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UNCERTAINTY PROPAGATION
IN MULTIRESPONSE OPTIMIZATION
USING A DESIRABILITY INDEX

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Uncertainty Propagation in Multiresponse Optimization using a Desirability Index

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Abstract

Optimizing the quality of a product is widespread in the industry. Products have to be manufactured such that they best fit some quality properties. Varying the product settings leads to different product qualities and the aim of the manufacturer is to find the factors settings that simultaneously optimize the quality properties.

The classical approach to solve such optimization problem is based on response surface methodology. First, a designed experiment is used to collect data and to adjust models capturing the relationship between the responses of interest and the factors settings. Those fitted models can then predict the quality properties for any design point of the experimental domain. Secondly, a desirability index is built to combine the predicted properties into a value belonging to the $[0, 1]$ interval. This index provides a ranking of possible factors settings in the solutions space and the optimum can be found by an adequate optimization algorithm. But, as model predictions are suiled with error, so is the desirability index and the optimal solution found. In practice, in the related literature and design of experiment software, this error is neglected.

This paper proposes an optimization methodology based on the fact that a desirability index is a random variable. The expectation of this index is taken as the criteria to be optimized and, since it can only be estimated, confidence and predicted intervals are constructed to take into account the propagation of the models error on the expected or predicted desirability index. The stochastic character of the index leads also to an uncertainty on the optimum and a methodology is proposed to build an equivalence zone containing no significantly different optimal solutions. This methodology is illustrated on a simulated example and compared to the classical optimization methodology.

Keywords: Multiresponse optimization, desirability, experimental design, error propagation, confidence interval, equivalence zone.

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1 Introduction

1.1 Classical approach to multiresponse optimization

Improving the quality of a product is a challenge that industries face daily. A food industry may want to improve the quality of its cakes, a rubber industry the quality of a tire tread compound, a pharmaceutical industry the quality of drug candidates, *etc.*

If a set of factors, $\mathbf{x} = (x_1, x_2, \ldots, x_k)$, can be chosen during manufacturing leading to different product qualities, $\mathbf{Y} = (Y_1, Y_2, \ldots, Y_p)$, modifying the x_j's makes the Y_i's varying. Producers want to find the factors settings that simultaneously optimize the p quality responses.

The classical approach to this optimization problem assumes that statistical models are available to predict the responses, Y_i's, from the factors, x_j's. To avoid to much expensive and time consuming trials, data are usually collected following an experimental design and models fitted to the data by multiple polynomial regression (Box and Draper, 1986; Khuri and Cornell, 1987; Myers *et al.*, 1989; Myers and Montgomery, 2002). For each Y_i, an adequate optimization algorithm can then be used to find the optimal factors settings in the experimental domain, denoted χ.

As the optimal x_j's for the Y_i's are usually different, the Y_i's responses may be competitive and it is often impossible to improve one response without deterioring another. The best compromise has to be found taking into account the relative importance of each response. A possible approach to transform the multiresponse optimization into a single objective optimization is to use *distance* or *loss* function measuring the departure from the individual responses optima. This methodology is not treated in this paper. For a review of this subject, see Khuri and Conlon (1981) or Ko *et al.* (2005).

In the context of industrial statistics and experimental design, the balance between the different responses is usually measured by a *desirability index*, a concept introduced by Harrington (1965). Harrington suggests to associate a value belonging to $[0, 1]$, $D(\mathbf{x})$, to each combination of factors levels, $\mathbf{x}$, representing the desirability of the resulting product quality. The desirability index has to be maximized. It allows to transform the multiresponse optimization into a unique objective optimization. $D(\mathbf{x})$ is usually defined as a combination of *desirability functions*, $d_i(Y_i), i = 1, 2, \ldots, p$, representing the confinity of each individual response to its specifications. Different types of desirability functions are proposed in the literature, the most well known are coming from Derringer and Suich (1980). Nowadays, such optimization methodology is commonly used by practitionners and implemented in most experimental design softwares (JMP, MODDE, Design-Expert,...).

In spite of this success, this methodology has a main drawback : it neglects the models prediction errors. For nearly all kinds of models, it is possible to quantify the uncertainty when using fitted models to estimate the expected responses for a new experimental domain point. The uncertainty of estimated expected responses propagates on the desirability index but this information is not taken into account in the classical optimization approach. Desirability indexes of two solutions are compared as if they were exact although they are random variables. This paper proposes a methodology that takes into account the uncertainty of the desirability index in multicritera optimization.

1.2 Stochastic approach to multiresponse optimization

As predictions provided by response models are affected by prediction error due to experimental error and model uncertainty, a desirability index built from these predictions becomes a random variable with a statistical distribution depending on the distribution of the predicted responses $\hat{Y}_1, \hat{Y}_2, ..., \hat{Y}_p$ in $\mathbf{x}$, a point of interest in the factors domain χ.

Steuer (2000) is the first author to discuss this problem in the context of desirability optimization. He points out that the random error term is neglected and suggests to take it into account by maximizing the expected desirability index over the factors domain instead of the desirability index of the estimated expected response as in the classical approach. The derived optimum $\mathbf{x}_{opt}$ represents the factors settings which give, in average, the highest desirability index.

Other problems follow from the stochastic character of the desirability index. First, due to response model uncertainty, the expected desirability index can only be estimated. A formula for this estimator must then be derived and one may also be interested to calculate a confidence interval to quantify the incertitude of this estimator. Second, the incertitude on the estimated expected desirability index leads to an incertitude on the estimated optimal factors settings, $\hat{\mathbf{x}}_{opt}$, and an equivalence zone may also be derived to delimit the subset of the factors domain which contains no significantly different optimal solutions. Third, real experiments are always affected by experimental error. An experiment performed at the optimal factors settings will never give the expected response and desirability index even if the models fit "perfectly" the average responses. For a solution $\mathbf{x}$ in the factors domain, the calculation of a prediction interval for the (observed) desirability index is then also a question of interest.

This problem is partially discussed in the literature. When a single response is concerned, Box and Hunter (1954) proposed an exact method to derive a confidence region for the stationary point of an estimated second order polynomial model. Stablein *et al.* (1983) generalized it to the constraint experimental region using Lagrange multipliers. Böckenholt (1989) summarized the results of the former authors and proposed a method to test if the optima of different response surfaces are statistically different. Still for the single response problem, del Castillo and Cahya (2001) and Peterson *et al.* (2002) proposed an improvement of the Stablein *et al.* method which can be used for general linear regression models and is more easy to apply provided that an adapted computer program is available.

For the multiple response case, Steuer (2000) pointed out the interest to work on the expected desirability index. Weber and Weihs (2003) derived analytically the statistical distribution of the desirability index for Harringon desirability functions. Cahya (2002) proposed a way to derive a confidence zone for optimal factors settings based on the Delta theorem and Trautmann and Weihs (2004) proposed a way to derive an equivalence zone for the optima based on a prediction interval for the desirability index.

1.3 Goal and overview of the paper

This paper proposes a general framework to take into account model and desirability index uncertainty in multicriteria optimization. Under general assumptions over the form of response models and desirability functions and for the geometric mean desirability index, it proposes formulas to estimate the expected desirability index, calculate related confidence

and prediction intervals and derive an equivalence zone for the optimum. Most results are based on variations of the Delta method theorem that shows, through simulations, to perform very well in this context.

In the next section, some notations are introduced for the assumed models linking responses to factors. In section 3, the literature on desirability indexes is reviewed and the classical optimization problem is formally expressed in terms of maximizing the desirability index of the expected responses.

Then the new optimization approach based on the expected desirability index is formalized in section 4. The computation procedures of Steuer (2000) and Trautmann and Weihs (2004) are reviewed and the need of taking prediction error into account emphasized.

In section 5, a new technique to estimate the expected desirability index based on the Delta method (von Mises, 1947) is proposed. The Delta method is first used to approximate the expected desirability index and estimate it. Then the Delta method theorem is used to quantify the uncertainty of this estimation by constructing confidence intervals. This constitutes section 6.

Once the factors settings that maximize the expected desirability index have been found by an adequate algorithm, the Delta method theorem can also be used to determine the set of equivalent solutions, *i.e.* factors settings that do not have significantly different expected desirability index. Details can be found in section 7.

Section 8 explains then how to construct a prediction interval for the desirability index when applying desirability index directly on predicted responses. This problem is related to the classical optimization approach and emphasises the danger of neglecting prediction error.

Finally, in section 9, the methodology is applied on a simulated optimization example to show its preformance.

2　Model and notations

Each response defining the quality of the product, Y_i $(i = 1, 2, \ldots, p)$, is assumed to be related to the same set of varying factors, x_j's $(j = 1, 2, \ldots, k)$. The objective is to find the factors settings $\mathbf{x} = (x_1, x_2, \ldots, x_k)$ in the factors domain of interest χ that simultaneously optimize the p responses $\mathbf{Y} = (Y_1, Y_2, \ldots, Y_p)$.

Multiresponse optimization is a common problem in industries. As they can not face testing all possible combinations of factors levels and measure the quality of resulting products, a model capturing the relationship between each response and factors is assumed over the domain of interest through an equation of the form

$$Y_i = f_i\left(\mathbf{x}, \boldsymbol{\beta_i}\right) + \epsilon_i \tag{1}$$

where the true link function f_i is unknown as well as the model parameters $(k \times 1)$ vector $\boldsymbol{\beta_i}$. The experimental errors ϵ_i are assumed to be of zero mean with variance $\sigma_{\epsilon_i}{}^2$ leading to the equalities $E[Y_i|\mathbf{x}] = f_i\left(\mathbf{x}, \boldsymbol{\beta_i}\right)$ and $V(Y_i|\mathbf{x}) = \sigma_{\epsilon_i}^2$. Moreover, for two different responses Y_i and Y_j, the corresponding conditional errors ϵ_i and ϵ_j are supposed to be independent.

Using experimental design tools, a set of independent experiments within χ can be adequately chosen and performed to collect data on which the assumed models can be fitted.

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For each property, the estimated model is denoted by

$$\hat{Y}_i = \hat{f}_i\left(\mathbf{x}, \hat{\boldsymbol{\beta}_i}\right). \tag{2}$$

Thanks to equation (2), the expected responses can be estimated for any point $\mathbf{x}$ in the experimental domain χ. In this paper, we suppose that $\hat{Y}_i = \hat{E}(Y_i|\mathbf{x})$ is an unbiased estimator of $E(Y_i|\mathbf{x})$ and that a formula is available to estimate the uncertainty of this estimate and of the prediction : $\hat{V}(\hat{E}(Y_i|\mathbf{x}))$ and $\hat{V}(\hat{Y}_i|\mathbf{x})$. We suppose also that those variances estimators are unbiased.

In this framework, the most well-known class of models is the multiple linear regression model usually used in experimental design. The link between the ith response Y_i and the factors $\mathbf{x}$ is assumed to follow an equation of the form

$$Y_i = \mathbf{z'_i}\boldsymbol{\beta_i} + \epsilon_i \tag{3}$$

where $\mathbf{z_i}$ is a $(q_i \times 1)$ vector of linear, polynomial or nonlinear transformations of the factors settings $\mathbf{x}$ (q_i is the number of model parameters).

On the basis of n_i independent experiments, each model can be fitted to data by least squares, leading to the prediction formula :

$$\hat{Y}_i = \mathbf{z'_i}\hat{\boldsymbol{\beta}_i} = \mathbf{z'_i}(\mathbf{Z'_i Z_i})^{-1}\mathbf{Z'_i y_i} = \hat{E}(Y_i|\mathbf{x}) \quad i = 1, 2, \ldots, p. \tag{4}$$

where $\mathbf{Z_i}$ is the $(n_i \times q_i)$ model matrix for response i and $\mathbf{y_i}$ the corresponding $(n_i \times 1)$ vector of observed responses y_{ij}, $(j = 1, 2, \cdots, n_i)$. When using this fitted model for prediction in a new point $\mathbf{x}$, the uncertainty of the estimated expected response $\hat{E}[Y_i|\mathbf{x}]$ and the uncertainty of the predicted response $\hat{Y}_i|\mathbf{x}$ can respectively be quantified by

$$\hat{V}\left[\hat{E}[Y_i|\mathbf{x}]\right] = \hat{\sigma}_{\epsilon_i}{}^2 \mathbf{z'_i}(\mathbf{Z'_i Z_i})^{-1}\mathbf{z_i} \tag{5}$$

and

$$\hat{V}\left[\hat{Y}_i|\mathbf{x}\right] = \hat{\sigma}_{\epsilon_i}{}^2 \cdot \left(1 + \mathbf{z'_i}(\mathbf{Z'_i Z_i})^{-1}\mathbf{z_i}\right) \tag{6}$$

where $\hat{\sigma}_{\epsilon_i}^2 = \frac{1}{n_i - q_i}\sum_{j=1}^{n_i}\left(y_{ij} - \hat{y}_{ij}\right)^2$ is the residual variance estimator.

3 Desirability functions and desirability indexes

The concept of *desirability* was introduced by Harrington (1965) to provide a solution to multiresponse optimization problems. It allows to balance the optimized properties Y_i's one against the other, taking into account their target value, their relative importance and their scale.

Harrington proceeds in two steps. First, each response Y_i is transformed to the same scale using a *desirability function*, denoted by d_i, such that $d_i(Y_i) \in [0, 1]$. If $d_i(Y_i) = 0$, the product is not at all acceptable according to the specifications of the ith property and if $d_i(Y_i) = 1$, the product fullfields them perfectly. The most well-known desirability functions are the one of Harrington (1965) based on the exponential function of a linear transformation of the Y_i's and the one of Derringer and Suich (1980) based on a power of a

linear transformation of the Y_i's. Gibb *et al.* (2001) and Govaerts and Le Bailly de Tilleghem (2005) propose smoother and differentiable desirability functions based on the logit function, normal density and normal distribution functions. These four types of desirability functions are presented in Figure 1 and Table 1 for the cases where the response must be maximized, minimized or reach a target value.
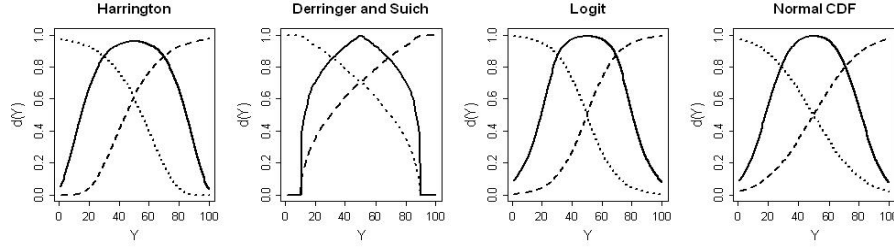

Figure 1: Different desirability functions. The continuous lines represent cases of targeted property and the dotted and dashed lines represent cases of minimized and maximized property respectively.

	Maximum	Minimum	Target Value
Harrington (1965)	$exp(-exp(-a-bY))$	$1-exp(-exp(-a-bY))$	$exp(-\|\frac{Y-T}{b}\|^n)$
Derringer and Suich (1980)	$\begin{array}{ll} 0 & \text{if } Y<a \\ (\frac{Y-a}{b-a})^s & \text{if } a\leq Y\leq b \\ 1 & \text{if } Y>b \end{array}$	$\begin{array}{ll} 1 & \text{if } Y<b \\ (\frac{a-Y}{a-b})^s & \text{if } b\leq Y\leq a \\ 0 & \text{if } Y>a \end{array}$	$\begin{array}{ll} 0 & \text{if } Y<a_1 \\ (\frac{Y-a_1}{T-a_1})^s_1 & \text{if } a_1\leq Y\leq T \\ (\frac{a_2-Y}{a_2-T})^s_2 & \text{if } T\leq Y\leq a_2 \\ 0 & \text{if } Y>a_2 \end{array}$
Gibb *et al* (2001)	$(1+exp(-\frac{Y-a}{b}))^{-1}$	$(1-exp(-\frac{Y-a}{b}))^{-1}$	$exp(-\frac{1}{2}(\frac{Y-T}{b})^2)$
Le Bailly and Govaerts (2005)	$\Phi(\frac{Y-a}{b})$	$1-\Phi(\frac{Y-a}{b})$	$\sqrt{\Phi(\frac{Y-a_1}{b_1})(1-\Phi(\frac{Y-a_2}{b_2}))}$

Table 1: Examples of desirability functions. Y is a response; the target value T and the parameters a and b have to be adjusted according to the specifications; Φ is the cumulative distribution function of the standard normal.

Secondly, the transformed properties $d_i(Y_i)$ are aggregated in a single value still in the $[0, 1]$ interval, the *desirability index*, representing the overall desirability of the product. The weighted arithmetic mean or the weighted geometric mean of the desirability functions (Derringer, 1994), as well as their minimum (Kim and Lin, 2000) are the three most often used desirability indexes, denoted by $D(\mathbf{x})$: $D(\mathbf{x}) = \sum_{i=1}^{p} w_i \cdot d_i(Y_i)$, $D(\mathbf{x}) = \prod_{i=1}^{p}(d_i(Y_i))^{w_i}$ with $\sum_{i=1}^{p} w_i = 1$ or $D(\mathbf{x}) = \min_i d_i(Y_i)$.

The desirability index transforms the multicriteria optimization into a single objective optimization and establishes a ranking in the solution space. The aim of the manufacturer is to find the factors levels $\mathbf{x} \in \chi$ that maximize the desirability index.

This paper treats general desirability functions of the form $d_i : \Re \rightarrow]0, 1]$, that are two times continuously differentiable and supposes that they are aggregated with the weighted geometric mean desirability index. This differentiability property is not verified for the Derringer and Suich desirability function and for the Harrington one when a target value

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is sought. A similar methodology may also be applied to desirability index defined as the weighted arithmetic mean using the same tools to develop analogue formulas. In the following, desirability functions are abbreviated by *DF* and desirability index by *DI*.

If statistical models of the form (2) are available to predict the responses Y_i's for any point $\mathbf{x} = (x_1, x_2, \ldots, x_k)$ in χ, the DI optimization problem, is classically solved by maximizing the following expression :

$$\max_{\mathbf{x} \in \chi} \prod_{i=1}^{p} \left(d_i \left(\hat{Y}_i \right) \right)^{w_i} = \max_{\mathbf{x} \in \chi} \prod_{i=1}^{p} \left(d_i \left(\hat{E}[Y_i | \mathbf{x}] \right) \right)^{w_i} \tag{7}$$

This is the classical use of DI proposed by Harrington (1965) and Derringer and Such (1980) in their respective papers with different DF's. Both do not discuss the fact that the Y_i's are random variables which can not be predicted exactly and that the predictions $\hat{Y}_i$ are only uncertain estimators of $E(Y_i | \mathbf{x})$.

Defining

$$\hat{D}^C(\mathbf{x}) = \prod_{i=1}^{P} \left(d_i \left(\hat{E}[Y_i | \mathbf{x}] \right) \right)^{w_i} \tag{8}$$

and using an adequate optimization algorithm, the solution of (8) can be found and is denoted by $\hat{\mathbf{x}}_{opt}^C = arg \max_{\mathbf{x} \in \chi} \hat{D}^C(\mathbf{x})$. The hats stand for estimations as opposed to true (but unknown) quantities: $\mathbf{x}_{opt}^C = arg \max_{\mathbf{x} \in \chi} D^C(\mathbf{x})$ with $D^C(\mathbf{x}) = \prod_{i=1}^{P} \left(d_i \left(E[Y_i | \mathbf{x}] \right) \right)^{w_i}$.

4 Uncertainty of the responses, the desirability index and the optimum

For any point $\mathbf{x} \in \chi$, each corresponding responses $Y_i | \mathbf{x}$ is a random variable, each desirability function $d_i (Y_i | \mathbf{x})$ is a random variable and the desirability index $D(\mathbf{x}) = \prod_{i=1}^{p} \left(d_i (Y_i | \mathbf{x}) \right)^{w_i}$ is also a random variable. To take this into account, Steuer (2000) proposes an *improved optimization procedure* by rewriting the optimization problem (7) as :

$$\max_{\mathbf{x} \in \chi} D^N(\mathbf{x}) = \max_{\mathbf{x} \in \chi} E(D(\mathbf{x})) = \max_{\mathbf{x} \in \chi} E \left[\prod_{i=1}^{p} \left(d_i (Y_i | \mathbf{x}) \right)^{w_i} \right] \tag{9}$$

Let's note $\mathbf{x}_{opt}^N$ the solution of this maximization problem. In an experimental context, this optimal solution will provide the factors settings which, on average, give the maximum desirability. Each single experiment at $\mathbf{x}_{opt}^N$ will not give this expected DI but will provide a realisation of the random variable $D(\mathbf{x}_{opt}^N)$. The idea of maximising the expected DI instead of the DI of expected responses is the same as in the utility theory field as defined by von Neumann and Morgenstern (1944). The expected utility function, u, is maximized instead of the utility function of expected results, R, to take risk factors into account: $\max E[u(R)]$ instead of $\max u(E[R])$.

As the expectation of a random variable function is the function of the random variable expectation if and only if the transformation is linear, most of the time, $D^N(\mathbf{x}) = E \left[\prod_{i=1}^{P} \left(d_i (Y_i | \mathbf{x}) \right)^{w_i} \right] \neq \prod_{i=1}^{P} \left(d_i \left(E[Y_i | \mathbf{x}] \right) \right)^{w_i} = D^C(\mathbf{x})$ and $\mathbf{x}_{opt}^N \neq \mathbf{x}_{opt}^C$.

As, in practice, the quantity $D^N(\mathbf{x})$ is unknown, it has to be estimated. Steuer (2000) proposed to approximate for each design point $\mathbf{x} \in \chi$ the distribution of $D(\mathbf{x})$ by Monte-Carlo simulations on the basis of the model error distribution often assumed to be Normal. This is an heavy procedure, especially if there is more than two optimized properties and a large experimental domain χ to explore. In addition, his procedure does not allow to quantify the uncertainty of the estimated $D^N(\mathbf{x}) : \hat{D}^N(\mathbf{x})$.

To avoid intensive use of Monte-Carlo simulations, Weber and Weihs (2003) and Govaerts and Le Bailly de Tilleghem (2005) suggest to derive analytically the distribution of $D(\mathbf{x})$ on the basis of the model random error distribution using the density transformation theorem. Unfortunatly this is a complex task, often impossible due to the step of responses aggregation. In addition, like Steuer simulations based procedure, the propagation of the uncertainty of the estimated parameters on the distribution of $D(\mathbf{x})$ and its expectation can not be quantified.

There is a clear need of a general method, easily applicable in pratice, to estimate $D^N(\mathbf{x})$. More precisely, the rest of the paper proposes solutions to the following problems:

Section 5: Estimation of the expected desirability $D^N(\mathbf{x})$.

> The Delta method is first proposed to approximate $D^N(\mathbf{x})$ as a function of $E[Y_i|\mathbf{x}]$ and $V[Y_i|\mathbf{x}]$. Then, an estimator $\hat{D}^N(\mathbf{x})$ is defined by replacing the unknown quantities in the approximation by their estimators $\hat{E}[Y_i|\mathbf{x}]$ and $\hat{V}[Y_i|\mathbf{x}]$.

Section 6: Quantification of the uncertainty of $\hat{D}^N(\mathbf{x})$.

> The Delta method theorem is used to construct a nonsymmetric confidence interval for $D^N(\mathbf{x})$.

Section 7: Construction of an equivalence zone around the optimal solution in χ.

> By an adequate optimization algorithm, the factors settings $\hat{\mathbf{x}}_{opt}^N$ that maximize $\hat{D}^N(\mathbf{x})$ over χ must first be found. Then, as the uncertainty of $\hat{D}^N(\hat{\mathbf{x}}_{opt}^N)$ and the uncertainty of $\hat{D}^N(\mathbf{x})$ for any point $\mathbf{x} \in \chi$ can be quantified, this information can be used to search through χ the set of points $\mathbf{x}$ that do not have significantly different expected desirabilities. This is called the *optimal equivalence zone.*

Section 8: Construction of a prediction interval on $D(\mathbf{x})$ for any $\mathbf{x}$ in χ.

> The exact distribution of $D(\mathbf{x})$ or simulations can be applied to construct a prediction interval on $D(\mathbf{x})$.

5 Estimation of the expected desirability index $D^N(\mathbf{x})$

The Delta method is often used to approximate the variance of a function of random variables. This method can also be used to approximate expectation. Indeed, on the basis of the Taylor expansion of a differentiable function h of random variables $Y_1, Y_2, \ldots, Y_p$, it can be shown that the following second order approximations hold (Hahn and Shapiro, 1969):

$$E\left[h\left(Y_1, Y_2, ..., Y_p\right)\right] \approx h\left(E[Y_1], E[Y_2], ..., E[Y_p]\right) \tag{10}$$
$$+ \frac{1}{2}\sum_{i=1}^{p}\left[\frac{\partial^2 h}{\partial Y_i^2}V[Y_i]\right] + \sum_{i<j}^{p}\left[\frac{\partial^2 h}{\partial Y_i \partial Y_j}Cov(Y_i, Y_j)\right]$$

$$V\left[h\left(Y_1, Y_2, ..., Y_p\right)\right] \approx \sum_{i=1}^{p}\left[\left(\frac{\partial h}{\partial Y_i}\right)^2 V[Y_i]\right] \tag{11}$$
$$+ 2\sum_{i<j}^{p}\left[\left(\frac{\partial h}{\partial Y_i}\right)\left(\frac{\partial h}{\partial Y_j}\right)Cov(Y_i, Y_j)\right]$$

where the derivatives are evaluated in the expectation of the random variables : $Y_i = E[Y_i]$.

If we assume that, conditionally to $\mathbf{x}$, the responses are independent, *i.e.* $(Y_i|\mathbf{x})\,\text{II}\,(Y_j|\mathbf{x})$ $\forall i \neq j$, the approximation (10) can be rewritten as

$$E\left[h\left(Y_1, ..., Y_p\right)|\mathbf{x}\right] \approx h\left(E[Y_1|\mathbf{x}], ..., E[Y_p|\mathbf{x}]\right) + \frac{1}{2}\sum_{i=1}^{p}\left[\frac{\partial^2 h}{(\partial Y_i)^2}V[Y_i|\mathbf{x}]\right] \tag{12}$$

where the derivatives are evaluated in the conditional expectations $E[Y_i|\mathbf{x}]$.

As the DI is a function of the random responses $Y_1|\mathbf{x}, Y_2|\mathbf{x}, \ldots, Y_p|\mathbf{x}$, formula (12) can be applied to approximate the expected DI conditionally to $\mathbf{x}$ to the second order as :

$$D^N(\mathbf{x}) = E\left[D(\mathbf{x})\right] = E\left[\prod_{i=1}^{p}\left(d_i\left(Y_i\right)\right)^{w_i}|\mathbf{x}\right] \approx \left[\prod_{i=1}^{p}\left(d_i\left(E\left[Y_i|\mathbf{x}\right]\right)\right)^{w_i}\right]\cdot(1 + B(\mathbf{x})) \tag{13}$$

where $B(\mathbf{x})$ is given by :

$$B(\mathbf{x}) = \frac{1}{2}\sum_{i=1}^{p}\left[\left(w_i(w_i-1)\left(\frac{\frac{\partial d_i(Y_i)}{\partial Y_i}}{d_i(E[Y_i|\mathbf{x}])}\right)^2 + w_i\frac{\frac{\partial^2 d_i(Y_i)}{\partial Y_i^2}}{d_i(E[Y_i|\mathbf{x}])}\right)\cdot V[Y_i|\mathbf{x}]\right] \tag{14}$$

The first part of (13) is the classical desirability $D^C(\mathbf{x})$, and the half sum $B(\mathbf{x})$ in the second term is a kind of bias correction. This approximation of $D^N(\mathbf{x})$ is possible for differentiable DF. This is not the case for the Derringer and Suich DF but those functions can be easely approximated by other differentiable functions as shown in Figure 1 or by the DF proposed by del Castillo *et al.* (1996).

$D^N(\mathbf{x})$ can be estimated by replacing in the approximation (13-14) the unknown quantities $E[Y_i|\mathbf{x}]$ and $V[Y_i|\mathbf{x}]$ by their usual estimators, the predictions given by the estimated models $\hat{E}(Y_i|\mathbf{x})$ and the estimators of the residual variances $\hat{V}(Y_i|\mathbf{x}) = \hat{\sigma}^2_{\epsilon_i}$. These are given explicitly in section 2 for the linear regression model. In $B(\mathbf{x})$, the first and second derivatives of $d_i(Y_i)$ are also evaluated in $\hat{E}(Y_i|\mathbf{x})$.

For any point $\mathbf{x} \in \chi$, formulas (13-14) provide then a general method to approximate and estimate the new desirability criteria $D^N(\mathbf{x})$ defined in (9). This allows to find estimated optimal factors settings $\hat{\mathbf{x}}^N_{opt}$ in χ using an adequate algorithm. This optimal solution may be different of the classical one $\hat{\mathbf{x}}^C_{opt}$ due to the bias term $B(\mathbf{x})$ present in the new desirability criteria :

$$\hat{D}^N(\mathbf{x}) = \hat{E}[D(\mathbf{x})] = \hat{D}^C(\mathbf{x})\cdot(1 + \hat{B}(\mathbf{x})) \tag{15}$$

6 Quantification of the uncertainty on $\hat{E}\left[D(\mathbf{x})\right]$.

The Delta method theorem (von Mises, 1947) can be used to derive the asymptotic properties of our estimator $\hat{D}^N(\mathbf{x})$ and build a confidence interval for $D^N(\mathbf{x})$.

The Delta method theorem: Suppose that $\boldsymbol{\theta}$ is a vector of parameters estimated on n observations by $\hat{\boldsymbol{\theta}}$ with $\sqrt{n}(\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}) \xrightarrow{d} \mathbf{N}(\mathbf{0}, \boldsymbol{\Sigma})$ and g is a continuously differentiable function then $\sqrt{n}(g(\hat{\boldsymbol{\theta}}) - g(\boldsymbol{\theta})) \xrightarrow{d} \mathbf{N}(\mathbf{0}, \frac{\partial g}{\partial \boldsymbol{\theta}} \boldsymbol{\Sigma} \frac{\partial g'}{\partial \boldsymbol{\theta}})$.

In order to apply this theorem to $\hat{D}^N(\mathbf{x}) = \hat{D}^C(\mathbf{x}) \cdot \left(1 + \hat{B}(\mathbf{x})\right)$, let us first note that the uncertainty on $\hat{B}(\mathbf{x})$ is negligeable compared to the uncertainty of the term $\hat{D}^C(\mathbf{x})$. In addition, as $\hat{D}^C(\mathbf{x})$ is a continuously differentiable function of $\hat{E}(\mathbf{Y}|\mathbf{x}) = (\hat{E}(Y_1|\mathbf{x}), ..., \hat{E}(Y_p|\mathbf{x}))$, $\hat{E}(\mathbf{Y}|\mathbf{x})$ becomes $\hat{\boldsymbol{\theta}}$ in the Delta theorem with expected value $E(\mathbf{Y}|\mathbf{x})$ and variance-covariance matrix $\boldsymbol{\Sigma} = diag(V(\hat{E}(Y_1|\mathbf{x})), ..., V(\hat{E}(Y_p|\mathbf{x})))$ since, conditionally to $\mathbf{x}$, the Y_i's are considered as independent. In the linear case, $V(\hat{E}(Y_i|\mathbf{x}))$ is given by (5).

On the other hand, the conclusion that $\hat{E}\left[D(\mathbf{x})\right]$ would be asymptotically normal is not realistic since it is bounded on the $[0,1]$ interval. In order to better fullfil this normality assumption, Cahya (2002) and Ding *et al.* (2003) suggest to apply a logit transformation to $\hat{E}\left[D(\mathbf{x})\right]$ before applying the theorem to get an unbounded support $(-\infty, \infty)$. In addition this insures that resulting confidence intervals are included in the interval $[0,1]$.

As $\mathrm{logit}(\hat{E}\left[D(\mathbf{x})\right])$ is also a continuously differentiable function of $\hat{E}(\mathbf{Y}|\mathbf{x})$, the Delta method theorem leads to the following result:

$$\mathrm{logit}\left(\hat{E}\left[D(\mathbf{x})\right]\right) \xrightarrow{d} N\left(\mathrm{logit}\left(E\left[D(\mathbf{x})\right]\right), V\left[\mathrm{logit}\left(\hat{E}\left[D(\mathbf{x})\right]\right)\right]\right) \tag{16}$$

The variance $V\left[\mathrm{logit}\left(\hat{E}\left[D(\mathbf{x})\right]\right)\right]$ can be estimated as a function of $\hat{E}[Y_i|\mathbf{x}]$ and $\hat{V}[Y_i|\mathbf{x}]$:

$$\hat{V}\left[\mathrm{logit}\left(\hat{E}[D(\mathbf{x})]\right)\right] \approx \frac{1}{\left(\hat{E}[D(\mathbf{x})].\left(1 - \hat{E}[D(\mathbf{x})]\right)\right)^2} \cdot \hat{V}[\hat{E}[D(\mathbf{x})]] \tag{17}$$

where

$$\hat{V}[\hat{E}[D(\mathbf{x})]] \approx \left(1 + \hat{B}(\mathbf{x})\right)^2 \cdot \hat{V}[\hat{D}^C(\mathbf{x})] \tag{18}$$

and

$$\hat{V}[\hat{D}^C(\mathbf{x})] \approx \sum_{i=1}^{p} \left[\left(w_i \cdot \frac{\frac{\partial d_i(\hat{E}[Y_i|\mathbf{x}])}{\partial \hat{E}[Y_i|\mathbf{x}]}}{d_i(\hat{E}[Y_i|\mathbf{x}])} \cdot \hat{D}^C(\mathbf{x}) \right)^2 \cdot \hat{V}\left[\hat{E}[Y_i|\mathbf{x}]\right] \right] \tag{19}$$

An *asymptotic* $(1-\alpha) \cdot 100\%$ *confidence interval* for $\mathrm{logit}\left(E[D(\mathbf{x})]\right)$ can then be derived as

$$\mathrm{logit}\left(\hat{E}[D(\mathbf{x})]\right) \pm z_{1-\alpha/2} \cdot \sqrt{\hat{V}\left[\mathrm{logit}\left(\hat{E}[D(\mathbf{x})]\right)\right]} \tag{20}$$

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Then, a $(1-\alpha)\cdot 100\%$ confidence interval for $D^N(\mathbf{x})$ can be obtain by transforming (20) using the inverse logit transformation:

$$\frac{\exp^{\mathrm{logit}\left(\hat{\mathrm{D}}^{\mathrm{N}}(\mathbf{x})\right)\pm \mathrm{z}_{0,975}\cdot\sqrt{\hat{\mathrm{V}}\left[\mathrm{logit}\left(\hat{\mathrm{D}}^{\mathrm{N}}(\mathbf{x})\right)\right]}}}{1+\exp^{\mathrm{logit}\left(\hat{\mathrm{D}}^{\mathrm{N}}(\mathbf{x})\right)\pm \mathrm{z}_{0,975}\cdot\sqrt{\hat{\mathrm{V}}\left[\mathrm{logit}\left(\hat{\mathrm{D}}^{\mathrm{N}}(\mathbf{x})\right)\right]}}} \tag{21}$$

Such confidence interval can be constructed for any $\mathbf{x} \in \chi$ to quantify the uncertainty of the estimation $\hat{D}^N(\mathbf{x})$. This interval is included in the $[0,1]$ interval and is not necessarily symmetric.

7 Set up of an equivalence zone for $\mathbf{x}_{opt}^N$

Using the estimator $\hat{E}[D(\mathbf{x})]$ (15), a value between 0 and 1 can be associated to any point $\mathbf{x} \in \chi$ representing the estimation of the expected DI of the solution $\mathbf{x}$ and the optimum $\hat{\mathbf{x}}_{opt}^N$ that maximizes this quantity can be found using an adequate algorithm.

As the expected DI of the optimum found, $E[D(\hat{\mathbf{x}}_{opt}^N)]$, is not exactly known but estimated by $\hat{E}[D(\hat{\mathbf{x}}_{opt}^N)]$, $\hat{\mathbf{x}}_{opt}^N$ is not necessary the true optimum, $\mathbf{x}_{opt}^N$, and there is a subset of points in χ that are associated to expected desirabilities not significantly different of the one associated to the optimum found $\hat{\mathbf{x}}_{opt}^N$.

We propose to define the *optimal equivalence zone, EZ,* as the subset of points $\mathbf{x} \in \chi$ such that the hypothesis $E[D^N(\mathbf{x})] = E[D^N(\hat{\mathbf{x}}_{opt}^N)]$ can not be rejected. This equivalence zone contains solutions that can not statistically be differenciated from $\hat{\mathbf{x}}_{opt}^N$.

In the preceeding section, the asymptotic distribution of $\mathrm{logit}\left(\hat{E}[D(\mathbf{x})]\right)$ for any $\mathbf{x} \in \chi$ has been established using the Delta method theorem (16). Exactly the same tool can be used to derive the asymptotic distribution of any other differentiable transformation of $\hat{E}[D(\mathbf{x})]$ like the logarithm. Cahya (2002) observed in his simulations that a difference of *log* is better approximated by a Normal than a difference of *logit*. That's why we propose to construct the equivalence zone around $\hat{\mathbf{x}}_{opt}^N$ on the basis of the asymptotic distribution of the difference

$$\hat{\Delta}_D(\mathbf{x},\hat{\mathbf{x}}_{opt}^N) = \log\left(\hat{E}[D(\mathbf{x})]\right) - \log\left(\hat{E}[D(\hat{\mathbf{x}}_{opt}^N)]\right).$$

As both $\log\left(\hat{E}[D(\mathbf{x})]\right)$ and $\log\left(\hat{E}[D(\hat{\mathbf{x}}_{opt}^N)]\right)$ are asymptotically Normal, their difference is also asymptotically Normal:

$$\hat{\Delta}_D(\mathbf{x},\hat{\mathbf{x}}_{opt}^N) \xrightarrow{d} N\left(\Delta_D(\mathbf{x},\hat{\mathbf{x}}_{opt}^N), V(\hat{\Delta}_D(\mathbf{x},\hat{\mathbf{x}}_{opt}^N))\right) \tag{22}$$

with

$$\Delta_D(\mathbf{x},\hat{\mathbf{x}}_{opt}^N) = \log\left(E[D(\mathbf{x})]\right) - \log\left(E[D(\hat{\mathbf{x}}_{opt}^N)]\right) \tag{23}$$

and

$$\begin{aligned} V(\hat{\Delta}_D(\mathbf{x},\hat{\mathbf{x}}_{opt}^N)) \;=\;& V\left(\log\left(\hat{E}[D(\mathbf{x})]\right)\right) + V\left(\log\left(\hat{E}[D(\hat{\mathbf{x}}_{opt}^N)]\right)\right) \\ & -2\cdot Cov\left(\log\left(\hat{E}[D(\mathbf{x})]\right), \log\left(\hat{E}[D(\hat{\mathbf{x}}_{opt}^N)]\right)\right) \end{aligned} \tag{24}$$

A formula similar to (17) can be applied to estimate the variances $V\left(\log\left(\hat{E}[D(\mathbf{x})]\right)\right)$ and $V\left(\log\left(\hat{E}[D(\hat{\mathbf{x}}_{opt}^N)]\right)\right)$. The covariance between the two log cannot be neglected and can be estimated once more by the Delta method theorem:

$$\hat{C}ov\left(\log\left(\hat{E}[D(\mathbf{x})]\right),\log\left(\hat{E}[D(\hat{\mathbf{x}}_{opt}^N)]\right)\right)\approx \qquad (25)$$

$$\frac{1+\hat{B}(\mathbf{x})}{\hat{E}[D(\mathbf{x})]}\cdot\hat{C}ov\left[\hat{D}^C(\mathbf{x}),\hat{D}^C(\hat{\mathbf{x}}_{opt}^N)\right]\cdot\frac{1+\hat{B}(\hat{\mathbf{x}}_{opt}^N)}{\hat{E}[D(\hat{\mathbf{x}}_{opt}^N)]}$$

where

$$\hat{C}ov\left[\hat{D}^C(\mathbf{x}),\hat{D}^C(\hat{\mathbf{x}}_{opt}^N)\right]\approx \qquad (26)$$

$$\sum_{i=1}^p\left(w_i\frac{\frac{\partial d_i(\hat{E}[Y_i|\mathbf{x}])}{\partial\hat{E}[Y_i|\mathbf{x}]}}{d_i(\hat{E}[Y_i|\mathbf{x}])}\hat{D}^C(\mathbf{x})\right)\cdot\hat{C}ov\left[\hat{E}[Y_i|\mathbf{x}],\hat{E}[Y_i|\mathbf{x}_{opt}^N]\right]\cdot\left(w_i\frac{\frac{\partial d_i(\hat{E}[Y_i|\mathbf{x}_{opt}^N])}{\partial\hat{E}[Y_i|\hat{\mathbf{x}}_{opt}^N]}}{d_i(\hat{E}[Y_i|\mathbf{x}_{opt}^N])}\hat{D}^C(\mathbf{x}_{opt}^N)\right)$$

In the case of linear regression model, we have :

$$\hat{C}ov\left[\hat{E}[Y_i|\mathbf{x}],\hat{E}[Y_i|\mathbf{x}_{opt}^N]\right]=\hat{\sigma}_i^2\mathbf{z}'(\mathbf{Z_i'Z_i})^{-1}\hat{\mathbf{z}}_{\mathbf{opt}}^{\mathbf{N}}$$

For any point $\mathbf{x}\in\chi$, the asymptotic distribution of the difference $\hat{\Delta}_D(\mathbf{x},\hat{\mathbf{x}}_{opt}^N)$ (22) can then be used to construct a confidence interval for the true difference. The equivalence zone around the optimum found $\hat{\mathbf{x}}_{opt}^N$ is constructed by screening the solutions space χ to select points $\mathbf{x}$ for which this confidence interval contains 0. At a level $(1-\alpha)\cdot 100\%$, it can be formulated as follows :

$$EZ\equiv\{\mathbf{x}\in\chi:0\in\hat{\Delta}_D(\mathbf{x},\hat{\mathbf{x}}_{opt}^N)\pm z_{1-\alpha/2}\cdot\sqrt{\hat{V}(\hat{\Delta}_D(\mathbf{x},\hat{\mathbf{x}}_{opt}^N))}\} \qquad (27)$$

The confidence interval for $\Delta_D(\cdot,\cdot)$ can also be applied to any pair of points $\mathbf{x}_1$ and $\mathbf{x}_2$ in χ to check if their desirabilities are significantly different.

A similar methodology has been developed by Cahya (2002) but he works with the classical index $D^C(\mathbf{x})$, the linear regression model and applies the Delta theorem to transformations of the regression parameters instead of transformations of the expected predicted responses. Moreover, his goal is to build a confidence zone for the true optimum $\mathbf{x}_{opt}^C$, as done in all former literature, while here we are only looking for a set of operating conditions $\mathbf{x}\in\chi$ for which the expected desirability does not significantly differ from the one of the estimated optimum $\hat{\mathbf{x}}_{opt}^N$. The advantage of our approach is that the equivalence zone is much more simple to calculate. The Cahya methodology necessitates indeed to optimize an objective function on χ for each $\mathbf{x}$ to decide if it belongs or not to the confidence zone.

8 Prediction interval for $D(\mathbf{x})$

As experimental responses are random variables, the result of a single experiment at a point $\mathbf{x}$ of χ can not exactly be predicted and individual values prediction intervals are usually

calculated to quantify this uncertainty. In the linear model, the prediction variance for a single observation Y_i is given by $V(\hat{Y}_i|\mathbf{x})$ in (6).

This implies that the DI for a single observation is also an unpredictable quantity and one may be interested to derive a prediction interval for the desirability in $\mathbf{x}$, $D(\mathbf{x})$.

In this context, Trautmann and Weihs (2004) proposed a methodology to construct such prediction interval from the analytical distribution function of $D(\mathbf{x})$ that can be derived for Harrington type DFs. From this interval, they construct a sort of optimal zone as a subset of $\mathbf{x}$ in χ around the optimum $\mathbf{x}_{opt}^N$ such that the probability of having $D(\mathbf{x})$ lying in a prediction interval around $\hat{D}^C(\mathbf{x}_{opt}^N)$ is high. They take into account only the random model error, ϵ, and neglect the propagation of the estimation error of their regression prediction models (2) on $D^N(\mathbf{x})$.

Similarly, Govaerts and Le Bailly de Tilleghem (2005) have derived the analytical distribution of D($\mathbf{x}$) for cumulative Normal DFs and can derive similar results.

When no analytical form for the distribution function of the DI exists, the best approach is to derive the prediction interval through simulations. In the classical regression model, one may simulate S possible responses in $\mathbf{x}$, $Y_i|\mathbf{x}$, using the statistical distribution of $\hat{Y}_i$:

$$\frac{Y_i - \hat{Y}_i}{\hat{\sigma}_{\epsilon_i}{}^2 . (1 + \mathbf{z_i'}(\mathbf{Z_i'Z_i})^{-1}\mathbf{z_i})} \sim t(n_i - q_i) \tag{28}$$

Each simulated vector $\mathbf{Y}^s = (Y_1^s, Y_2^s, ...Y_p^s)$, $s = 1, 2, \ldots, S$, will allow to calculate one possible DI $D(\mathbf{x})^s$ and the prediction interval will be derived from the the quantiles of the empirical distribution of $(D(\mathbf{x})^1, \ldots, D(\mathbf{x})^S)$.

9   Simulations study

To demonstrate that the confidence interval formula (21) for $D^N(\mathbf{x})$ works as well as the equivalence zone around the optimum found (27), simulations are performed on a simple optimization example.

Two responses, Y_1 and Y_2, have to be simultaneously optimized on a one factor x domain ($x \in [0, 1]$). The first response, Y_1, has to be maximized and the second response, Y_2, has to be minimized. Two third order models have been chosen such that they are not too simple and such that their respective optimizations are not too competitive. They are represented in Figure 2.

The Normal cdf is used to construct DFs as presented in Table 1. They depend on parameters a and b fixed according to the acceptable responses values (Govaerts and Le Bailly de Tilleghem, 2005). The first response is of the kind the higher, the better. Let's suppose that all values smaller than 1.5 are not at all desired and all values greater than 3 are equivalently hugely desired. Those lower and upper limits, $LL_1 = 1.5$ and $UL_1 = 3$, are used to compute the two parameters of the desirability function as $a_1 = \frac{LL_1 + UL_1}{2} = 2.25$ and $b_1 = \frac{UL_1 - \frac{LL_1 + UL_1}{2}}{2} = 0.375$. In this way, accordingly to the properties of the standard Normal $c.d.f.$, $d_1(1.5) = 0.023$ and $d_1(3) = 0.977$ and between 1.5 and 3, the desirability increases. This DF is represented in Figure 3 as a function of Y_1. The second response has to be minimized. Let's suppose that all values greater than $UL_2 = 1.25$ are not at all desired and all values smaller than $LL_2 = 0.5$ are equivalently hugely desired. Those limits are used

to compute the two parameters $a_2 = \frac{LL_2 + UL_2}{2} = 0.875$ and $b_2 = \frac{UL_2 - \frac{LL_2 + UL_2}{2}}{2} = 0.1875$. In this way, $d_2(1.25) = 0.023$ and $d_2(0.5) = 0.977$ and between 0.5 and 1.25, the desirability decreases. This DF is represented in Figure 3 as a function of Y_2. Both DFs are also represented in Figure 4 as a function of x and, over the $[0, 1]$ interval, the respective optima are 0.373 for Y_1 and 0.226 for Y_2. Finally, the geometric mean DI is used to summarize those two DFs, giving the same weight to both properties.

In this example, the difference between the 2 indexes, $D^N(x)$ and $D^C(x)$, is small as shown in Figure 5. The resulting optima are closed to each other: $x_{opt}^N = 0.288$ and $x_{opt}^C = 0.285$.
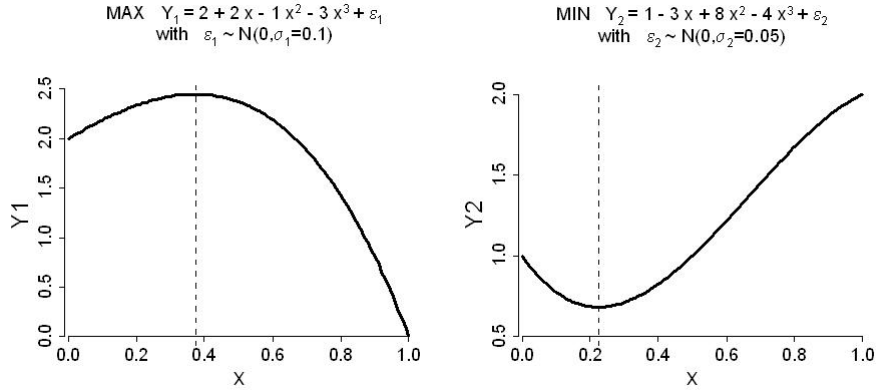
Figure 2: Two responses, Y_1 and Y_2, to be respectively maximized and minimized on $[0, 1]$. The respective optima are marked by vertical dashed lines and are 0.373 for Y_1 and 0.226 for Y_2
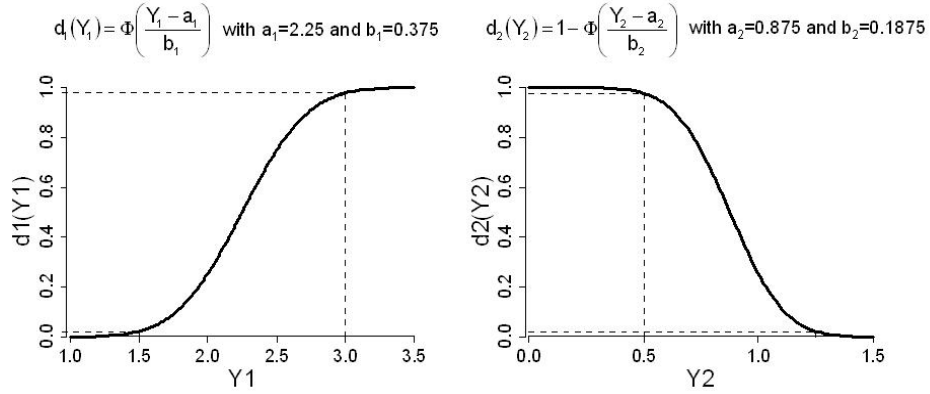
Figure 3: Desirability functions for Y_1 and Y_2 based on the Normal cdf: $d_1(Y_1)$ and $d_2(Y_2)$.

To first check the adequacy of the confidence interval for $D^N(x)$, the next simulation was repeated 10000 times:

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$$d_1(Y_1) = \Phi\left(\frac{Y_1 - a_1}{b_1}\right) \text{ with } a_1 = 2.25 \text{ and } b_1 = 0.375 \qquad d_2(Y_2) = 1 - \Phi\left(\frac{Y_2 - a_2}{b_2}\right) \text{ with } a_2 = 0.875 \text{ and } b_2 = 0.1875$$
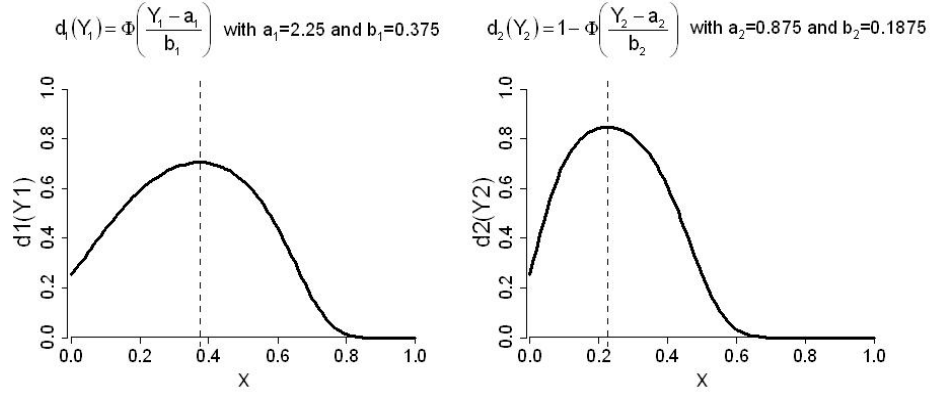
Figure 4: Desirability functions for Y_1 and Y_2 based on the Normal *cdf* as functions of x. The respective optima are marked by vertical dashed lines and are 0.373 for Y_1 and 0.226 for Y_2.
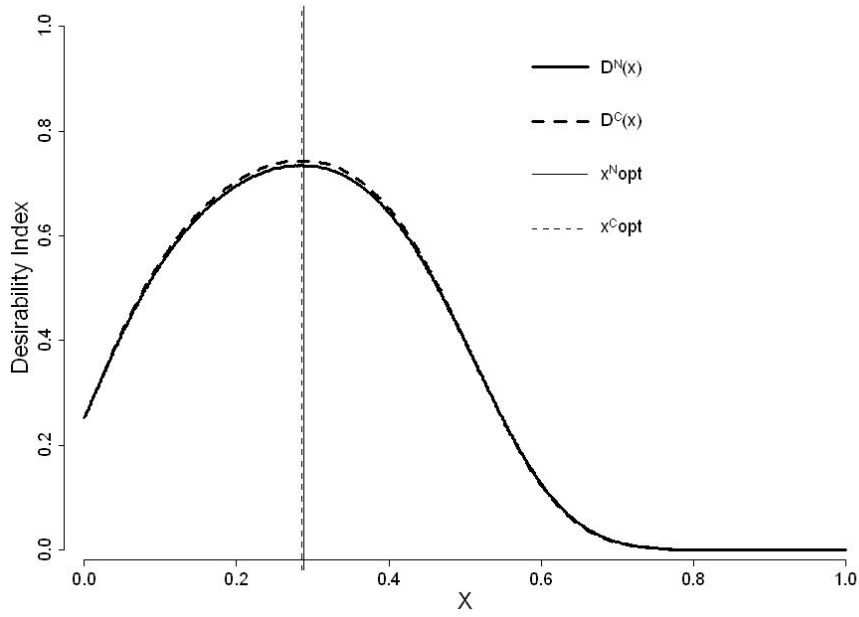

Figure 5: Difference between the classical use and the new use of desirability index: $D^N(x)$ and $D^C(x)$ are represented by a continuous and a dashed thick curves respectively. The respective optima are marked by vertical thin continuous and dashed lines, $x_{opt}^N = 0.288$ and $x_{opt}^C = 0.285$.

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Step 1: For each response, Y_1 and Y_2, generation of a sample of size $n = 10$ following the the models given in Figure 2 and fit of a cubic regression model to the simulated data (Figure 6).

Step 2: Estimation of $D^N(x)$ over the factor domain $\chi = [0, 1]$ using the fitted models and our estimator (15) (Figure 7).
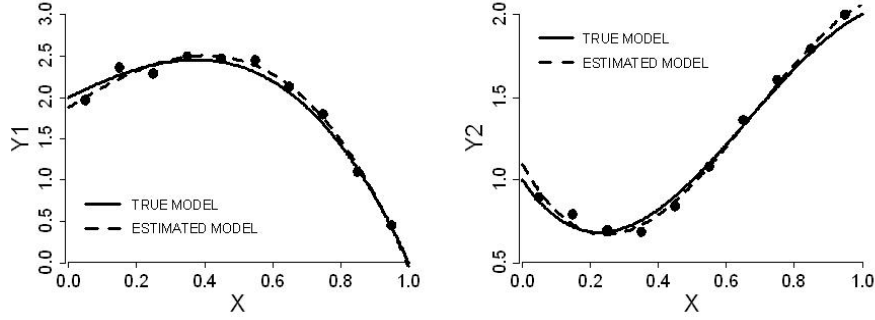

Figure 6: Example of the first step for one simulation run: the dots represent the generated datasample on which the models are fitted. The continuous and the dashed lines represent respectively the true and the estimated models.
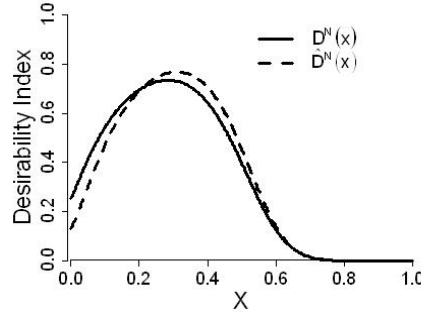
Figure 7: Example of the second step for one simulation run: the continuous and the dashed lines represent respectively the true and the estimated expected desirabilities.

From run to run, the estimated expected desirability can have very different shapes. For any $x \in \chi = [0, 1]$, we have 10000 realisations of the distribution of our estimator $\hat{D}^N(x)$. Figure 8 compares the 2.5% and 97.5% quantiles of this simulated distribution and the theoretical 95% confidence interval for $D^N(x)$ given by formula (21), using the true $D^N(x)$ (12). The theoretical formula provides confidence intervals really similar to the simulations.
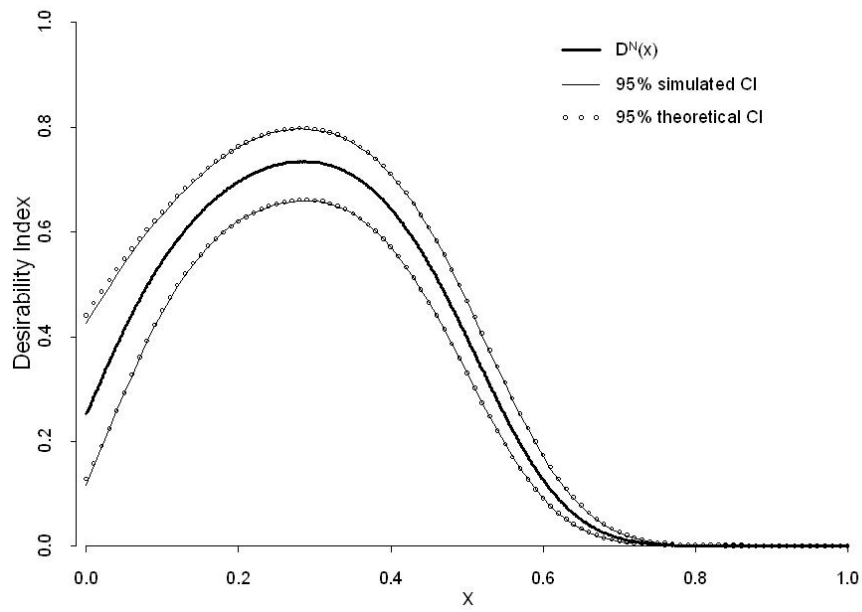
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Figure 8: Validation of the confidence interval: comparison of the 95% theoretical confidence interval for $D^N(x)$ given by formula (21) using the true $D^N(x)$ - empty dots - and 95% simulated confidence interval constructed on the basis of the quantiles 2.5% and 97.5% of the simulated distribution for the estimator $\hat{D}^N(x)$ - continuous thin lines -.

We can conclude that the approximated asymptotic distribution given by the Delta method theorem provides, in this example, quite accurate confidence intervals even if the number of data is small.

Secondly, to check the adequacy of the equivalence zone around the optimum found, the next simulation was repeated 10000 times:

Step 1: For each response, Y_1 and Y_2, generation of a sample of size $n = 10$ following the models given in Figure 2 and fit of a cubic regression model to the simulated data (Figure 6).

Step 2: Estimation of the difference between $D^N(x)$ and $D^N(x_{opt}^N)$ by computing $\hat{D}^N(x) - \hat{D}^N(x_{opt}^N)$ over the factors domain $\chi = [0, 1]$ using the fitted models (Figure 9).
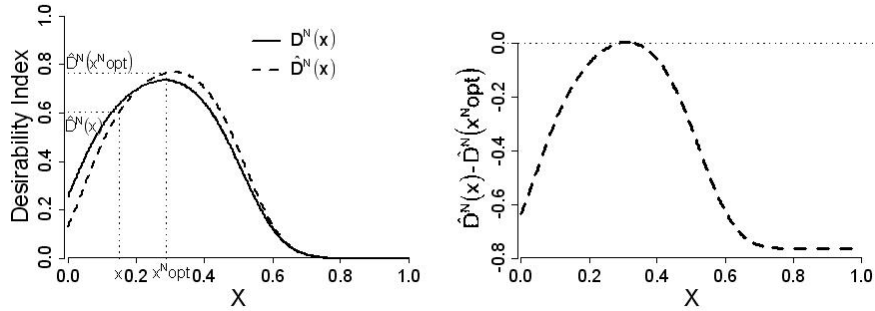

Figure 9: Example of the second step for one simulation run: the first graph compares the true espected desirability index $D^N(x)$ (continuous curve) and the estimated one $D^N(x)$ (dashed curve) and the second graph presents the resulting estimated difference of expected desirability between any point x in $[0, 1]$ and the optimum x_{opt}^N, $\hat{D}^N(x) - \hat{D}^N(x_{opt}^N)$.

For any x in $[0, 1]$, we have 10000 realisations of the distribution of the estimator $\hat{D}^N(x) - \hat{D}^N(x_{opt}^N)$. The simulated equivalence zone around the optimum x_{opt}^N is constructed by retaining points x for which the intervals determined by the 2.5% and 97.5% quantiles of this simulated distribution contain 0, meaning that, for those points x, $D^N(x)$ is not significantly different of $D^N(x_{opt}^N)$. This simulated equivalence zone is compared on Figure 10 with the theoretical equivalence zone around x_{opt}^N, *i.e.* as defined by (27) where true quantities are used instead of estimators. On this example, the theoretical equivalence zone is exactlty the same as the one obtained by simulations: all points $x \in [0.220, 0.333]$ are equivalent to the optimum x_{opt}^N.

Note also that, in all performed simulations, the difference between $D^C(\mathbf{x})$ and $D^N(\mathbf{x})$ is small compared to the uncertainty of the corresponding quantities $\hat{D}^C(\mathbf{x})$ and $\hat{D}^N(\mathbf{x})$. On the presented example of this section, the difference between $D^C(x)$ and $D^N(x)$ on Figure 5 is indeed negligeable compared to the size of confidence intervals drawn in Figure 8. Similarly, the difference between the two optima x_{opt}^C and x_{opt}^N (Figure 5) is small compared to the size of the equivalence zone around the optimum (Figure 10).
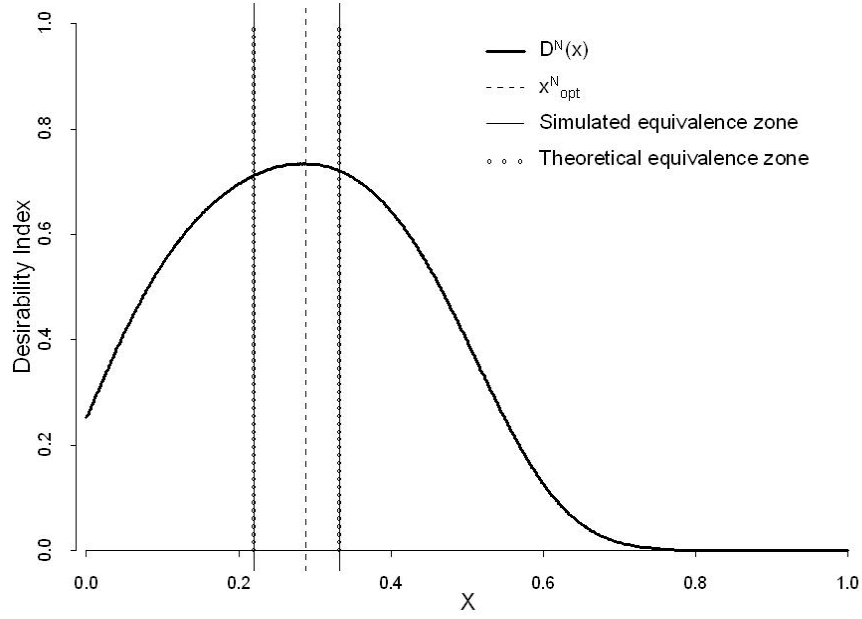
Figure 10: Validation of the equivalence zone around x^N_{opt}. Comparison of the equivalence zone obtained by simulations of the distribution of estimated differences $\hat{D}^N(x) - \hat{D}^N(x^N_{opt})$ (continuous thin vertical line) and the equivalence zone obtained with the theoretical formula (27) (dotted vertical line). Both are the same, $[0.220, 0.333]$. The thick continuous curve is $D^N(x)$ and the thick dashed vertical line is the true optimum x^N_{opt}.

10 Conclusion

This paper proposes a new use of DI and a new methodology to quantify uncertainty of estimated DI and estimated optimum. It generalizes and integrates existing literature on the subject.

As Steuer (2000) emphasized, due to the model error term ϵ_i, each response for given factors levels $\mathbf{x}$, $Y_i|\mathbf{x}$, is a random variable. The classical use of DI as introduced by Harrington consists of summarising the desirability of expected optimized properties by a single value between 0 and 1 ($D^C(\mathbf{x})$) and neglecting the error term. Assuming that $\epsilon_i \sim N(0, \sigma^2_{\epsilon_i})$ with known variance $\sigma^2_{\epsilon_i}$, Steuer suggested to take this available information into account by considering the DI as a random variable and maximizing the expected DI of the responses ($D^N(\mathbf{x})$), applying to DI an idea previously introduced by von Neumann and Morgenstern (1944) in utility theory field. To avoid intensive simulations, as the exact distribution of the DI random variable can not, in most cases, be handeled easely, the Delta method is used to approximate the expected DI up to second order terms. This is possible if the DFs are two times differentiable.

The approximation of the expected DI by the Delta method depends on expected responses $E[Y_i|\mathbf{x}]$ and on response variances $V[Y_i|\mathbf{x}]$. By replacing these usually unknown quantities by their classical estimators, an estimator for the expected DI is obtained ($\hat{D}^N(\mathbf{x})$). The Delta method theorem allows to derive the asymptotic distribution of our estimator and build a $(1-\alpha) \cdot 100\%$ confidence interval for the true expected DI. This theorem may also be used to derive the asymptotic distribution of the difference of the estimated expected DI of two solutions and construct an equivalence zone around the estimated optimum, gathering factors levels having non-significantly different expected DI as the optimum found.

Though simulations, we found that the Delta method provides a good second order approximation of the expected DI. In most cases, the difference between the classical use of DI, $D^C(\mathbf{x})$, and the new one, $D^N(\mathbf{x})$, is small as well as the resulting optima, $\mathbf{x}^C_{opt}$ and $\mathbf{x}^N_{opt}$. The most important improvement is the new methodology based on the Delta method theorem to measure the prediction error propagation on the estimated expected DI. This allows to compare the estimated expected DI of two solutions taking into account their incertitude and constructing an equivalence zone around the optimum found. Simulations reveals that this uncertainty porpagation is much more important in practice than the bias correction between $D^C(\mathbf{x})$ and $D^N(\mathbf{x})$.

11 Acknowledgment

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