Uncertainty of the Optimum Influence Factor Levels in Multicriteria Optimization Using the Concept of Desirability

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Abstract:
The Desirability Index (DI) is a widely used method for multicriteria optimization in industrial quality control, by which optimal levels of the process influencing factors are determined in order to achieve maximum process quality. In practice however situations may occur in which slight changes of these factor levels lead to lower production costs or to a facilitation of the production process and therefore would be preferred. In this paper an innovative approach for measuring the effect of these changes on the DI based on its distribution is introduced.

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1 Introduction

The approach for multicriteria optimization based on the concept of desirabilities and introduced by [HAR65] has become an appropriate means in the range of Multicriteria Decision Making Techniques (see [HEN92] for a review). It consists of a complexity reduction in industrial quality optimization and furthermore makes use of design of experiment methods, by which polynomial models are set up reflecting the functional relationships between the quality measures and the process influencing factors. In the first step Desirability Functions (DFs) transfer the values of the quality measures into desirabilities onto a unitless scale in the domain $[0, 1]$ regarding the desirability of their feasible realizations. The Desirability Index (DI) then represents a univariate and unitless measure for the overall process quality by combining the individual desirabilities usually using the geometric mean. The closer its value comes to the maximum value of 1 the more satisfying the process quality proves. As the DI is not only a function of the quality measures but also of the influence factors — using their functional relationships with the quality measures resulting from the design of experiment phase — the DI and thus the overall process quality can be optimized by nonlinear optimization of the levels of the influence factors, optimizing all often competing quality measures simultaneously.

Usually the process then is set up based on the optimal levels of the influence factors. Regarding the convenience of the process flow or the production costs however sometimes slight modifications of these levels would be preferred in practice. In this paper an innovative approach for measuring the effect of these changes on the DI in the course of the process is introduced, which makes use of the distribution of the DI ([WEB03]) and results in ranges of the influence factors that ensure that the prediction interval of the optimized DI still covers the values of the DI in the ongoing process with a predefined probability.

Chapter 2 reviews the type of the DF and the DI introduced by [HAR65], whereas in Chapter 3 an overview of the proposed approach is given. Afterwards the latter is illustrated in detail by two simulated practical examples in Chapters 4 and 5. Conclusions and a short summary are provided in Chapter 6.

2 Harrington's Desirability Functions and the Desirability Index

Harrington introduced two types of DFs, which transform the quality measures onto a unitless scale between 0 and 1. One aimes at maximization of the quality measure (one-sided specification) whereas the other one reflects a target value problem (two-sided specification) (Fig. 1).

1. **Two-Sided Specification:** For a quality measure Y_i $(i = 1, \ldots, k)$ the transformation requires two specification limits $(LSL_i,\ USL_i)$ symmetrically around the target value, which are associated with a desirability of $1/e$. Then the DF resulting in desirabilites d_i is defined as:

$$d_i(Y_i') = e^{-|Y_i'|^{n_i}}, \qquad i = 1, \ldots, k;\ 0 < n_i < \infty \quad \text{with} \tag{1}$$

$$Y_i' = \frac{2Y_i - (USL_i + LSL_i)}{USL_i - LSL_i}, \qquad i = 1, \ldots, k. \tag{2}$$

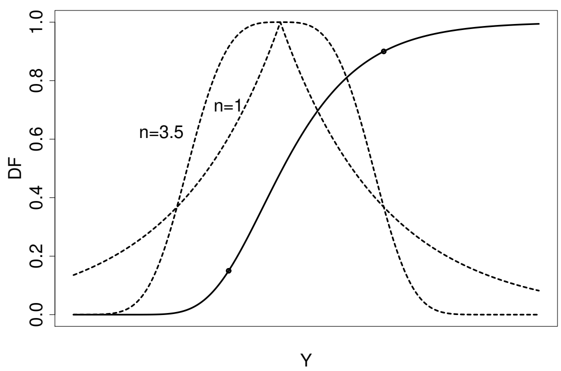

Figure 1: Harrington's one- and two-sided DFs with n as in (1). Predefined points (Y_i, d_i) for one-sided DF are marked.

The parameter n_i is to be chosen so that the resulting kurtosis of the function adequately meets the expert's preferences.

2. **One-Sided Specification:** The one-sided DF uses a special form of the Gompertz-Curve:

$$d_i(Y_i') = e^{-e^{-Y_i'}}, \qquad i = 1, \ldots, k, \tag{3}$$

whereby the kurtosis of the function is determined by the solution of a system of two linear equations that require two values of Y_i and associated values of d_i using

$$Y_i' \;=\; -[\ln(-\ln d_i)] = b_{0i} + b_{1i} Y_i, \qquad i = 1, \ldots, k. \tag{4}$$

The DI combines the k individual desirabilities into one overall quality value by

$$D := (\prod_{i=1}^{k} d_i)^{1/k} \text{ or as a modification of Harrington's approach} \tag{5}$$

$$D := \min_{i=1,\ldots,k} d_i \quad ([\text{KIM00}]). \tag{6}$$

A central element of the approach proposed is the knowledge of the distribution of the DI. In [WEB03] the distributions of the above two types of DIs, namely the geometric mean (5) and the minimum of the DFs (6) based on Harrington's one-sided or two-sided DFs are derived. When using the geometric mean an approximative approach arises as most suitable for the one-sided case, whereas for the two-sided case the distribution of the DI is made available only for two quality measures Y_i (i=1,2) and $n_i = 1\ \forall i$.

As the proposed procedure is based on the distribution function of the DI, as a review only this is presented in the following for different types of DIs.

Theorem 1 (DI Geometric Mean) *Given k quality measures Y_i ($i = 1, \ldots, k$) with $Y_i \sim \mathcal{N}(\mu_i, \sigma_i^2)$ and DFs d_i (1) resp. (3), the DI defined as $D := (\prod_{i=1}^k d_i)^{1/k}$ has the following distribution function:*

$$
\begin{aligned}
F_{\mathcal{D}}(D) &\approx 1 - \Phi\left[\frac{\log(k) + \log(-\log(D)) - \mu^*}{\sigma^*}\right] \textit{ with } \mu^* \textit{ and } \sigma^{*2} \textit{as defined in [SCH82]} \\
&\quad \textit{resp. [WEB03] in the one-sided case,} \\
&\quad \textit{and in the two-sided case for } k = 2 \textit{ and } n_i = 1\ (i = 1, 2) \\
F_{\mathcal{D}}(D) &= \int_0^D f_{\mathcal{D}}(D) d(D) \textit{ with} \\
f_{\mathcal{D}}(D) &= \frac{\sqrt{2}}{2D\sqrt{\pi(\tilde{\sigma_2}^2 + \tilde{\sigma_1}^2)}} \cdot \left(exp\left(-\frac{(-2\log(D) - \tilde{\mu_1} - \tilde{\mu_2})^2}{2(\tilde{\sigma_2}^2 + \tilde{\sigma_1}^2)} \right) \right. \\
&\quad \cdot erf\left(\frac{((-2\log(D))\tilde{\sigma_2}^2 - \tilde{\mu_1}\tilde{\sigma_2}^2 + \tilde{\mu_2}\tilde{\sigma_1}^2)}{\tilde{\sigma_2}\tilde{\sigma_1}\sqrt{2}\sqrt{\tilde{\sigma_2}^2 + \tilde{\sigma_1}^2}} \right) \\
&\quad + exp\left(-\frac{(-2\log(D) - \tilde{\mu_1} + \tilde{\mu_2})^2}{2(\tilde{\sigma_2}^2 + \tilde{\sigma_1}^2)} \right) erf\left(\frac{((-2\log(D))\tilde{\sigma_2}^2 - \tilde{\mu_1}\tilde{\sigma_2}^2 - \tilde{\mu_2}\tilde{\sigma_1}^2)}{\tilde{\sigma_2}\tilde{\sigma_1}\sqrt{2}\sqrt{\tilde{\sigma_2}^2 + \tilde{\sigma_1}^2}} \right) \\
&\quad + exp\left(-\frac{(-2\log(D) + \tilde{\mu_1} - \tilde{\mu_2})^2}{2(\tilde{\sigma_2}^2 + \tilde{\sigma_1}^2)} \right) erf\left(\frac{((-2\log(D))\tilde{\sigma_2}^2 + \tilde{\mu_1}\tilde{\sigma_2}^2 + \tilde{\mu_2}\tilde{\sigma_1}^2)}{\tilde{\sigma_2}\tilde{\sigma_1}\sqrt{2}\sqrt{\tilde{\sigma_2}^2 + \tilde{\sigma_1}^2}} \right) \\
&\quad + exp\left(-\frac{(-2\log(D) + \tilde{\mu_1} + \tilde{\mu_2})^2}{2(\tilde{\sigma_2}^2 + \tilde{\sigma_1}^2)} \right) erf\left(\frac{((-2\log(D))\tilde{\sigma_2}^2 + \tilde{\mu_1}\tilde{\sigma_2}^2 - \tilde{\mu_2}\tilde{\sigma_1}^2)}{\tilde{\sigma_2}\tilde{\sigma_1}\sqrt{2}\sqrt{\tilde{\sigma_2}^2 + \tilde{\sigma_1}^2}} \right) \\
&\quad + exp\left(-\frac{(-2\log(D) - \tilde{\mu_1} - \tilde{\mu_2})^2}{2(\tilde{\sigma_2}^2 + \tilde{\sigma_1}^2)} \right) erf\left(\frac{((-2\log(D))\tilde{\sigma_1}^2 + \tilde{\mu_1}\tilde{\sigma_2}^2 - \tilde{\mu_2}\tilde{\sigma_1}^2)}{\tilde{\sigma_2}\tilde{\sigma_1}\sqrt{2}\sqrt{\tilde{\sigma_2}^2 + \tilde{\sigma_1}^2}} \right) \\
&\quad + exp\left(-\frac{(-2\log(D) - \tilde{\mu_1} + \tilde{\mu_2})^2}{2(\tilde{\sigma_2}^2 + \tilde{\sigma_1}^2)} \right) erf\left(\frac{((-2\log(D))\tilde{\sigma_1}^2 + \tilde{\mu_1}\tilde{\sigma_2}^2 + \tilde{\mu_2}\tilde{\sigma_1}^2)}{\tilde{\sigma_2}\tilde{\sigma_1}\sqrt{2}\sqrt{\tilde{\sigma_2}^2 + \tilde{\sigma_1}^2}} \right) \\
&\quad + exp\left(-\frac{(-2\log(D) + \tilde{\mu_1} - \tilde{\mu_2})^2}{2(\tilde{\sigma_2}^2 + \tilde{\sigma_1}^2)} \right) erf\left(\frac{((-2\log(D))\tilde{\sigma_1}^2 - \tilde{\mu_1}\tilde{\sigma_2}^2 - \tilde{\mu_2}\tilde{\sigma_1}^2)}{\tilde{\sigma_2}\tilde{\sigma_1}\sqrt{2}\sqrt{\tilde{\sigma_2}^2 + \tilde{\sigma_1}^2}} \right) \\
&\quad \left. + exp\left(-\frac{(-2\log(D) + \tilde{\mu_1} + \tilde{\mu_2})^2}{2(\tilde{\sigma_2}^2 + \tilde{\sigma_1}^2)} \right) erf\left(\frac{((-2\log(D))\tilde{\sigma_1}^2 - \tilde{\mu_1}\tilde{\sigma_2}^2 + \tilde{\mu_2}\tilde{\sigma_1}^2)}{\tilde{\sigma_2}\tilde{\sigma_1}\sqrt{2}\sqrt{\tilde{\sigma_2}^2 + \tilde{\sigma_1}^2}} \right) \right) \\
&\quad \textit{and}
\end{aligned}
$$

$$\begin{aligned}
\tilde{\mu}_i &= \frac{2}{USL_i - LSL_i} \cdot \mu_i - \frac{USL_i + LSL_i}{USL_i - LSL_i} \text{ and } \tilde{\sigma}_i^2 = (\frac{2}{USL_i - LSL_i})^2 \cdot \sigma_i^2; \\
erf(x) &= 2 \cdot \Phi(\sqrt{2}x) - 1 \quad \textit{(Gaussian Error Function)}, \\
\Phi(x) &:= \textit{Distribution function of } \mathcal{N}(0,1).
\end{aligned}$$

When using the minimum of the DFs (6) as a DI the distribution function of the DI comes out as follows:

Theorem 2 (DI Minimum DFs) *Given k quality measures Y_i $(i = 1, \ldots, k)$ with $Y_i \sim \mathcal{N}(\mu_i, \sigma_i^2)$ and DFs d_i (1) resp. (3), the DI D defined as $D := \min_{i=1,\ldots,k} d_i$ has the following distribution function:*

$$\begin{aligned}
F_{\mathcal{D}}(D) &= 1 - \prod_{i=1}^{k} \Phi\left[\frac{(\log(-\log(D)) - \tilde{\mu}_i)}{\tilde{\sigma}_i}\right] \quad (\textit{One-sided DFs}) \textit{ with} \\
&\quad \tilde{\mu}_i = -(b_{0i} + b_{1i} \cdot \mu_i) \text{ and } \tilde{\sigma}_i^2 = (b_{1i})^2 \cdot \sigma_i^2, \\
F_{\mathcal{D}}(D) &= 1 - \prod_{i=1}^{k} \left(-1 + \Phi\left[\frac{((-\log(D))^{1/n_i} - \tilde{\mu}_i)}{\tilde{\sigma}_i}\right] + \Phi\left[\frac{((-\log(D))^{1/n_i} + \tilde{\mu}_i)}{\tilde{\sigma}_i}\right]\right) \\
&\quad (\textit{Two-sided DFs }) \textit{ with } \tilde{\mu}_i \textit{ and } \tilde{\sigma}_i^2 \textit{ as defined in Theorem 1.}
\end{aligned}$$

In the course of time some alternative DFs were introduced (e.g. [DER80], [CAS96], [NOB00]), the most important one in form of more flexible DFs that allow nonsymmetric specifications around the target value ([DER80]). The procedure presented in the following chapter in principle can be applied to all kind of DFs and DIs if the distribution of the DI is known or has been approximated accurately enough. We focus on Harrington's DFs as so far only for these an analytical representation for the distribution of the DI exists.

3 Overview: Stepwise Approach

As a starting point a process is assumed, which was optimized regarding k quality measures $Y_1, \ldots, Y_k$ using a DI D and Harrington's DFs (1) resp. (3). Optimal Levels $X_1^{opt}, ..., X_n^{opt}$ of the process influencing factors $X_1, ..., X_n$ are therefore assumed to be given, which have been determined via design of experiment methods and nonlinear optimization techniques. Usually the optimization problem is stated as

$$\min_{X_1,\ldots,X_n \in F} -\hat{D}(X_1, \ldots, X_n) = -D(d_1(E(Y_1)), \ldots, d_n(E(Y_n))), \tag{7}$$

with F specifying the domain of $X_1, \ldots, X_n$ and $Y_i = f(X_1, \ldots, X_n, \varepsilon_i)$ ($\varepsilon_i \sim \mathcal{N}(0, \sigma_i^2)$) determined by polynomial models resulting from design of experiment methods. By taking the expectation $E(Y_i)$ and thus ignoring the variance of the error term biased and non-optimal optimization results may occur ([STE00]). Therefore a more appropriate approach is the optimization problem

$$\min_{X_1,\ldots,X_n \in F} -E(D(X_1, \ldots, X_n)) = -E(D(d_1(Y_1), \ldots, d_n(Y_n))), \tag{8}$$

which can be handled knowing the distribution of the Desirability Index and simultaneously taking into account the model uncertainty of the design of experiment phase. This optimization approach is therefore used in the examples of the following chapters. A detailed overview of the advantages and drawbacks of the usual optimization procedures applied is given in [STE00].

Using the levels $X_1^{opt}, ..., X_n^{opt}$ the expectation of D as well as the respective prediction interval can be calculated based on its distribution in order to measure the uncertainty of the optimization result. In order to determine how slight changes of the influence factors X_i^{opt} ($i \in 1, \ldots, n$) affect the probability that the prediction interval covers the realizations of the DI, the following **procedure** was developed, which is illustrated via exemplary practical cases in the next chapters. Note that a simulation-based procedure is used due to the very complicated distribution functions of the DI. An analytical approach therefore seems to be impossible.

1. At first determine the distribution function $F_{\mathcal{D}}(D)$ of the DI D (see Theorem 1 resp. 2) for $Y_i \sim \mathcal{N}(\mu_i, \sigma_i^2)$ ($i = 1, ..., k$) resulting from model building in the design of experiment phase, where polynomial models are calculated in order to reflect the relationship between the process influencing factors and the quality measures using linear regression techniques (see [WEI95] or [WEI99] for a review).

2. Compute $[Q_{0.025}, Q_{0.975}]$ as a prediction interval for D, which covers the true value of the DI in the optimum with a probability of 95 %, where Q_α is the α-%-quantile of $F_{\mathcal{D}}(D)$. By means of this the uncertainty of the optimization of the DI is expressed.

3. Select the kind of influence factors which are intended to be varied in predefined intervals $[X_i^{min}, X_i^{max}]$ in order to determine the effect on the DI and specify the step width within the intervals. Usually only selective influence factors are chosen, for which slight modifications would be more convenient in the process flow.

4. Determine the distribution function $F_{\mathcal{D}_{shift}}(D_{shift})$ for each combination of shifted influence factors (i.e. $Y_i \sim \mathcal{N}(\mu_i + c_i, \sigma_i^2)$), where D_{shift} is the DI when shifted influence factors are used, c_i caused by shifts in X_i.

5. Compute the probability that D is yet covered by the original prediction interval

$$\begin{aligned} P_{int} &:= P(D_{shift} \in [Q_{0.025}, Q_{0.975}] \,|\, Y_i \sim \mathcal{N}(\mu_i + c_i, \sigma_i^2)\,\forall\, i) \\ &= F_{\mathcal{D}_{shift}}(Q_{0.975}) - F_{\mathcal{D}_{shift}}(Q_{0.025}). \end{aligned}$$

   For visualizing the resulting probability surface generate a plot (influence factors vs. P_{int}) if up to two influence factors have been selected in Step 3. Otherwise the shift of the remaining factors has to be set to a constant value and usually several different plots have to be prepared.

6. Specify lower limit P_{min} as the least acceptable value of P_{int} and generate a plot as above with the restriction $P_{int} > P_{min}$ and a table with all combinations of shifts of the influence factors which lead to a value of P_{int} in this region.

7. Create a plot that visualizes the factor region(s) which result in an acceptable probability that D will be covered by the initially computed interval $[Q_{0.025}, Q_{0.975}]$ as in Step 1. Therefore the influence factor regions which fulfill the condition $P_{int} > P_{min}$ are plotted against each other.

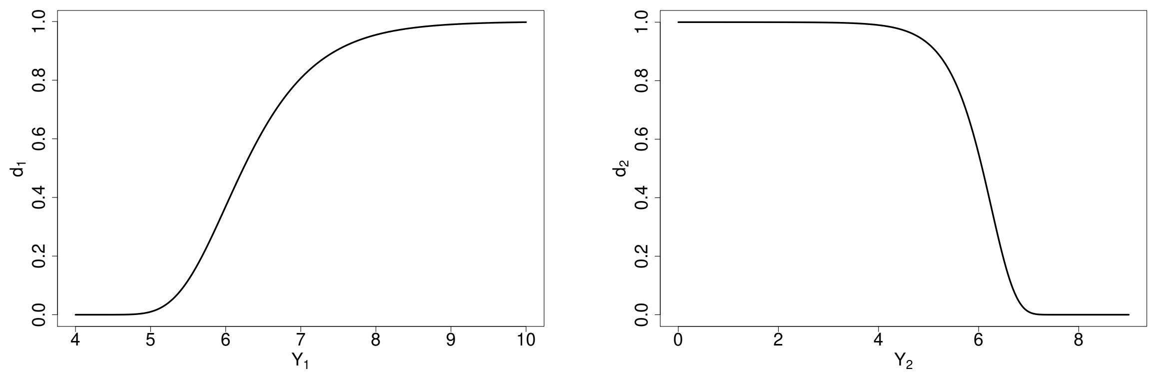

Figure 2: Desirability Functions of flavor (Y_1) and price (Y_2)

4 Example I: Fruit Juice Mixture

A fruit juice mixture consisting of watermelon (X_1)-, pineapple (X_2)-, orange (X_3)- and grapefruit-juice (X_4) has to be optimized regarding the quality measures flavor (Y_1), measured on a scale from 0 to 10, and price (Y_2), measured in Euros (see [WEI99], p. 177). For both quality measures Harrington's one-sided desirability functions d_i (i=1,2) as in (3) are utilized in order to reflect the expert's preferences. As displayed in Fig. 2 maximization of flavor while simultaneously minimizing the price is desired.

For optimization purposes of the DI $D := (\prod_{i=1}^{2} d_i)^{1/2}$ design of experiment methods were used to determine polynomial models reflecting the relationship between the proportions of the influence factors $X_1, \ldots, X_4$ and the quality measures on the side-condition $\sum_{i=1}^{4} X_i = 100$ (%):

$$\hat{Y_1} = 4.713 - 0.0927 \cdot X_1 + 0.0590 \cdot X_3 + 0.0933 \cdot X_4 \quad (9)$$

$$\text{with standard deviation } sd_1 = 0.288, \quad (10)$$

$$\hat{Y_2} = 3.797 - 0.0333 \cdot X_1 + 0.0212 \cdot X_3 + 0.0585 \cdot X_4 \text{ with } sd_2 = 0.239. \quad (11)$$

Thus assuming validity of these models, $Y_i \sim \mathcal{N}(\mu_i, \sigma_i^2)$ with $\mu_i = \hat{Y_i}$ and $\sigma_i = sd_i$ as specified in (9) and (11), therefore the approximative distribution of the resulting DI can be derived as follows using the results of [WEB03]:

$$f_{\mathcal{D}}(D) \approx -\frac{1}{\sqrt{2\pi} \cdot \sigma^* \cdot \log(D) \cdot D} \cdot \exp\left[-\frac{1}{2\sigma^{*2}}(\log(-2 \cdot \log(D)) - \mu^*)^2\right] \quad (12)$$

with μ^* and σ^{*2} as defined in [WEB03] resp. [SCH82] and

No.	X_1	X_2	X_3	X_4	$E(D)$	$D(\hat{Y}_1, \hat{Y}_2)$
1	35	10	55	0	3.7 E-17	2.8 E-91
2	30	3	0	67	0.244	0.226
3	68	7	25	0	2.5 E-82	0
4	30	3	0	67	0.244	0.226
5	30	20	50	0	1.1 E-07	9.3 E-19
6	55	20	0	25	1.4 E-07	2.4 E-18
7	30	20	0	50	0.628	0.647
8	30	3	67	0	1.4 E-16	1.6 E-84
9	68	7	0	25	7.5 E-30	0

Table 1: Expected values $E(D)$ of the DI as well as $D(\hat{Y}_1, \hat{Y}_2)$ for each experiment.

$$F_{\mathcal{D}}(D) \approx 1 - \Phi\left[\frac{\log(2) + \log(-\log(D)) - \mu^*}{\sigma^*}\right]. \tag{13}$$

By means of the knowledge of this distribution the expected value of the DI can be optimized, which can be seen as an improved optimization procedure for the DI as in the classic approach the DI is calculated based on the values of $\hat{Y}_i$ and therefore the model uncertainty is not taken into account (see [STE00]). Thus for each experiment the expected value $E(D)$ of the DI is determined as displayed in Table 1. Additionally in comparison the values following the classic approach are displayed so that the differences become obvious. Note that as a side restriction X_3 and X_4 may not be used simultaneously.

These results indicate that exceeding 30 % the proportion of watermelon-juice (X_1) leads to undesirable values of the quality measures. Furthermore experiment 7 is the one with the maximal value of $E(D)$ followed by experiments 2 and 4, which all make use of grapefruit-juice (X_4). Regarding the factor settings of the experiments 2, 4 and 7 a grid search was carried out in order to find the optimal factor settings which lead to the optimal expected value of the DI. As X_2 is not included in the models (9) and (11) — it follows from $\sum_{i=1}^{4} X_i = 100$ % — only X_1 and X_4 are varied on a grid with ranges $10 \leq X_1 \leq 40$ and $30 \leq X_4 \leq 80$ and step width 0.1. The optimal factor settings come out as

$$X_1^{opt} = 30, X_4^{opt} = 50.6 \text{ and } X_2^{opt} = 19.4 \text{ with } E(D_{opt}) = 0.67 \tag{14}$$

$$\text{leading to } \mu^* = -0.25 \text{ and } \sigma^{*2} = 0.105, \tag{15}$$

whereby the following domain restrictions of the influence factors had to be met:

$$30\% \leq X_1 \leq 100\%, \tag{16}$$

$$X_3 = 0\% \vee X_4 = 0\%, \tag{17}$$

$$0\% \leq X_2 \leq 20\% \Leftrightarrow X_1 + X_3 \text{ resp. } X_4 \geq 80\%, \tag{18}$$

$$X_1 + X_2 \leq 75\% \Leftrightarrow 25\% \leq X_3 \text{ resp. } X_4 \text{ and} \tag{19}$$

$$0.1 \cdot X_1 \leq X_2. \tag{20}$$

Following the procedure described in Chapter 3 the distribution function of the DI is determined based on (13) and the optimal factor settings (14). The 95 % prediction-interval for the true DI in the optimum comes out as

$$[Q_{0.025}, Q_{0.975}] = [0.66, 0.89] \text{ with } Q_\alpha := \alpha \text{ \%-quantile of } F_{\mathcal{D}}(D). \tag{21}$$

Whereas the resulting interval reflects the uncertainty of D_{opt}, in practice an analysis of the effects of varying the optimal factor levels can also be of interest, which somehow reflects the uncertainty of the levels regarding D_{opt}. For example in a production process a slight change of one influence factor may lead to lower production costs or may just be more convenient in the process flow.
As a first example only the effect of shifts of X_1 is focussed assuming that the proportion of X_4 is not affected. Of course this also leads to a modification of X_2 but X_2 is not included in the models (9) and (11). For all possible shifts of X_1 in the interval $[-30, 70]$ and step width 0.01, ignoring the restriction $\sum_{i=1}^{4} X_i = 100\%$ at the moment, the distribution function of the DI is calculated and the probability that the interval (21) still covers the values of the DI is determined as

$$P_{int} := P(D_{shift} \in [Q_{0.025}, Q_{0.975}] \,|\, Y_i \sim \mathcal{N}(\mu_i + c_i, \sigma_i^2)) = F_{\mathcal{D}_{shift}}(Q_{0.975}) - F_{\mathcal{D}_{shift}}(Q_{0.025}), \tag{22}$$

where D_{shift} is the DI when shifted values of X_1 are used, i.e $Y_i \sim \mathcal{N}(\mu_i + c_i, \sigma_i^2)$.

Fig. 3 illustrates the shape of this probability in the range X_1 is shifted. Additionally lines are included which reflect the restrictions listed in (16)-(20). The gray-shaded region mirrors the domain in which all these restrictions are met. Thus the part of the displayed curve falling inside this region indicates the range in which X_1 can be varied so that all restrictions are met and the desired minimal probability P_{min} is exceeded, which was

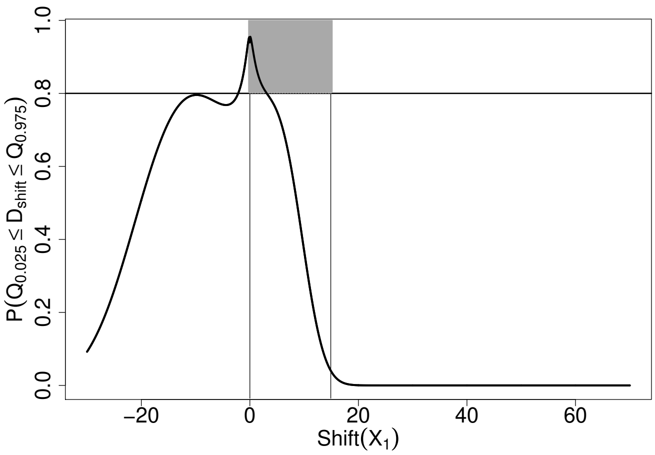

Figure 3: Probability that $[Q_{0.025}, Q_{0.975}]$ covers the values of the DI when X_1 is shifted

chosen as $P_{min} = 0.8$.

In case shifts of both influence factors X_1 and X_4 are of interest the procedure is carried out analogously. For all combinations of shifts in the ranges $[-30, 70]$ (X_1) and $[-50.6, 49.4]$ (X_4) with step width 0.2, again ignoring the restriction $\sum_{i=1}^{4} X_i = 100\%$ at the moment, the probabilities as in (22) are computed. Fig. 4 visualizes P_{int} plotted against the shifts of X_1 and X_4, where in this stage only the restriction $\sum_{i=1}^{4} X_i = 100$ % is considered. Furthermore in Fig. 4 the same surface when the condition $P_{int} \geq P_{min} = 0.8$ is satisfied is shown below.

For the purpose of including all restrictions (16)-(20) and in order to get a better overview regarding the range of possible shifts of the influence factors X_1 and X_4, in Fig. 5 X_1 and X_4 are plotted against each other where the lines reveal the restrictions mentioned. As in the example above the gray-shaded region reflects the region in which all restrictions are met. The black area inside again reflects the range of possible shifts of the influence factors X_1 and X_4 with regard to meeting all restrictions and exceeding the desired minimal probability $P_{min} = 0.8$. Thus due to the factor restrictions only a quite small part of the theoretically possible range is allowed for shifting.

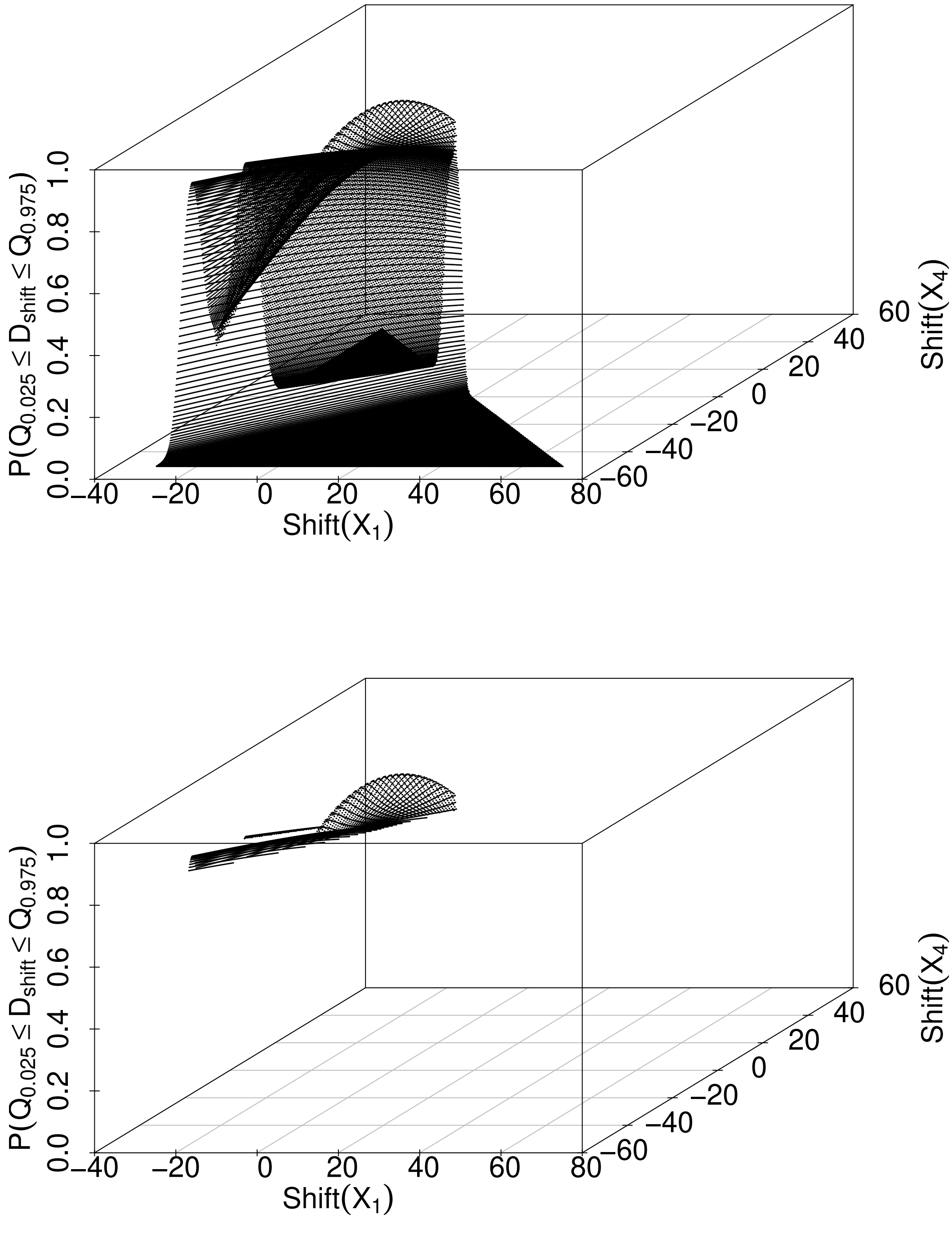

Figure 4: Probability that $[Q_{0.025}, Q_{0.975}]$ covers the values of the DI when X_1 and X_4 are shifted; below: Same Surface with $P(Q_{0.025} \leq D_{shift} \leq Q_{0.975}) \geq P_{min} = 0.8$.

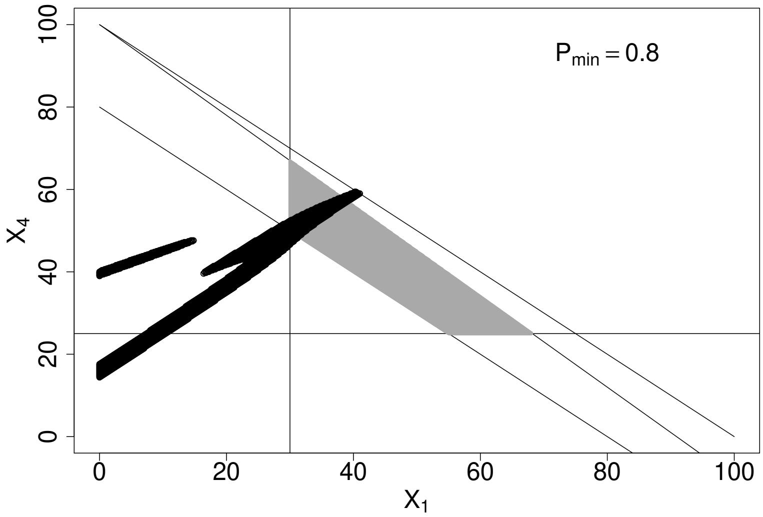

Figure 5: Ranges of X_1 and X_4 so that $[Q_{0.025}, Q_{0.975}]$ covers the value of the DI with a probability of at least 80 %.

5 Example II: Tire Tread Compound

In the following we revert to the example used by [DER80], which is modified in terms of differently specified DFs. An optimal compound of a tire tread, consisting of "Hydrated silica" (X_1), "Silane coupling agent" (X_2) and "Sulfur" (X_3) has to be found, where its quality is measured by the variables "PICO Abrasion Index" (Y_1), "200%-Modulus" (Y_2), "Elongation at Break" (Y_3) and "Hardness" (Y_4). The assumed related one-sided DFs as in (3), which express the desirability of different values of Y_1-Y_4, are displayed in Fig. 6. In this case another kind of DI is used, namely $D := \min_{i=1,\ldots,4} d_i$. That implies a "maximin-approach", i.e. the minimum desirability is to be maximized over time. The optimization of the DI follows the same procedure as outlined in Chapter 4 using the models

$$\begin{aligned} \hat{Y_1} &= 139.1 + 16.5X_1 + 17.9X_2 + 10.9X_3 - 4X_1^2 - 3.5X_2^2 - 1.6X_3^2 + 5.1X_1X_2 \\ &\quad +7.1X_1X_3 + 7.9X_2X_3 \text{ with } sd_1 = 5.6, \qquad (23) \\ \hat{Y_2} &= 1261.1 + 268.2X_1 + 246.5X_2 + 139.5X_3 - 83.6X_1^2 - 124.8X_2^2 + 199.2X_3^2 \\ &\quad +69.4X_1X_2 + 94.1X_1X_3 + 104.4X_2X_3 \text{ with } sd_2 = 328.7, \qquad (24) \\ \hat{Y_3} &= 400.4 - 99.7X_1 - 31.4X_2 - 73.9X_3 + 7.9X_1^2 + 17.3X_2^2 + 0.4X_3^2 + 8.8X_1X_2 \\ &\quad +6.3X_1X_3 + 1.3X_2X_3 \text{ with } sd_3 = 20.6 \text{ and} \qquad (25) \end{aligned}$$

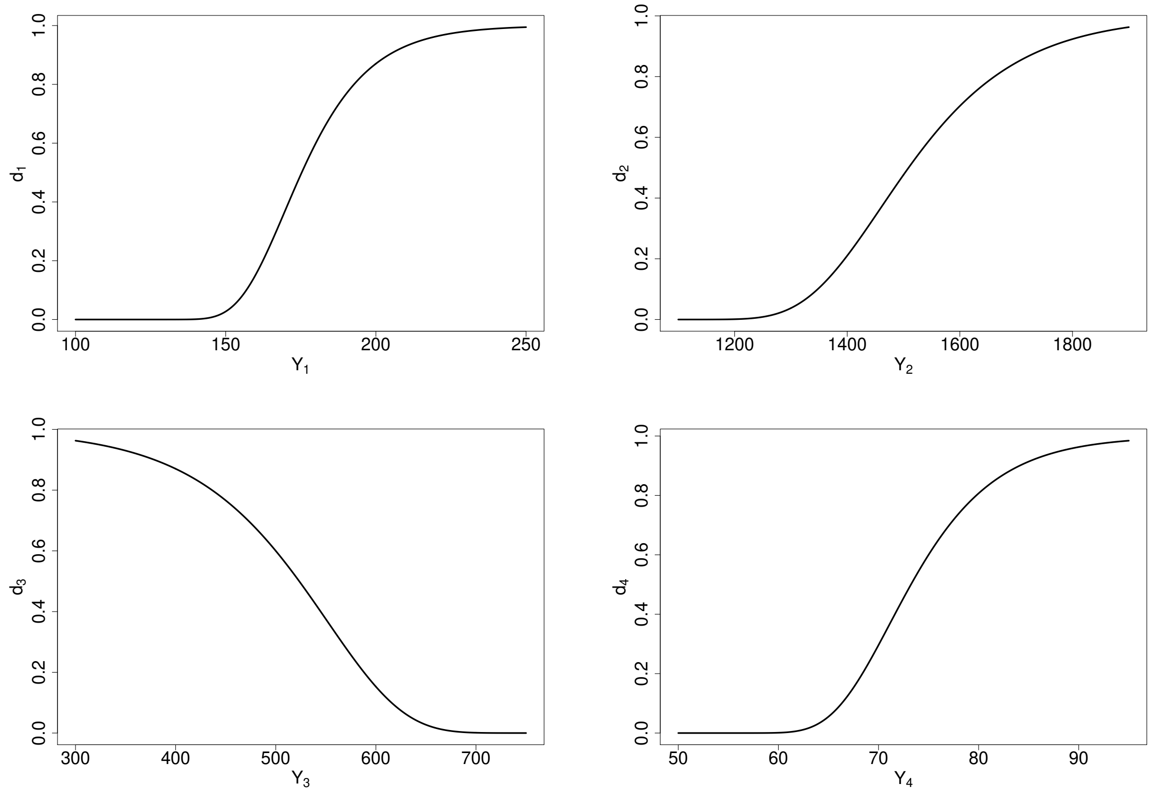

Figure 6: Desirability Functions of PICO Abrasion Index(Y_1), 200%-Modulus (Y_2), Elongation at Break (Y_3) and Hardness (Y_4)

$$\begin{aligned}\hat{Y_4} &= 68.9 - 1.4X_1 + 4.3X_2 + 1.6X_3 + 1.6X_1^2 + 0.1X_2^2 - 0.3X_3^2 - 1.6X_1X_2 \\ &\quad +0.1X_1X_3 - 0.3X_2X_3 \text{ with } sd_4 = 1.27. \end{aligned} \tag{26}$$

Again the mentioned innovated approach of optimizing the expectation of the DI instead of $\hat{D} := \min_{i=1,\ldots,4} d_i(\hat{Y_i})$ is applied, where from [WEB03]

$$E(D) = \int_0^1 -\frac{1}{\log(D)} \sum_{i=1}^{4} \left(\frac{1}{\tilde{\sigma}_i} \phi \left(\frac{\log(-\log(D)) - \tilde{\mu}_i}{\tilde{\sigma}_i} \right) \prod_{\substack{j=1 \\ j \neq i}}^{4} \Phi \left(\frac{\log(-\log(D)) - \tilde{\mu}_j}{\tilde{\sigma}_j} \right) \right) d\,(D) \tag{27}$$

$$\text{with } \tilde{\mu}_i = -(b_{0i} + b_{1i} \cdot \mu_i), \tilde{\sigma}_i^2 = (b_{1i})^2 \cdot \sigma_i^2 \text{ and} \tag{28}$$

$\phi(x)$ resp. $\Phi(x)$: Density resp. Distribution function of $\mathcal{N}(0,1)$.

A grid search on coded influence factors was carried out, where we assumed possible ranges $-2 \leq X_i \leq 2$ $(i = 1, \ldots, 3)$ resulting in the optimal influence factor levels

$$X_1^{opt} = 0.7,\ X_2^{opt} = 1.3 \text{ and } X_3^{opt} = 1.3 \text{ with } E(D_{opt}) = 0.577. \tag{29}$$

Taking into account the uncertainty of the optimization resulting from the model errors in (23)-(26) and starting with the procedure described in Chapter 3, the 95%-prediction interval for D_{opt} is calculated based on

$$F_{\mathcal{D}}(D) = 1 - \prod_{i=1}^{4} \Phi \left[\frac{(\log(-\log(D)) - \tilde{\mu}_i)}{\tilde{\sigma}_i} \right] \text{ with } \tilde{\mu}_i \text{ and } \tilde{\sigma}_i^2 \text{ as in (28)} \tag{30}$$

(Theorem 2) and comes out as

$$[Q_{0.025}, Q_{0.975}] = [0.43, 0.70] \text{ with } Q_\alpha := \alpha\% - \text{quantile of } F_{\mathcal{D}}(D). \tag{31}$$

The influence factors X_1 and X_3 were selected for shifting in their full domain of $-2 \leq X_i \leq 2$ $(i = 1, 3)$ in order to measure the effect onto D_{opt}. Analogously to the example in Chapter 4 hereby the uncertainty of the optimal factor levels regarding D_{opt} is determined using equation (22). In Fig. 7 the shifted values of X_1 and X_3 are plotted against the probability P_{int} that the prediction interval as in (31) still covers the realizations of the DI. Assuming that at least a probability of 80% has to be achieved the lower graphic of Fig. 7 shows the range of P_{int} that meets this condition.

In order to facilitate the analysis of this range, in Fig. 8 the respective values of X_1 and X_3 are plotted against each other. In this case no additional restrictions regarding the influence factors have to be taken into account. It becomes obvious that a quite wide scope of possible shifts of X_1 and X_3 exists.

6 Summary and Conclusion

Considering the examples in Chapters 4 and 5 it can be seen that the method described provides an appropriate means for analyzing and visualizing the regions of possible shifts of influence factors which lead to an acceptable probability that the DI will be covered by the prediction interval constructed using the optimal factor settings. As an innovative approach the distribution of the DI is taken into account. But it is also obvious that this analysis becomes more and more complicated the more influence factors are allowed for shifting as

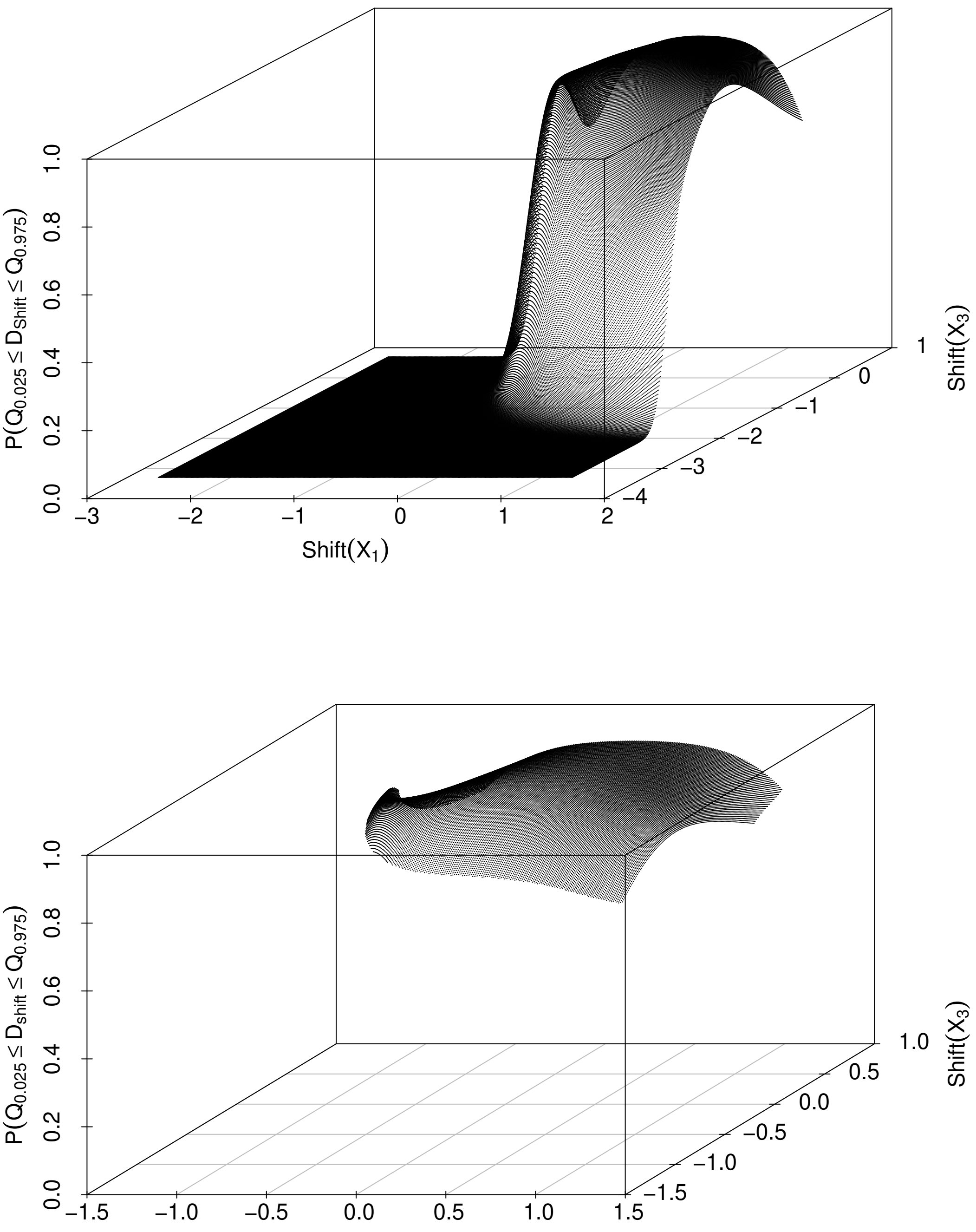

Figure 7: Probability that $[Q_{0.025}, Q_{0.975}]$ covers the values of the DI when X_1 and X_3 are shifted;below: Same Surface with $P(Q_{0.025} \leq D_{shift} \leq Q_{0.975}) \geq P_{min} = 0.8$.

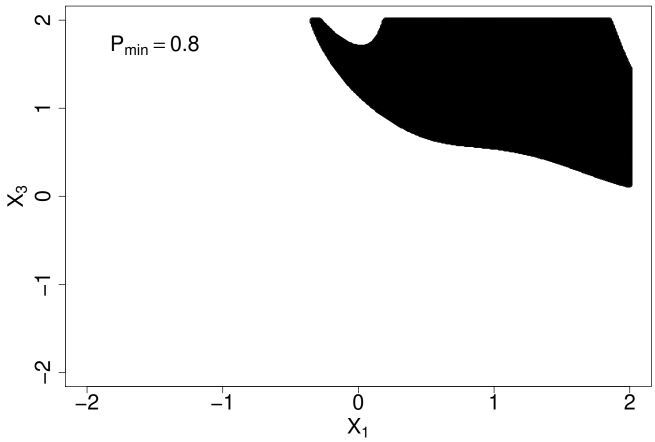

Figure 8: Ranges of X_1 and X_3 so that $[Q_{0.025}, Q_{0.975}]$ covers the values of the DI with a probability of at least 80 %.

- graphical illustration is difficult for more than two factors. From three dimensions on plots as in Fig. 4 can only be generated by fixing the remaining factors to a constant value. Therefore in this case tables should be provided additionally.
- the resulting region does not need to be cohesive as can be seen in Chapter 4 and
- the number of possible combinations of shifted influence factors which lead to a DI within the desired prediction interval heavily increases.

Therefore and because of very complex density and distribution functions of the DI a general analytical approach will be highly complicated if not impossible so that the proposed procedure will provide appropriate assistance in practice.
In case the distribution of other types of is known, the procedure can be applied analogously without any modification.

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