Multiple response optimisation: Multiobjective stochastic programming methods

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Abstract
The multiresponse surface problem is modelled as one of multiobjective stochastic optimisation, and diverse solutions are proposed. Several crucial differences are highlighted between this approach and others that have been proposed. Finally, in a numerical example, some particular solutions are applied and described in detail.

1 Introduction
Many (perhaps most) real-world design problems are in fact multiobjective optimisation problems in which the designer seeks to optimise simultaneously several performance attributes of a design, and an improvement in one objective is often only gained at the cost of deteriorations in others, and so a trade-off is necessary. Similar situations are met in the study of natural phenomena and in experimental trials.

Moreover, the response variables, perhaps the controllable variables and even some parameters involved in these studies may have a random (or stochastic) character.

A very useful statistical tool in the study of these designs, phenomena and experiments is that of the response surfaces methodology, in its multivariate version. This approach makes it possible to determine an analytical relationship between the response and control variables, through a process of continuous improvement and optimisation. Similarly, it allows us to obtain an approximate vector function (termed the multiresponse surface or predicted response vector) with a smaller amount of data and fewer experimental runs, see Khuri and Cornell (1987), Kleijnen (2008a), Myers, and Montgomery (2002) and Kleijnen (2008b).

Although the response variables are random and in consequence the estimated multiresponse surface contains shape parameters that are estimated in the regression stage (i.e.

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a polynomial regression model in terms of \( x \) where \( Y \) as a function of \( x \) is described by

\[
Y(x) = \beta_0 + \beta_1 x + \ldots + \beta_p x^p + \varepsilon
\]

where \( \varepsilon \sim N(0, \Sigma) \) and \( \Sigma \) is a positive definite matrix, where

\( \beta \) are unknown constant parameters, and \( x \) is an \( n \)-dimensional vector of coded variables (also termed factors) \( x_1, x_2, \ldots, x_n \). We assume that the response variables can be modelled by a second order polynomial regression model in terms of \( x_j^2 \). Hence, the \( k^{th} \) response model can be written as

\[
Y_k = X_k \beta_k + \varepsilon_k
\]

where \( Y_k \) is an \( N \times 1 \) vector of observations on the \( k^{th} \) response, \( X_k \) is an \( N \times p \) matrix of rank \( p \) termed the design or regression matrix, \( p = 1 + n + n(n + 1)/2 \), \( \beta_k \) is a \( p \times 1 \) vector of unknown constant parameters, and \( \varepsilon_k \) is a random error vector associated with the \( k^{th} \) response. In the present case, it is assumed that \( X_1 = \cdots = X_r = X \). Hence, (2) can be written as

\[
Y = XB + \varepsilon
\]

where \( Y = [Y_1; Y_2; \ldots; Y_r] \), \( B = [\beta_1; \beta_2; \ldots; \beta_r] \) and \( \varepsilon = [\varepsilon_1; \varepsilon_2; \ldots; \varepsilon_r] \), such that

\[
\varepsilon \sim N_{N \times r}(0, I_N \otimes \Sigma)
\]

i.e. \( \varepsilon \) has an \( N \times r \) matrix multivariate normal distribution with \( \varepsilon(\varepsilon) = 0 \) and \( \text{Cov}(\text{vec}\varepsilon') = I_N \otimes \Sigma \), where \( \Sigma \) is a \( r \times r \) positive definite matrix, where

\( \text{Cov}(\text{vec}\varepsilon') = I_N \otimes \Sigma \), where \( \Sigma \) is a \( r \times r \) positive definite matrix, where
if \( \mathbf{A} = [\mathbf{A}_1; \mathbf{A}_2; \ldots; \mathbf{A}_m] \), then \( \text{vec} \mathbf{A} = (\mathbf{A}_1', \mathbf{A}_2', \ldots, \mathbf{A}_m')' \) and \( \otimes \) denotes the direct (or Kronecker) product of matrices, see Muirhead (1982, Theorem 3.2.2, p. 79). In addition let

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

- \( \mathbf{\hat{B}} = [\mathbf{\hat{\beta}}_1; \mathbf{\hat{\beta}}_2; \ldots; \mathbf{\hat{\beta}}_r] \): The least squares estimator of \( \mathbf{B} \) given by \( \mathbf{\hat{B}} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} \), from where \( \mathbf{\hat{\beta}}_k = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}_k, k = 1, 2, \ldots, r \). Moreover, under the assumption that \( \mathbf{E} \sim N_{N \times r}(0, \mathbf{I}_N \otimes \Sigma) \), then \( \mathbf{\hat{B}} \sim N_{p \times r}(\mathbf{\hat{B}}, (\mathbf{X}'\mathbf{X})^{-1} \otimes \Sigma) \), with \( \text{Cov}(\text{vec} \mathbf{\hat{B}}') = (\mathbf{X}'\mathbf{X})^{-1} \otimes \Sigma \).

- \( \mathbf{z}(\mathbf{x}) = (1, x_1, x_2, \ldots, x_n, x_1^2, x_2^2, \ldots, x_n^2, x_1 x_2, x_1 x_3, \ldots, x_{n-1} x_n)' \).

- \( \mathbf{\hat{Y}}(\mathbf{x}) = (\hat{Y}_1(\mathbf{x}), \hat{Y}_2(\mathbf{x}), \ldots, \hat{Y}_r(\mathbf{x}))' \): The multiresponse surface or predicted response vector at the point \( \mathbf{x} \).

- \( \mathbf{\hat{\Sigma}} = \frac{\mathbf{Y}'(\mathbf{I}_N - \mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}}{N - p} \): The estimator of the variance-covariance matrix \( \Sigma \) such that \( (N - p)\mathbf{\hat{\Sigma}} \) has a Wishart distribution with \( (N - p) \) degrees of freedom and the parameter \( \Sigma \); this fact is denoted as \( (N - p)\mathbf{\hat{\Sigma}} \sim W_r(N - p, \Sigma) \). Here, \( \mathbf{I}_m \) denotes an identity matrix of order \( m \).

Finally, note that

\[
E(\mathbf{\hat{Y}}(\mathbf{x})) = E(\mathbf{\hat{B}}'\mathbf{z}(\mathbf{x})) = \mathbf{\hat{B}}'\mathbf{z}(\mathbf{x})
\]  

and

\[
\text{Cov}(\mathbf{\hat{Y}}(\mathbf{x})) = \mathbf{z}'(\mathbf{x})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{z}(\mathbf{x})\Sigma.
\]  

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

\[
\mathbf{\hat{Cov}}(\mathbf{\hat{Y}}(\mathbf{x})) = \mathbf{z}'(\mathbf{x})(\mathbf{X}'\mathbf{X})^{-1}\mathbf{z}(\mathbf{x})\mathbf{\hat{\Sigma}}.
\]  

### 3 Multiresponse optimisation

In the following sections, we make use of multiresponse optimisation and multiobjective (or more general multicriteria) optimisation. For convenience, the concepts and notation required are listed below in terms of the estimated model of multiresponse surface optimisation. Definitions and detailed properties may be found in Khuri and Cornell (1981), Khuri and Cornell (1987), Rios et al. (1989), Steuer (1986), Miettinen (1999), Vajda (1972) and Prékopa (1995).

The multiresponse optimisation (MRO) problem in general is proposed as

\[
\min_{\mathbf{x}} \mathbf{\hat{Y}}(\mathbf{x}) = \min_{\mathbf{x}} \left( \begin{array}{c} \hat{Y}_1(\mathbf{x}) \\ \hat{Y}_2(\mathbf{x}) \\ \vdots \\ \hat{Y}_r(\mathbf{x}) \end{array} \right)
\]

subject to

\[
\mathbf{x} \in \mathbf{X},
\]
which is a deterministic nonlinear multiobjective optimisation problem, see Steuer (1986), Ríos et al. (1989) and Miettinen (1999); and where \( \mathcal{X} \) denotes the experimental region, which in general is defined as a hypercube

\[
\mathcal{X} = \{x| l_i < x_i < u_i, \quad i = 1, 2, \ldots, n\},
\]

where \( l = (l_1, l_2, \ldots, l_n)^t \) defines the vector of lower bounds of factors and \( u = (u_1, u_2, \ldots, u_n)^t \) defines the vector of upper bounds of factors. Alternatively, the experimental region is defined as a hypersphere

\[
\mathcal{X} = \{x| x^t x \leq c^2, c \in \mathbb{R}\},
\]

where, in general, \( c \) is determined by the experimental design model used, see Khuri and Cornell (1987). Alternatively (7) can be written as

\[
\min_{x \in \mathcal{X}} \mathbf{\hat{Y}}(x)
\]

In the response surface methodology context, observe that in multiobjective optimisation problems, there rarely exists a point \( \mathbf{x}^* \) which is considered as an optimum, i.e. few cases satisfy the requirement that \( \mathbf{\hat{Y}}_k(\mathbf{x}) \) is minimum for all \( k = 1, 2, \ldots, r \). From the viewpoint of multiobjective optimisation, this justifies the following notion of the Pareto point, which is more weakly defined than is an optimum point:

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

Existence criteria for Pareto points in a multiobjective optimisation problem and the extension of scalar optimisation (Kuhn-Tucker’s conditions) to the vectorial case are established in Steuer (1986), Ríos et al. (1989) and Miettinen (1999).

Methods for solving a multiobjective optimisation problem are based on the information possessed 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, where

\[
\text{The value function is a function } f: \mathbb{R}^n \to \mathbb{R} \text{ such that } \min \mathbf{\hat{Y}}(\mathbf{x}^*) < \min \mathbf{\hat{Y}}(\mathbf{x}_1) \Leftrightarrow f(\mathbf{\hat{Y}}(\mathbf{x}^*)) < f(\mathbf{\hat{Y}}(\mathbf{x}_1)), \quad \mathbf{x}^* \neq \mathbf{x}_1.
\]

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 material an appropriate solution can be found too.

As can be observed, all the approaches proposed in the literature are particular cases of the models studied in multiobjective optimisation, and in particular of the \( \epsilon \)-constraint model and the value function model or a combination of the two. Accordingly, the equivalent nonlinear scalar optimisation problem of (7) is of the form

\[
\min_{\mathbf{x}} f(\mathbf{\hat{Y}}(\mathbf{x})) \quad \text{subject to} \quad \mathbf{x} \in \mathcal{X} \cap \mathcal{S},
\]

where \( \mathcal{S} \) is a subset generated by additional potential constraints, which derive from the particular technique used for establishing the equivalent deterministic scalar optimisation
problem (8). In some particular cases of (8), a new fixed parameter may appear, such as a \( w = (w_1, w_2, \ldots, w_r)' \), vector of response weights and/or \( \tau = (\tau_1, \tau_2, \ldots, \tau_r)' \), vector of target values for the response vector. Particular examples of this equivalent univariate objective optimisation are the use of goal programming, see Kazemzadeh et al. (2008), and of the \( \epsilon \)-constraint model, see Biles (1972), among many others.

When uncertainty is assumed in an MRO problem, in other words, when the MRO problem is considered as a stochastic program, different approaches have been proposed, see Nari (2008), Chiao and Hamada (2001), Amiri et al. (2008), Khuri and Conlon (1981) and Khuri and Cornell (1987). In particular some of these approaches can be established as

\[
\begin{align*}
\min_x f(\hat{Y}(x)) \\
\text{subject to} \\
\hat{B} \sim N_{p \times r}(B, (X'X)^{-1} \otimes \Sigma) \\
(N - p)\Sigma \sim W_r(N - p, \Sigma),
\end{align*}
\]

where \( \hat{B} \) and \( \hat{\Sigma} \) are independent.

In addition, it is sometimes assumed that \( w \) and/or \( \tau \) are stochastic, and diverse strategies have been proposed to obtain particular values for these, including Group Decision Making, among others, see Khuri and Conlon (1981) and Hejazi et al. (2010).

In general terms, thus, the MRO problem under uncertainty has been addressed as follows:

1. It is considered as a deterministic multiobjective optimisation problem (7).
2. An equivalent deterministic univariate optimisation problem, such as goal programming, is proposed (8).
3. In the equivalent deterministic univariate optimisation problem, uncertainty is assumed (9).

### 4 Proposed approach

In the univariate case, Díaz-García et al. (2005) considered the problem as a stochastic optimisation program. The approach proposed in the present paper consists in extending this idea to multiresponse optimisation. Specifically, we propose the MRO as the following nonlinear multiobjective stochastic optimisation problem from the beginning:

\[
\begin{align*}
\min_x \tilde{Y}(x, \tilde{B}) \\
\text{subject to} \\
\tilde{B} \sim N_{p \times r}(B, (X'X)^{-1} \otimes \Sigma) \\
(N - p)\Sigma \sim W_r(N - p, \Sigma).
\end{align*}
\]

where \( \tilde{Y}(x, \tilde{B}) \equiv \tilde{Y}(x) \) and \( \tilde{Y}_k(x, \tilde{B}_k) \equiv \tilde{Y}_k(x) \).

The solution of (10) can be applied to any model (technique, method or solution) under multiobjective stochastic optimisation, which in general, is a multidimensional extension of stochastic optimisation models, see Vajda (1972), Díaz-García et al. (2005) and Prékopa (1995).
4.1 Multiobjective stochastic optimisation approaches

In this subsection we propose under diverse multiobjective stochastic optimisation approaches. The properties of the solution obtained under the different approaches are described in detail by Kataoka (1963), Stancu-Minasian (1984) and Prékopa (1995).

As shown below, each multiobjective stochastic optimisation approach can be proposed in several ways. In some cases, this possibility is a consequence of assuming that the response variables are correlated or not.

4.1.1 Multiobjective expected value solution, multiobjective E-model

Point \( x \in X \) is the expected value solution to (10) if it is an efficient solution in the Pareto sense to the following deterministic multiobjective optimisation problem

\[
\min_{x \in X} E \left( \hat{Y} \left( x, \hat{B} \right) \right)
\]

4.1.2 Multiobjective minimum variance solution, multiobjective V-model

The \( x \in X \) point is the minimum variance solution to problem (10) if it is an efficient solution in the Pareto sense of the deterministic multiobjective optimisation problem

\[
\min_{x \in X} \begin{pmatrix}
\text{Var} \left( \hat{Y}_1(x) \right) \\
\text{Var} \left( \hat{Y}_2(x) \right) \\
\vdots \\
\text{Var} \left( \hat{Y}_r(x) \right)
\end{pmatrix}
\]

This efficient solution is adequate if it is assumed that the response variables are Uncorrelated. However, if the response variables are assumed to be correlated a better one is:

\[
\min_{x \in X} \text{Cov} \left( \hat{Y} \left( x, \hat{B} \right) \right)
\]

4.1.3 Multiobjective expected value standard deviation solution, multiobjective modified E-model

Point \( x \in X \) is an expected value standard deviation solution to the problem (10) if it is an efficient solution in the Pareto sense of the mixed deterministic multiobjective-matrix optimisation problem

\[
\min_{x \in X} \begin{pmatrix}
E \left( \hat{Y} \left( x, \hat{B} \right) \right) \\
\text{Cov} \left( \hat{Y} \left( x, \hat{B} \right) \right)^{1/2}
\end{pmatrix}
\]

where \((A^{1/2})^2 = A\), see Muirhead (1982, Appendix).

We now define the concept of the efficient solution of multiobjective minimum risk of joint aspiration level \( \tau = (\tau_1, \tau_2, \ldots, \tau_r)' \) and the efficient solution with a joint probability \( \alpha \). The two solutions are obtained by applying the multivariate versions of minimum risk and the Kataoka criteria, respectively, referred to in the literature as criteria of maximum probability or satisfying criteria, due to the fact that, as shown below, in both cases the criteria to be used provide, in one way or another, “good” solutions in terms of probability, see Kataoka (1963).
4.1.4 Multiobjective minimum risk solution of joint aspiration level $\tau$, multiobjective modified P-model

Point $x \in X$ is a minimum risk solution of joint aspiration level $\tau$ to problem (10) if it constitutes an efficient solution in the Pareto sense of the multiobjective stochastic optimisation problem

$$\min_{x \in X} \begin{pmatrix} P\left(\hat{Y}_1(x) \leq \tau_1\right) \\ P\left(\hat{Y}_2(x) \leq \tau_2\right) \\ \vdots \\ P\left(\hat{Y}_r(x) \leq \tau_r\right) \end{pmatrix}.$$  \hfill (15)

It is also possible to consider the following alternative multiobjective P-model

$$\min_{x \in X} P \begin{pmatrix} \hat{Y}_1(x) \leq \tau_1 \\ \hat{Y}_2(x) \leq \tau_2 \\ \vdots \\ \hat{Y}_r(x) \leq \tau_r \end{pmatrix}.$$  \hfill (16)

Again, (16) is more adequate if the response variables are correlated. However, (16) is considerably more complicated to solve than (15). When $r = 2$, Prékopa (1970) proposed an algorithm for a similar problem (probabilistic constrained programming), which can be applied to solve (16).

4.1.5 Multiobjective Kataoka solution with probability $\alpha$

Point $x \in X$ is a multiobjective Kataoka solution with probability $\alpha$ (fixed) to problem (10) if it is an efficient solution in the Pareto sense of the multiobjective optimisation problem

$$\min_{x, \tau} \tau \begin{pmatrix} \tau_1 \\ \tau_2 \\ \vdots \\ \tau_r \end{pmatrix} \text{ subject to } \begin{pmatrix} P\left(\hat{Y}_k(x) \leq \tau_k\right) = \alpha, k = 1, 2, \ldots, r \\ x \in X \end{pmatrix}.$$  \hfill (17)

Alternatively, (17) can be proposed as

$$\min_{x, \tau} \tau \begin{pmatrix} \tau_1 \\ \tau_2 \\ \vdots \\ \tau_r \end{pmatrix} \text{ subject to } \begin{pmatrix} P\left(\hat{Y}_1(x) \leq \tau_1\right) \\ P\left(\hat{Y}_2(x) \leq \tau_2\right) \\ \vdots \\ P\left(\hat{Y}_r(x) \leq \tau_r\right) = \alpha \\ x \in X \end{pmatrix}.$$  \hfill (18)

Note that (17) and (18) are multiobjective probabilistic constrained programming, see Charnes and Cooper (1963), Stancu-Minasian (1984) and Prékopa (1995).

Many other approaches can be used to solve (10). For example, Stancu-Minasian (1984) proposed a stochastic version of the sequential technique, termed the Lexicographic method, for solving (12) and (15) or direct application to (10); among many other options.
In all cases, observe that
\[ E\left( \hat{Y}(x, \hat{B}) \right) = Y(x, B) \quad \text{and} \quad \text{Cov}\left( \hat{Y}(x, \hat{B}) \right) = z'(x)(X'X)^{-1}z(x)\Sigma, \]
in general are unknown. Then, from a practical point of view, and having the final expression of the equivalent deterministic problem of (10), \( E\left( \hat{Y}(x, \hat{B}) \right) \) and \( \text{Cov}\left( \hat{Y}(x, \hat{B}) \right) \) should be replaced by their corresponding estimators
\[ E\left( \hat{Y}(x, \hat{B}) \right) = \hat{Y}(x, \hat{B}) \quad \text{and} \quad \text{Cov}\left( \hat{Y}(x, \hat{B}) \right) = z'(x)(X'X)^{-1}z(x)\Sigma. \]

5 Equivalent deterministic programs

In this section we study several particular equivalent deterministic programs from (13) in detail.

5.1 Multiobjective V-model

Taking into account the final comment in Section 4, our intention is to solve the matrix optimisation problem
\[ \min_{x \in X} \text{Cov}\left( \hat{Y}(x, \hat{B}) \right). \quad (19) \]

For the sake of convenience, in this section we denote \( \text{Cov}\left( \hat{Y}(x, \hat{B}) \right) \) as \( \text{Cov}\left( \hat{Y}(x) \right) \). Obviously, the difficulty in expressing the problem in this way lies in defining the meaning of the minimum of a matrix function. The idea of minimising a matrix function, and in particular a matrix of variance-covariance, has been studied with respect to various areas of statistical theory. For example, when regression estimators are determined for a multivariate general linear model, this is done by minimising the determinant or the trace of sums of squares and cross-products matrix of the error, see [Giri 1977]. Similarly, the choice or comparison of experimental design models is done by minimising a function of the variance-covariance matrix of treatment estimators, see [Khuri and Cornell 1987] and [Azais and Druilhet 1997].

Fortunately, it is possible to reduce the nonlinear matrix minimisation problem (19) to a univariate nonlinear minimisation problem by taking into account the following considerations. Observe that the procedure described here is just one of various possible options, see [Rios et al. 1989] and [Miettinen 1999].

Assume that \( \text{Cov}\left( \hat{Y}(x) \right) \) is a positive definite matrix for all \( x \), denoting it as \( \text{Cov}\left( \hat{Y}(x) \right) > 0 \). Now, let \( x_1 \) and \( x_2 \) be two possible values of the vector \( x \) and let \( B = \text{Cov}\left( \hat{Y}(x_1) \right) - \text{Cov}\left( \hat{Y}(x_2) \right) \). Then we say that
\[ \text{Cov}\left( \hat{Y}(x_1) \right) < \text{Cov}\left( \hat{Y}(x_2) \right) \iff B < 0, \quad (20) \]
i.e. if the matrix \( B \) is a negative definite matrix. Moreover, note that \( \hat{Y}(x_1) \) and \( \hat{Y}(x_2) \), are diagonalizable. Then, let \( D_{x_1} \) and \( D_{x_2} \) be the diagonal matrixes associated with \( \text{Cov}\left( \hat{Y}(x_1) \right) \) and \( \text{Cov}\left( \hat{Y}(x_2) \right) \), respectively; with \( D_{x_1} = \text{diag}(\alpha_1, \ldots, \alpha_r) \), \( \alpha_1 > \cdots > \alpha_r > 0 \) and \( D_{x_2} = \text{diag}(\gamma_1, \ldots, \gamma_r) \), \( \gamma_1 > \cdots > \gamma_r > 0 \), where \( \alpha_j \) and \( \gamma_j \) denote
the eigenvalues of \( \hat{\text{Cov}} \left( \hat{Y} (x_1) \right) \) and \( \hat{\text{Cov}} \left( \hat{Y} (x_2) \right) \), respectively. Thus, expression (20) can alternatively be presented as:

\[
\hat{\text{Cov}} \left( \hat{Y} (x_1) \right) < \hat{\text{Cov}} \left( \hat{Y} (x_2) \right) \iff D_{x_1} - D_{x_2} < 0,
\]

i.e.

\[
\hat{\text{Cov}} \left( \hat{Y} (x_1) \right) < \hat{\text{Cov}} \left( \hat{Y} (x_2) \right) \iff \alpha_j - \gamma_j < 0, \quad j=1,\ldots,r
\]

and \( \hat{\text{Cov}} \left( \hat{Y} (x_1) \right) \neq \hat{\text{Cov}} \left( \hat{Y} (x_2) \right) \); which defines a weak Pareto order, see Steuer (1986), Rios et al. (1989) and Miettinen (1999). Then from Steuer (1986), Rios et al. (1989) and Miettinen (1999), there exists a function \( g : \mathcal{S} \rightarrow \mathbb{R} \), such that

\[
\hat{\text{Cov}} \left( \hat{Y} (x_1) \right) < \hat{\text{Cov}} \left( \hat{Y} (x_2) \right) \iff g \left( \hat{\text{Cov}} \left( \hat{Y} (x_1) \right) \right) < g \left( \hat{\text{Cov}} \left( \hat{Y} (x_2) \right) \right),
\]

where \( \hat{\text{Cov}} \left( \hat{Y} (x) \right) \in \mathcal{S} \subset \mathbb{R}^{r(r+1)/2} \) and \( \mathcal{S} \) is the set of positive definite matrices. From Steuer (1986), Rios et al. (1989) and Miettinen (1999) prove that the non-linear matrix minimisation problem (19) is reduced in the following scalar non-linear minimisation problem

\[
\min_{x \in \mathcal{X}} g \left( \hat{\text{Cov}} \left( \hat{Y} (x, \hat{B}) \right) \right).
\]

Unfortunately or otherwise, the function \( g(\cdot) \) is not unique. For example, in other statistical contexts we can find the following commonly used functions \( g(\cdot) \), see Giri (1977):

1. The trace of the matrix \( \hat{\text{Cov}} \left( \hat{Y} (x) \right) \):

\[
g \left( \hat{\text{Cov}} \left( \hat{Y} (x) \right) \right) = \operatorname{tr} \left( \hat{\text{Cov}} \left( \hat{Y} (x) \right) \right)
\]

\[
= z'(x)(X'X)^{-1}z(x) \sum_j \hat{\sigma}_{jj}.
\]

2. The determinant of the matrix \( \hat{\text{Cov}} \left( \hat{Y} (x) \right) \):

\[
g \left( \hat{\text{Cov}} \left( \hat{Y} (x) \right) \right) = \left| \hat{\text{Cov}} \left( \hat{Y} (x) \right) \right|
\]

\[
= \left| z'(x)(X'X)^{-1}z(x) \right|^r \left| \hat{\Sigma} \right|
\]

3. The sum of all the elements of the matrix \( \hat{\text{Cov}} \left( \hat{Y} (x) \right) \):

\[
g \left( \hat{\text{Cov}} \left( \hat{Y} (x) \right) \right) = z'(x)(X'X)^{-1}z(x) \sum_{j,k=1}^r \hat{\sigma}_{jk}.
\]

4. \( g \left( \hat{\text{Cov}} \left( \hat{Y} (x) \right) \right) = \lambda_{\text{max}} \left( \hat{\text{Cov}} \left( \hat{Y} (x) \right) \right) \), where \( \lambda_{\text{max}} \) is the maximum eigenvalue of the matrix \( \hat{\text{Cov}} \left( \hat{Y} (x) \right) \).

5. \( g \left( \hat{\text{Cov}} \left( \hat{Y} (x) \right) \right) = \lambda_{\text{min}} \left( \hat{\text{Cov}} \left( \hat{Y} (x) \right) \right) \), where \( \lambda_{\text{min}} \) is the minimum eigenvalue of the matrix \( \hat{\text{Cov}} \left( \hat{Y} (x) \right) \).
6. \( g \left( \hat{\text{Cov}} \left( \hat{\mathbf{Y}}(\mathbf{x}) \right) \right) = \lambda_j \left( \hat{\text{Cov}} \left( \hat{\mathbf{Y}}(\mathbf{x}) \right) \right) \), where \( \lambda_j \) is the \( j \)-th eigenvalue of the matrix \( \hat{\text{Cov}} \left( \hat{\mathbf{Y}}(\mathbf{x}) \right) \), among others.

But observe that

\[
\lambda_j \left( \hat{\text{Cov}} \left( \hat{\mathbf{Y}}(\mathbf{x}) \right) \right) = \lambda_j \left( \mathbf{z}'(\mathbf{x}) \mathbf{X}' \mathbf{X}^{-1} \mathbf{z}(\mathbf{x}) \hat{\Sigma} \right)
= \mathbf{z}'(\mathbf{x}) \mathbf{X}' \mathbf{X}^{-1} \mathbf{z}(\mathbf{x}) \lambda_j \left( \hat{\Sigma} \right).
\]

Hence we can conclude that as a consequence of the structure of the covariance matrix \( \hat{\text{Cov}} \left( \hat{\mathbf{Y}}(\mathbf{x}) \right) \), for all the particular definitions of the function \( g \) considered above, the scalar non-linear minimisation problem (23) has a unique solution given by the solution of the non-linear minimisation problem

\[
\min_{\mathbf{x} \in \mathbf{X}} \mathbf{z}'(\mathbf{x}) \mathbf{X}' \mathbf{X}^{-1} \mathbf{z}(\mathbf{x}). \tag{24}
\]

5.2 Multiobjective P-model

Proceeding as in Díaz-García et al. (2002), the equivalent multiobjective deterministic problem to (10) via the P-model (15) is

\[
\min_{\mathbf{x} \in \mathbf{X}} \begin{pmatrix}
\tau_1 - \mathbf{z}'(\mathbf{x}) \hat{\beta}_1 \\
\sqrt{\sigma_{11}} \mathbf{z}'(\mathbf{x}) \mathbf{X}' \mathbf{X}^{-1} \mathbf{z}(\mathbf{x}) \\
\tau_2 - \mathbf{z}'(\mathbf{x}) \hat{\beta}_2 \\
\sqrt{\sigma_{22}} \mathbf{z}'(\mathbf{x}) \mathbf{X}' \mathbf{X}^{-1} \mathbf{z}(\mathbf{x}) \\
\vdots \\
\tau_r - \mathbf{z}'(\mathbf{x}) \hat{\beta}_r \\
\sqrt{\sigma_{rr}} \mathbf{z}'(\mathbf{x}) \mathbf{X}' \mathbf{X}^{-1} \mathbf{z}(\mathbf{x})
\end{pmatrix}. \tag{25}
\]

5.3 Multiobjective Kataoka model

From Díaz-García et al. (2005), the equivalent multiobjective deterministic problem to (10) via the Kataoka model (17) is given by

\[
\min_{\mathbf{x} \in \mathbf{X}} \begin{pmatrix}
\mathbf{z}'(\mathbf{x}) \hat{\beta}_1 + \Phi^{-1}(\delta) \sqrt{\sigma_{11}} \mathbf{z}'(\mathbf{x}) \mathbf{X}' \mathbf{X}^{-1} \mathbf{z}(\mathbf{x}) \\
\mathbf{z}'(\mathbf{x}) \hat{\beta}_2 + \Phi^{-1}(\delta) \sqrt{\sigma_{22}} \mathbf{z}'(\mathbf{x}) \mathbf{X}' \mathbf{X}^{-1} \mathbf{z}(\mathbf{x}) \\
\vdots \\
\mathbf{z}'(\mathbf{x}) \hat{\beta}_r + \Phi^{-1}(\delta) \sqrt{\sigma_{rr}} \mathbf{z}'(\mathbf{x}) \mathbf{X}' \mathbf{X}^{-1} \mathbf{z}(\mathbf{x})
\end{pmatrix}. \tag{26}
\]

where \( \Phi \) denotes the distribution function of the standard Normal distribution.

Similar equivalent multiobjective deterministic problems to (10) are obtained by applying the other stochastic solutions described in Section 4. Note that, if each stochastic solution is combined with each multiobjective optimisation technique, an infinite number of possible solutions to (10) is obtained. For example, note that the function of value \( f(\cdot) \) may take an infinite number of forms. One of these particular forms is the weighting method. Under this approach, problem (26) can be restated as:

\[
\min_{\mathbf{x} \in \mathbf{X}} \sum_{k=1}^{r} w_k \left\{ \mathbf{z}'(\mathbf{x}) \hat{\beta}_k + \Phi^{-1}(\delta) \sqrt{\sigma_{kk}} \mathbf{z}'(\mathbf{x}) \mathbf{X}' \mathbf{X}^{-1} \mathbf{z}(\mathbf{x}) \right\}. \tag{27}
\]
such that \( \sum_{k=1}^{r} w_k = 1, w_k \geq 0 \ \forall \ k = 1, 2, \ldots, r \): where \( w_k \) weights the importance of each characteristic. The solution \( x \in \mathcal{X} \) of (27) can be termed the multiobjective Kataoka solution with probability \( \alpha \) to problem (10), via the weighting method.

Similarly, \( x \in \mathcal{X} \) is the multiobjective Kataoka solution with probability \( \alpha \) to the problem (10), via goal programming if \( x \in \mathcal{X} \) is

\[
\min_{x \in \mathcal{X}} \sum_{k=1}^{p} w_k (d_k^+ + d_k^-)
\]

subject to

\[
z'(x) \beta_k + \Phi^{-1}(\delta) \sqrt{\sigma_{kk}} z'(x)(X'X)^{-1}z(x) - d_k^+ + d_k^- = \tau_k, \ k = 1, 2, \ldots, r,
\]

where

\[
d_k^+ = \frac{1}{2} \left( \left| z'(x) \beta_k + \Phi^{-1}(\delta) \sqrt{\sigma_{kk}} z'(x)(X'X)^{-1}z(x) - \tau_k \right| + \left( z'(x) \beta_k + \Phi^{-1}(\delta) \sqrt{\sigma_{kk}} z'(x)(X'X)^{-1}z(x) - \tau_k \right) \right),
\]

\[
d_k^- = \frac{1}{2} \left( \left| z'(x) \beta_k + \Phi^{-1}(\delta) \sqrt{\sigma_{kk}} z'(x)(X'X)^{-1}z(x) - \tau_k \right| - \left( z'(x) \beta_k + \Phi^{-1}(\delta) \sqrt{\sigma_{kk}} z'(x)(X'X)^{-1}z(x) - \tau_k \right) \right).
\]

6 Application

A real case from the literature is analysed by applying several approaches and particular solutions from multiobjective stochastic optimisation.

In the following example, taken from Pignatiello (1993), there are two response variables \( Y = (Y_1, Y_2)' \) with 4 replicates and three setting variables \( x = (x_1, x_2, x_3)' \). The experimental data are shown in Table 1. It is assumed that the targets of the responses are \( \tau = (\tau_1, \tau_2)' = (103, 73)' \).

| Replicate | 1 | 2 | 3 | 4 | 1 | 2 | 3 | 4 |
|-----------|---|---|---|---|---|---|---|---|
| D | x_1 | x_2 | x_3 | Y_1 | | | | Y_2 |
| 8 | 1 | 1 | 1 | 104.45 | 103.63 | 99.79 | 104.92 | 76.90 | 77.03 | 67.99 | 75.77 |
| 4 | 1 | 1 | -1 | 104.12 | 104.80 | 104.20 | 104.34 | 72.99 | 74.25 | 73.94 | 73.28 |
| 6 | 1 | -1 | 1 | 98.73 | 99.36 | 102.84 | 94.24 | 67.10 | 63.61 | 68.65 | 62.42 |
| 2 | 1 | -1 | -1 | 100.19 | 99.63 | 100.27 | 100.60 | 67.03 | 66.18 | 66.58 | 67.94 |
| 7 | -1 | 1 | 1 | 103.15 | 106.96 | 107.62 | 103.44 | 71.68 | 76.27 | 77.50 | 76.37 |
| 3 | -1 | 1 | -1 | 106.08 | 105.64 | 105.67 | 105.39 | 72.94 | 72.85 | 72.58 | 72.38 |
| 5 | -1 | -1 | 1 | 113.52 | 111.12 | 112.85 | 106.67 | 68.29 | 68.47 | 68.96 | 64.71 |
| 1 | -1 | -1 | -1 | 109.90 | 109.76 | 110.70 | 109.77 | 67.70 | 67.24 | 67.96 | 66.93 |

Equations (29) and (30) are response surfaces for \( Y_1 \) and \( Y_2 \).

\[
\hat{Y}_1(x) = 104.86 - 3.147x_1 - 0.142x_2 - 0.199x_3 + 2.379x_1x_2 - 0.35x_1x_3 - 0.106x_2x_3
\]

\[
\hat{Y}_2(x) = 70.45 - 0.348x_1 + 3.59x_2 + 0.28x_3 + 0.323x_1x_2 - 0.45x_1x_3 + 0.614x_2x_3
\]

(29)

(30)

From which the multiresponse optimisation problem is given as

\[
\min_{x \in \mathcal{X}} \hat{Y}(x) = \min_{x \in \mathcal{X}} \left( \begin{array}{c} \hat{Y}_1(x) \\ \hat{Y}_2(x) \end{array} \right)
\]

(31)
where $\mathcal{X} = \{ x | x_i \in [-1, 1], i = 1, 2, 3 \}$.

Now, assume that the importance of each response variable must be assessed from the decision makers’ viewpoint. For the purposes of this example, consider $w = (w_1, w_2)' = (0.285, 0.715)'$.

From [20] and [30]

$$
\hat{B} = \begin{bmatrix}
\hat{\beta}_0 \\
\hat{\beta}_1 \\
\hat{\beta}_2 \\
\hat{\beta}_3 \\
\hat{\beta}_{12} \\
\hat{\beta}_{13} \\
\hat{\beta}_{23}
\end{bmatrix} = \begin{bmatrix}
104.86 \\
-3.147 \\
-0.142 \\
-0.199 \\
2.379 \\
-0.35 \\
-0.106
\end{bmatrix}'
$$

Also,

$$
\hat{\Sigma} = \begin{bmatrix}
4.190 & 3.546 \\
3.546 & 4.666
\end{bmatrix}
$$

From

$$
\widehat{\text{Cov}}(\text{vec} \, \hat{B}) = \hat{\Sigma} \otimes (X'X)^{-1}
$$

$$
= \begin{bmatrix}
4.190 & 3.546 \\
3.546 & 4.666
\end{bmatrix} \otimes 0.03125 I_7.
$$

In particular, $\widehat{\text{Cov}}(\hat{\beta}_1) = 0.131 I_7$ and $\widehat{\text{Cov}}(\hat{\beta}_2) = 0.145 I_7$. Therefore, the estimator of the covariance matrix of response surfaces according to equation (6) is

$$
\widehat{\text{Cov}}(Y(x)) = (1 + x_1^2 + x_2^2 + x_3^2 + x_1^2x_2^2 + x_1^2x_3^2 + x_2^2x_3^2) \begin{bmatrix}
0.131 & 0.111 \\
0.111 & 0.145
\end{bmatrix}.
$$

Next, we propose diverse multiobjective stochastic solutions and their deterministic equivalent corresponding programs:

- **Equivalent multiobjective V-model**

$$
\min_{x \in \mathcal{X}} \begin{bmatrix}
\text{Var} \left( \hat{Y}_1(x, \hat{\beta}_1) \right) \\
\text{Cov} \left( \hat{Y}_1(x, \hat{\beta}_1), \hat{Y}_2(x, \hat{\beta}_2) \right) \\
\text{Var} \left( \hat{Y}_2(x, \hat{\beta}_2) \right)
\end{bmatrix},
$$

And its corresponding deterministic equivalent program is

$$
\min_{x \in \mathcal{X}} z'(x)(X'X)^{-1} z(x).
$$

- **Equivalent deterministic multiobjective modified E-model**

$$
\min_{x \in \mathcal{X}} \begin{bmatrix}
\hat{Y}(x, \hat{\beta})
\end{bmatrix},
$$

where

$$
\hat{Y}(x, \hat{\beta}) = \begin{bmatrix}
\hat{Y}_1(x, \hat{\beta}_1) \\
\hat{Y}_2(x, \hat{\beta}_2)
\end{bmatrix},
$$

and $\left( \text{Cov} \left( \hat{Y}(x, \hat{\beta}) \right) \right)^{1/2}$ is

$$
\left( \begin{bmatrix}
\text{Var} \left( \hat{Y}_1(x, \hat{\beta}_1) \right) \\
\text{Cov} \left( \hat{Y}_1(x, \hat{\beta}_1), \hat{Y}_2(x, \hat{\beta}_2) \right) \\
\text{Var} \left( \hat{Y}_2(x, \hat{\beta}_2) \right)
\end{bmatrix} \right)^{1/2},
$$

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In this case the deterministic equivalent program can be stated as (among many other options, including lexicographic or \( \epsilon \)-constraint models)

\[
\min_{x \in X} r_1 f \left( \hat{Y} \left( x, \hat{\beta} \right) \right) + r_2 \ g \left( \left( \text{Cov} \left( \hat{Y} \left( x, \hat{\beta} \right) \right) \right)^{1/2} \right),
\]

where \( r_j \geq 0, j = 1, 2 \) are constants such that \( r_1 + r_2 = 1 \) (in general), whose values indicate the relative importance of the expectation and matrix covariance of \( \hat{Y} \left( x, \hat{\beta} \right) \), and \( f \) and \( g \) are value functions.

In particular, using (24), a deterministic equivalent program via the weighting method is

\[
\min_{x \in X} \left( w_1 \ z'(x)\hat{\beta}_1 + w_2 \ z'(x)\hat{\beta}_2 \right) + r_2 \ z'(x)(X'X)^{-1}z(x),
\]

and assuming that the primary objective function is \( g \), via the \( \epsilon \)-constraint model we have

\[
\min_{x \in X} z'(x)(X'X)^{-1}z(x)
\]

subject to

\[
\begin{align*}
\tau_1 - z'(x)\hat{\beta}_1 = \tau_1 \\
\tau_2 - z'(x)\hat{\beta}_2 = \tau_2.
\end{align*}
\]

- **Equivalent deterministic multiobjective \( P \)-model**

\[
\min_{x \in X} \left( \frac{\tau_1 - z'(x)\hat{\beta}_1}{\sqrt{\sigma_{11} z'(x)(X'X)^{-1}z(x)}} \right) + \left( \frac{\tau_2 - z'(x)\hat{\beta}_2}{\sqrt{\sigma_{22} z'(x)(X'X)^{-1}z(x)}} \right).
\]

In this case the deterministic equivalent program via the weighting method is

\[
\min_{x \in X} \left\{ \frac{\tau_1 - z'(x)\hat{\beta}_1}{\sqrt{\sigma_{11} z'(x)(X'X)^{-1}z(x)}} \right\} + \left\{ \frac{\tau_2 - z'(x)\hat{\beta}_2}{\sqrt{\sigma_{22} z'(x)(X'X)^{-1}z(x)}} \right\}.
\]

And assuming that \( \hat{Y}_2 \left( x, \hat{\beta} \right) \) is the primary objective function, the deterministic equivalent program via the \( \epsilon \)-constraint method is

\[
\min_{x \in X} \frac{\tau_2 - z'(x)\hat{\beta}_2}{\sqrt{\sigma_{22} z'(x)(X'X)^{-1}z(x)}} \quad \text{subject to} \quad \frac{\tau_1 - z'(x)\hat{\beta}_1}{\sqrt{\sigma_{11} z'(x)(X'X)^{-1}z(x)}} = \tau_1.
\]

- **Equivalent deterministic multiobjective Kataoka model**

\[
\min_{x \in X} \left( z'(x)\hat{\beta}_1 + \Phi^{-1}(\delta) \frac{\sqrt{\sigma_{11} z'(x)(X'X)^{-1}z(x)}}{\sqrt{\sigma_{22} z'(x)(X'X)^{-1}z(x)}} \right) + \left( z'(x)\hat{\beta}_2 + \Phi^{-1}(\delta) \frac{\sqrt{\sigma_{11} z'(x)(X'X)^{-1}z(x)}}{\sqrt{\sigma_{22} z'(x)(X'X)^{-1}z(x)}} \right).
\]

The deterministic equivalent program via the weighting method is

\[
\min_{x \in X} \left\{ z'(x)\hat{\beta}_1 + \Phi^{-1}(\delta) \frac{\sqrt{\sigma_{11} z'(x)(X'X)^{-1}z(x)}}{\sqrt{\sigma_{22} z'(x)(X'X)^{-1}z(x)}} \right\} + \left\{ z'(x)\hat{\beta}_2 + \Phi^{-1}(\delta) \frac{\sqrt{\sigma_{11} z'(x)(X'X)^{-1}z(x)}}{\sqrt{\sigma_{22} z'(x)(X'X)^{-1}z(x)}} \right\}.
\]
Now assuming that $\hat{Y}_2(x, \hat{\beta}_2)$ is the primary objective function, the deterministic equivalent program via the $\epsilon$-constraint method is

$$\min_{x \in X} z'(x)\hat{\beta}_2 + \Phi^{-1}(\delta) \sqrt{\sigma_{22}} z'(x)(X'X)^{-1}z(x)$$

subject to

$$z'(x)\hat{\beta}_1 + \Phi^{-1}(\delta) \sqrt{\sigma_{11}} z'(x)(X'X)^{-1}z(x) = \tau_1.$$
Table 2: Comparison of the results of the proposed model and those derived by other methods.

| Stochastic programming method | $x_1$ | $x_2$ | $x_3$ | $F(x)$ | $\hat{Y}_1(x)$ | $\hat{Y}_2(x)$ | $\text{Var}(\hat{Y}_1(x))$ | $\text{Var}(\hat{Y}_2(x))$ | $\text{Cov}(\hat{Y}_1(x), \hat{Y}_2(x))$ |
|-------------------------------|-------|-------|-------|--------|----------------|----------------|---------------------------|---------------------------|-----------------------------|
| Chiao and Hamada (2001)       | -1.00 | -1.00 | -1.00 | -104.612 | 73.574         | 0.917          | 1.041                     | 0.788                     |
| Hejazi et al. (2010)$^c$      | 0.953 | 0.709 | 0.407 | -103.247 | 73.000         | 0.428          | 0.476                     | 0.362                     |
| Robust E-model                | 1.000 | 0.707 | 0.483 | -103.332 | 73.000         | 0.470          | 0.523                     | 0.397                     |
| Lexicographic (First $E(F(x))$) | 1.000 | 0.707 | 0.483 | -103.000 | 73.000         | 0.470          | 0.523                     | 0.397                     |
| Lexicographic (First $\text{Var}(F(x))$) | 0.000 | 0.000 | 0.000 | -104.865 | 70.453         | 0.131          | 0.146                     | 0.111                     |
| Modified V-model              | 0.000 | 0.000 | 0.000 | -104.865 | 70.453         | 0.131          | 0.146                     | 0.111                     |
| Multiobjective                | 0.522 | -1.000 | 0.108 | 39.588   | 102.100        | 66.449         | 0.336                     | 0.375                     | 0.285                      |
| Stochastic approaches         | 1.000 | 0.707 | 0.452 | 3.511    | 100.672        | 67.577         | 0.343                     | 0.382                     | 0.290                      |
| V-model                       | -0.349 | 1.000 | 0.548 | -2.672   | 104.893        | 74.630         | 0.377                     | 0.420                     | 0.320                      |
| Modified V-model              | 0.910 | -0.658 | 0.000 | 8.799    | 100.780        | 67.296         | 0.343                     | 0.382                     | 0.290                      |
| P-model                       | 1.000 | -1.000 | 1.000 | 74.989   | 99.039         | 65.405         | 0.917                     | 1.021                     | 0.776                      |
| Kataoka ($\epsilon$-constraint) | 0.541 | -1.000 | 0.851 | 67.296   | 101.780        | 66.096         | 0.556                     | 0.619                     | 0.470                      |
| Goal Programming              | 0.844 | 0.605 | 1.000 | 102.78  | 72.78   | 0.6764         | 0.6441                     | 0.4895                    |

$^a$Objective function
$^b$Squared euclidean distance
$^c$Where weights $w$ are considered deterministic
$^d|x_1| = |x_2| = 0.5$
$^e\delta = 0.95$
Note that while all of these optimisation techniques essentially provide the solution to the same practical problem, i.e. that of obtaining the critical value of the variables $x$, from a mathematical point of view and more precisely from the standpoint of mathematical programming, problem (9) as solved by Chiao and Hamada (2001) and Hejazi et al. (2010) and problem (10) examined in the present paper are not the same. Therefore, unless a reasonable basis for comparison is proposed, Table 2 should be taken simply as an example of different approaches and different solutions to the practical problem. From the latter, experts, researchers or decision makers can select the most suitable method for solving their own problem in terms of the particular context.

Conclusions

It should be emphasised that even a comparison between the diverse techniques proposed in this paper should be made with appropriate reservations, since the solutions discussed refer to different decision-making criteria. For example, Table 2 shows that the methods designed to minimise the variance actually obtain a lower variance than the other solutions, but perhaps the optimum response variables are a little further from the target. Likewise, the minimum risk models provide more conservative solutions.

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