{x})\right) + 2\lambda(\widehat{\mathbb{B}})\mathbf{x} = \mathbf{0} \quad (4.14)$$

$$\nabla_{\lambda} L(\mathbf{x}, \lambda; \widehat{\mathbb{B}}) = |\mathbf{x}|^2 - c^2 \leq 0 \quad (4.15)$$

$$\lambda(\widehat{\mathbb{B}})(|\mathbf{x}|^2 - c^2) = 0 \quad (4.16)$$

$$\lambda(\widehat{\mathbb{B}}) \geq 0 \quad (4.17)$$

In addition, assume that strict complementarity slackness holds at $\mathbf{x}^*(\mathbb{B})$ with respect to $\lambda^*(\mathbb{B})$, that is

$$\lambda^*(\mathbb{B}) > 0 \Leftrightarrow \|\mathbf{x}\|^2 - c^2 = 0. \quad (4.18)$$

Analogously, the Kuhn-Tucker condition (4.14) to (4.17) for $\widehat{\mathbb{B}} = \mathbb{B}$ are stated next.

Corollary 4.2. *The necessary and sufficient conditions that a point $\mathbf{x}^*(\mathbb{B}) \in \mathfrak{R}^n$ for arbitrary fixed $\mathbb{B} \in \mathfrak{R}^p$, be a unique global minimum of the convex program (1.3) is that, $\mathbf{x}^*(\mathbb{B})$ and the corresponding Lagrange multiplier $\lambda^*(\mathbb{B}) \in \mathfrak{R}$, fulfill the Kuhn-Tucker first order conditions*

$$\nabla_{\mathbf{x}}L(\mathbf{x}, \lambda; \mathbb{B}) = \nabla_{\mathbf{x}}f\left(\widehat{\mathbf{Y}}(\widehat{\mathbf{x}})\right) + 2\lambda(\mathbb{B})\mathbf{x} = \mathbf{0} \quad (4.19)$$

$$\nabla_{\lambda}L(\mathbf{x}, \lambda; \mathbb{B}) = \|\mathbf{x}\|^2 - c^2 \leq 0 \quad (4.20)$$

$$\lambda(\mathbb{B})(\|\mathbf{x}\|^2 - c^2) = 0 \quad (4.21)$$

$$\lambda(\mathbb{B}) \geq 0 \quad (4.22)$$

and $\lambda(\mathbb{B}) = 0$ when $\|\mathbf{x}\|^2 - c^2 < 0$ at $[\mathbf{x}^*(\mathbb{B}), \lambda^*(\mathbb{B})]'$.

Observe that, due to the strict convexity of the constraint and objective function, the second-order sufficient condition is evidently fulfilled for the convex program (3.10).

The next result states the existence of a once continuously differentiable solution to program (3.10), see Fiacco and Ghaemi (1982).

Theorem 4.3. *Assume that (4.18) holds and the second-order sufficient condition is satisfied by the convex program (3.10). Then*

1. $\mathbf{x}^*(\mathbb{B})$ is a unique global minimum of program (1.3) and $\lambda^*(\mathbb{B})$ is also unique.
2. For $\widehat{\mathbb{B}} \in V_{\varepsilon}(\mathbb{B})$ (is an ε -neighborhood or open ball), there exist a unique once continuously differentiable vector function

$$\mathbf{r}^*(\widehat{\mathbb{B}}) = \begin{bmatrix} \mathbf{x}^*(\widehat{\mathbb{B}}) \\ \lambda^*(\widehat{\mathbb{B}}) \end{bmatrix} \in \mathfrak{R}^{n+1}$$

satisfying the second order sufficient conditions of problem (1.3), such that $\mathbf{r}^*(\mathbb{B}) = [\mathbf{x}^*(\mathbb{B}), \lambda^*(\mathbb{B})]'$ and hence, $\mathbf{x}^*(\mathbb{B})$ is a unique global minimum of problem (3.10) with associated unique Lagrange multiplier $\lambda^*(\mathbb{B})$.

3. For $\widehat{\mathbb{B}} \in V_{\varepsilon}(\mathbb{B})$, the status of the constraint is unchanged and $\lambda^*(\widehat{\mathbb{B}}) > 0 \Leftrightarrow \|\mathbf{x}\|^2 - c^2 = 0$ holds.

5 Asymptotic normality of the critical point

This section considers the statistical and mathematical programming aspects of the sensitivity analysis of the optimum of a estimated multiresponse surface model.

Theorem 5.1. *Assume:*

1. For any $\widehat{\mathbb{B}} \in V_{\varepsilon}(\mathbb{B})$, the second-order sufficient condition is fulfilled for the convex program (3.10) such that the second order derivatives

$$\frac{\partial^2 L(\mathbf{x}, \lambda; \widehat{\mathbb{B}})}{\partial \mathbf{x} \partial \mathbf{x}'}, \quad \frac{\partial^2 L(\mathbf{x}, \lambda; \widehat{\mathbb{B}})}{\partial \mathbf{x} \partial \text{vec}' \widehat{\mathbb{B}}}, \quad \frac{\partial^2 L(\mathbf{x}, \lambda; \widehat{\mathbb{B}})}{\partial \mathbf{x} \partial \lambda}, \quad \frac{\partial^2 L(\mathbf{x}, \lambda; \widehat{\mathbb{B}})}{\partial \lambda \partial \mathbf{x}'}, \quad \frac{\partial^2 L(\mathbf{x}, \lambda; \widehat{\mathbb{B}})}{\partial \lambda \partial \text{vec} \widehat{\mathbb{B}}}$$

exist and are continuous in $[\mathbf{x}^*(\widehat{\mathbb{B}}), \lambda^*(\widehat{\mathbb{B}})]' \in V_\varepsilon([\mathbf{x}^*(\mathbb{B}), \lambda^*(\mathbb{B})]')$ and

$$\frac{\partial^2 L(\mathbf{x}, \lambda; \widehat{\mathbb{B}})}{\partial \mathbf{x} \partial \mathbf{x}'}$$

is positive definite.

2. $\widehat{\mathbb{B}}_\nu$, the estimator of the true parameter vector \mathbb{B}_ν , is based on a sample of size N_ν such that

$$\sqrt{N_\nu}(\widehat{\mathbb{B}}_\nu - \mathbb{B}_\nu) \sim \mathcal{N}_{p \times r}(\mathbb{B}, \Theta), \quad \frac{1}{N_\nu} \Theta = (\mathbf{X}' \mathbf{X})^{-1} \otimes \Sigma.$$

3. (4.18) holds for $\widehat{\mathbb{B}} = \mathbb{B}$. Then asymptotically

$$\sqrt{N_\nu} [\mathbf{x}^*(\widehat{\mathbb{B}}) - \mathbf{x}^*(\mathbb{B})] \xrightarrow{d} \mathcal{N}_n(\mathbf{0}_n, \Xi),$$

where the $n \times n$ variance-covariance matrix

$$\Xi = \left(\frac{\partial \mathbf{x}^*(\widehat{\mathbb{B}})}{\partial \text{vec } \widehat{\mathbb{B}}} \right) \widehat{\Theta} \left(\frac{\partial \mathbf{x}^*(\widehat{\mathbb{B}})}{\partial \text{vec } \widehat{\mathbb{B}}} \right)', \quad \frac{1}{N_\nu} \widehat{\Theta} = (\mathbf{X}' \mathbf{X})^{-1} \otimes \widehat{\Sigma}$$

such that all elements of $(\partial \mathbf{x}^*(\widehat{\mathbb{B}}) / \partial \text{vec } \widehat{\mathbb{B}})$ are continuous on any $\widehat{\mathbb{B}} \in V_\varepsilon(\mathbb{B})$; furthermore

$$\left(\frac{\partial \mathbf{x}^*(\widehat{\mathbb{B}})}{\partial \text{vec } \widehat{\mathbb{B}}} \right) = [\mathbf{I} - \mathbf{P}^{-1} \mathbf{Q} (\mathbf{Q}' \mathbf{P}^{-1} \mathbf{Q})^{-1} \mathbf{Q}'] \mathbf{P}^{-1} \mathbf{G},$$

where

$$\mathbf{P} = \frac{\partial^2 L(\mathbf{x}, \lambda; \widehat{\mathbb{B}})}{\partial \mathbf{x} \partial \mathbf{x}'}$$

$$\mathbf{Q} = \frac{\partial^2 L(\mathbf{x}, \lambda; \widehat{\mathbb{B}})}{\partial \lambda \partial \mathbf{x}}$$

$$\mathbf{G} = \frac{\partial^2 L(\mathbf{x}, \lambda; \widehat{\mathbb{B}})}{\partial \mathbf{x} \partial \text{vec}' \widehat{\mathbb{B}}}$$

Proof. According to Theorem 4.1 and Corollary 4.2, the Kuhn-Tucker conditions (4.14)–(4.17) at $[\mathbf{x}^*(\widehat{\mathbb{B}}), \lambda^*(\widehat{\mathbb{B}})]'$ and the conditions (4.19)–(4.22) at $[\mathbf{x}^*(\mathbb{B}), \lambda^*(\mathbb{B})]'$ are fulfilled for mathematical programs (1.3) and (3.10), respectively. From conditions (4.19)–(4.22) of Corollary 4.2, the following system equation

$$\nabla_{\mathbf{x}} L(\mathbf{x}, \lambda; \mathbb{B}) = \nabla_{\mathbf{x}} f(\widehat{\mathbf{Y}}(\mathbf{x})) + 2\lambda(\mathbb{B})\mathbf{x} = \mathbf{0} \quad (5.23)$$

$$\nabla_{\lambda} L(\mathbf{x}, \lambda; \mathbb{B}) = \|\mathbf{x}\|^2 - c^2 = 0, \quad (5.24)$$

has a solution $\mathbf{x}^*(\mathbb{B}), \lambda^*(\mathbb{B}) > 0, \mathbb{B}$.

The nonsingular Jacobian matrix of the continuously differentiable functions (5.23) and (5.27) with respect to \mathbf{x} and λ at $[\mathbf{x}^*(\widehat{\mathbb{B}}), \lambda^*(\widehat{\mathbb{B}})]'$ is

$$\begin{pmatrix} \frac{\partial^2 L(\mathbf{x}, \lambda; \widehat{\mathbb{B}})}{\partial \mathbf{x} \partial \mathbf{x}'} & \frac{\partial^2 L(\mathbf{x}, \lambda; \widehat{\mathbb{B}})}{\partial \lambda \partial \mathbf{x}} \\ \frac{\partial^2 L(\mathbf{x}, \lambda; \widehat{\mathbb{B}})}{\partial \mathbf{x}' \partial \lambda} & 0 \end{pmatrix}.$$

According to the implicit functions theorem, there is a neighborhood $V_\varepsilon(\mathbb{B})$ such that for arbitrary $\widehat{\mathbb{B}} \in V_\varepsilon(\mathbb{B})$, the system (5.23) and (5.27) has a unique solution $\mathbf{x}^*(\widehat{\mathbb{B}})$, $\lambda^*(\widehat{\mathbb{B}})$, $\widehat{\mathbb{B}}$ and by Theorem 4.3, the components of $\mathbf{x}^*(\widehat{\mathbb{B}})$, $\lambda^*(\widehat{\mathbb{B}})$ are continuously differentiable function of $\widehat{\mathbb{B}}$, see Bigelow and Shapiro (1974). Their derivatives are given by

$$\begin{pmatrix} \frac{\partial \mathbf{x}^*(\widehat{\mathbb{B}})}{\partial \text{vec } \widehat{\mathbb{B}}} \\ \frac{\partial \lambda^*(\widehat{\mathbb{B}})}{\partial \text{vec } \widehat{\mathbb{B}}} \end{pmatrix} = - \begin{pmatrix} \frac{\partial^2 L(\mathbf{x}, \lambda; \widehat{\mathbb{B}})}{\partial \mathbf{x} \partial \mathbf{x}'} & \frac{\partial^2 L(\mathbf{x}, \lambda; \widehat{\mathbb{B}})}{\partial \lambda \partial \mathbf{x}} \\ \frac{\partial^2 L(\mathbf{x}, \lambda; \widehat{\mathbb{B}})}{\partial \mathbf{x}' \partial \lambda} & 0 \end{pmatrix}^{-1} \begin{pmatrix} \frac{\partial^2 L(\mathbf{x}, \lambda; \widehat{\mathbb{B}})}{\partial \mathbf{x} \partial \text{vec}' \widehat{\mathbb{B}}} \\ 0 \end{pmatrix}. \quad (5.25)$$

The explicit form of $(\partial \mathbf{x}^*(\widehat{\mathbb{B}})/\partial \text{vec } \widehat{\mathbb{B}})$ follows from (5.25) and by the formula

$$\begin{pmatrix} \mathbf{P} & \mathbf{Q} \\ \mathbf{Q}' & \mathbf{0} \end{pmatrix}^{-1} = \begin{pmatrix} [\mathbf{I} - \mathbf{P}^{-1} \mathbf{Q} (\mathbf{Q}' \mathbf{P}^{-1} \mathbf{Q})^{-1} \mathbf{Q}'] \mathbf{P}^{-1} & \mathbf{P}^{-1} \mathbf{Q} (\mathbf{Q}' \mathbf{P}^{-1} \mathbf{Q})^{-1} \\ (\mathbf{Q}' \mathbf{P}^{-1} \mathbf{Q})^{-1} \mathbf{Q}' \mathbf{P}^{-1} & -(\mathbf{Q}' \mathbf{P}^{-1} \mathbf{Q})^{-1} \end{pmatrix},$$

where \mathbf{P} is symmetric and nonsingular.

Then from assumption 2, Rao (1973, (iii), p. 388) and Bishop *et al.* (1991, Theorem 14.6-2, p. 493) (see also Cramér (1946, p. 353)) we have

$$\sqrt{N_\nu} [\mathbf{x}^*(\widehat{\mathbb{B}}) - \mathbf{x}^*(\mathbb{B})] \xrightarrow{d} \mathcal{N}_n \left(\mathbf{0}_n, \left(\frac{\partial \mathbf{x}^*(\mathbb{B})}{\partial \text{vec } \widehat{\mathbb{B}}} \right) \Theta \left(\frac{\partial \mathbf{x}^*(\mathbb{B})}{\partial \text{vec } \widehat{\mathbb{B}}} \right)' \right). \quad (5.26)$$

Finally note that all elements of $(\partial \mathbf{x}^*/\partial \widehat{\mathbb{B}})$ are continuous on $V_\varepsilon(\mathbb{B})$, so that the asymptotical distribution (5.26) can be substituted by

$$\sqrt{N_\nu} [\mathbf{x}^*(\widehat{\mathbb{B}}) - \mathbf{x}^*(\mathbb{B})] \xrightarrow{d} \mathcal{N}_n \left(\mathbf{0}_n, \left(\frac{\partial \mathbf{x}^*(\widehat{\mathbb{B}})}{\partial \text{vec } \widehat{\mathbb{B}}} \right) \widehat{\Theta} \left(\frac{\partial \mathbf{x}^*(\widehat{\mathbb{B}})}{\partial \text{vec } \widehat{\mathbb{B}}} \right)' \right),$$

see Rao (1973, (iv), pp.388–389). □

As a particular case, assume that the functional in (3.10) is defined as

$$f(\widehat{\mathbf{Y}}(\mathbf{x})) = \sum_{k=1}^r w_k \widehat{Y}_k(\mathbf{x}), \quad \sum_{k=1}^r w_k = 1,$$

with w_k known constants. Then,

Corollary 5.2. *Suppose:*

1. For any $\widehat{\mathbb{B}} \in V_\varepsilon(\mathbb{B})$, the second-order sufficient condition is fulfilled for the convex program (3.10) such that the second order derivatives

$$\frac{\partial^2 L(\mathbf{x}, \lambda; \widehat{\mathbb{B}})}{\partial \mathbf{x} \partial \mathbf{x}'}, \quad \frac{\partial^2 L(\mathbf{x}, \lambda; \widehat{\mathbb{B}})}{\partial \mathbf{x} \partial \text{vec}' \widehat{\mathbb{B}}}, \quad \frac{\partial^2 L(\mathbf{x}, \lambda; \widehat{\mathbb{B}})}{\partial \mathbf{x} \partial \lambda}, \quad \frac{\partial^2 L(\mathbf{x}, \lambda; \widehat{\mathbb{B}})}{\partial \lambda \partial \mathbf{x}'}, \quad \frac{\partial^2 L(\mathbf{x}, \lambda; \widehat{\mathbb{B}})}{\partial \lambda \partial \text{vec } \widehat{\mathbb{B}}}$$

exist and are continuous in $[\mathbf{x}^*(\widehat{\mathbb{B}}), \lambda^*(\widehat{\mathbb{B}})]' \in V_\varepsilon([\mathbf{x}^*(\mathbb{B}), \lambda^*(\mathbb{B})]')$ and

$$\frac{\partial^2 L(\mathbf{x}, \lambda; \widehat{\mathbb{B}})}{\partial \mathbf{x} \partial \mathbf{x}'}$$

is positive definite.

2. $\widehat{\mathbb{B}}_\nu$, the estimator of the true parameter vector \mathbb{B}_ν , is based on a sample of size N_ν such that

$$\sqrt{N_\nu}(\widehat{\mathbb{B}}_\nu - \mathbb{B}_\nu) \sim \mathcal{N}_{p \times r}(\mathbb{B}, \Theta), \quad \frac{1}{N_\nu}\Theta = (\mathbf{X}'\mathbf{X})^{-1} \otimes \Sigma.$$

3. (4.18) holds for $\widehat{\mathbb{B}} = \mathbb{B}$. Then asymptotically

$$\sqrt{N_\nu} [\mathbf{x}^*(\widehat{\mathbb{B}}) - \mathbf{x}^*(\mathbb{B})] \xrightarrow{d} \mathcal{N}_n(\mathbf{0}_n, \Xi)$$

where the $n \times n$ variance-covariance matrix

$$\Xi = \left(\frac{\partial \mathbf{x}^*(\widehat{\mathbb{B}})}{\partial \text{vec } \widehat{\mathbb{B}}} \right) \widehat{\Theta} \left(\frac{\partial \mathbf{x}^*(\widehat{\mathbb{B}})}{\partial \text{vec } \widehat{\mathbb{B}}} \right)', \quad \frac{1}{N_\nu} \widehat{\Theta} = (\mathbf{X}'\mathbf{X})^{-1} \otimes \widehat{\Sigma}$$

such that all elements of $(\partial \mathbf{x}^*(\widehat{\mathbb{B}})/\partial \text{vec } \widehat{\mathbb{B}})$ are continuous on any $\widehat{\mathbb{B}} \in V_\varepsilon(\mathbb{B})$; furthermore

$$\left(\frac{\partial \mathbf{x}^*(\widehat{\mathbb{B}})}{\partial \text{vec } \widehat{\mathbb{B}}} \right) = \mathbf{S}^{-1} \left(\frac{\mathbf{x}^*(\widehat{\mathbb{B}})\mathbf{x}^*(\widehat{\mathbb{B}})'\mathbf{S}^{-1}}{\mathbf{x}^*(\widehat{\mathbb{B}})'\mathbf{S}^{-1}\mathbf{x}^*(\widehat{\mathbb{B}})} - \mathbf{I}_n \right) \mathbf{M}(\mathbf{x}^*(\widehat{\mathbb{B}})),$$

where

$$\mathbf{S} = \frac{\partial^2 L(\mathbf{x}, \lambda; \widehat{\mathbb{B}})}{\partial \mathbf{x} \partial \mathbf{x}'} = 2 \sum_{k=1}^r w_k \widehat{\mathbf{B}}_k - 2\lambda^*(\widehat{\mathbb{B}})\mathbf{I}_n.$$

and

$$\begin{aligned} \mathbf{M}(\mathbf{x}) &= \nabla_{\mathbf{x}} \mathbf{z}'(\mathbf{x}) = \frac{\partial \mathbf{z}'(\mathbf{x})}{\partial \mathbf{x}} \\ &= (\mathbf{0}; \mathbf{I}_n; 2 \text{diag}(\mathbf{x}); \mathbf{C}_1; \dots; \mathbf{C}_{n-1}) \in \mathfrak{R}^{n \times p}, \end{aligned}$$

with

$$\mathbf{C}_i = \begin{pmatrix} \mathbf{0}'_1 \\ \vdots \\ \mathbf{0}'_{i-1} \\ \mathbf{x}'\mathbf{A}_i \\ x_i \mathbf{I}_{n-i} \end{pmatrix}, \quad i = 1, \dots, n-1, \quad \mathbf{0}_j \in \mathfrak{R}^{n-i}, j = 1, \dots, i-1;$$

observing that when $i = 1$ (i.e. $j = 0$), this row does not appear in \mathbf{C}_1 ; and

$$\mathbf{A}_i = \begin{pmatrix} \mathbf{0}'_1 \\ \vdots \\ \mathbf{0}'_i \\ \mathbf{I}_{n-i} \end{pmatrix}, \quad \mathbf{0}'_k \in \mathfrak{R}^{n-i}, k = 1, \dots, i.$$

Proof. The required result follows from Theorem 5.1 and observing that in this particular case

$$\nabla_{\mathbf{x}} L(\mathbf{x}, \lambda; \mathbb{B}) = \left\{ \begin{array}{l} \mathbf{M}(\mathbf{x}) \sum_{k=1}^r w_k \boldsymbol{\beta}_k + 2\lambda(\mathbb{B})\mathbf{x} \\ \text{or} \\ \sum_{k=1}^r w_k [\boldsymbol{\beta}_{1k} + 2\mathbf{B}_k \mathbf{x}] + 2\lambda(\mathbb{B})\mathbf{x} \end{array} \right\} = \mathbf{0}$$

$$\nabla_{\lambda} L(\mathbf{x}, \lambda; \boldsymbol{\beta}) = \|\mathbf{x}\|^2 - c^2 = 0$$

□

Conclusions

As a consequence of Theorem 4.3 now is feasible to establish confidence regions and intervals and hypothesis tests on the critical point, see Bishop *et al.* (1991, Section 14.6.4, pp. 498–500); it is also possible to identify operating conditions as regions or intervals instead of isolated points.

The results of this paper can be taken as a good first approximation to the exact problem. However, unfortunately in many applications the number of observations is relatively small and perhaps the results obtained in this work should be applied with caution.

Acknowledgments

This paper was written during J. A. Díaz-García's stay as a professor at the Department of Statistics and O. R. of the University of Granada, España. F. Caro was supported by the project No. 158 of University of Medellin.

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