



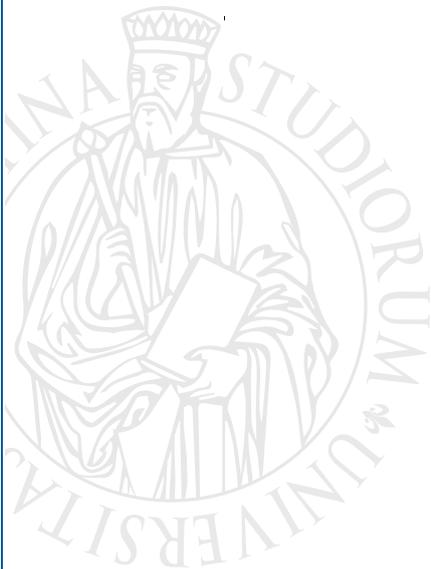
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**Split-plot designs and
multi-response process optimization:
a comparison between two approaches**

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SPLIT-PLOT DESIGNS AND MULTI-RESPONSE PROCESS OPTIMIZATION: A COMPARISON BETWEEN TWO APPROACHES

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Abstract: Nowadays split-plot designs play a crucial role in the technological field, both for their flexibility when applying a robust design approach and in relation to the modelling step, by considering Mixed Response Surface models and/or the class of Generalized Linear Mixed Models-GLMMs. In this paper, a split-plot design is studied in a process optimization scenario involving several response variables, e.g., a multi-response situation, in which a comparison between two optimization methods is performed. More precisely, by considering a real case study related to the improvement of a measurement process of a Numerical-Control machine (N/C machine) to measure dental implants, the optimization is carried out with the Pareto front approach and then compared with other analytical methods also used to optimize. The final discussion considers the advantages and disadvantages (of application) for both methods.

1. Introduction

Process optimization is a key step for statistical quality control, and its relevance has increased since the long and fruitful scientific debate related to the Taguchi’s two step procedure for robust design (Nair, 1992). Currently, the robust design approach involves an approach composed of 3 key-steps: experimental design, modeling, and optimization. The key to successful implementation is to incorporate noise factors involved in the experimental planning, which are then modeled and chosen based on a suitable analysis in the subsequent optimization. Therefore, we extend the concept of process optimization to robust process optimization, in which control and noise variables are jointly studied to achieve the best set of control factor levels to makes it possible to simultaneously reach the target value and minimize the process variability with a robust configuration. In this context, the process

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optimization step strictly depends on the chosen designed experiment and the class of statistical models applied. Specifically, we can use Response Surface Methodology (RSM) approaches (Myers et al., 2016), or plan a designed experiment outside the RSM context, and then model the experimental data with a more flexible class of statistical models, e.g. Generalized Linear Models-GLMs (McCullagh and Nelder, 1989; Nelder and Lee, 1991; Lee and Nelder, 2003) or Generalized Linear Mixed Models-GLMMs (Dror and Steinberg, 2006; Robinson et al., 2006; Berni and Bertocci, 2018).

Undoubtedly, the choices of designed experiment and modelling are related to the process to be studied and optimized, and the same reasoning should be applied when deciding on the number and type of response variables to consider. In fact, the multi-response situation should arise if, and only if, the real scenario shows that several response variables are naturally involved and are important to the whole process under study. If this is not the case, then collinearity, which may often arise among responses (Box et al., 1973; Chiao and Hamada, 2001), can lead to complications with analysis and optimization.

A further issue in a multi-response situation appears during the optimization process, since it is not feasible in practical terms to reach an ideal optimum simultaneously for all the responses. In this context many authors, starting from Derringer and Suich (1980), Khuri and Conlon (1981), have proposed methods to achieve an optimal solution as a compromise or balance between several response variables, Del Castillo et al. (1996), Copeland and Nelson (1996).

In addition, a further issue concerns the conjunction of a multi-response case and the dual response approach. In fact, optimization must take care of a double feature: the simultaneous optimization of several variables, jointly with the consideration of two statistical models, e.g., location and dispersion. Indeed, we should make a distinction when considering the differences between the dual response approach, or, alternatively, when a single response model, opportunely weighted for dispersion, is applied in a “true” multi-response case. In the latter case, the application of analytical methods for optimizing can give fruitful and satisfactory results, particularly by considering recent developments involving noise factors.

To this end, several optimization measures are suggested in the literature (Lin and Tu, 1995; Tang and Xu, 2002). The Pareto front approach is a multi-response optimization method of the analytical-qualitative type, consisting of two sequential steps: a first step based on objective conditions identifies the dominant solutions, and a second step based on selecting the best solution subjective conditions that match the experimenters’ priorities (Lu et al., 2011; Chapman et al., 2014a).

In this study, data from a split-plot experiment (Berni, 2010) are optimized through the Pareto front approach (Chapman et al., 2014b), and following, the results obtained are compared with a proposal of the analytical optimization method. More specifically, both methods are compared and discussed through an empirical example in the orthodontic field, in order to improve the accuracy in the measurements of a Numerical Control machine (N/C machine), which provides some automatic control of machining tools.

This paper is structured as follows: in Section 2, the basics of split-plot designs are reviewed and briefly illustrated. Section 3 provides a short description of both optimization methods, and Section 4 presents the case-study including optimization results. The paper concludes with discussion and final remarks.

2. Split-plot designs for statistical quality control: a review

The split-plot design (Cochran and Cox, 1957) has been developed and characterized over the years, becoming a type of designed experiment that is widely used in industrial, technological, and environmental fields.

In relation to the developments that the fractional factorial designs and the Response Surface Methodology-RSM have had since the 1980s, the split-plot design has experienced a particular renewal (Box and Jones, 1992), expounding its theoretical features, specific usefulness for the statistical quality control and robust design concepts, which were initially introduced by Genichi Taguchi, (Nair, 1992). In this context, the two seminal papers of Vining and Myers (1990) and Myers et al. (1992) extended the two-step procedure into the dual-response approach, and the combined-array is considered as a milestone for recent developments and robust process optimization. Within this methodological framework, the split-plot design plays a central role, starting from the tutorial by Box and Jones (1992), in which the authors proposed the split-plot design as an efficient alternative to Taguchi's product-array for a robust design approach, also in a fractional factorial setting (Bisgaard, 2000).

Currently, split-plot designs have great relevance for recent developments in robust process optimization, expounding the initial concept of the robust design approach, with a focus on the design and modeling steps (Kowalski and Potcner, 2003; Kowalski et al., 2007; Jones and Nachtsheim, 2009).

Furthermore, the split-plot design has been revised and included in the class of *crossed bi-randomized* experimental designs (Myers et al., 2016), given the possibility of including environmental/noise factors as Whole-Plot (WP) factors and process factors as Sub-Plot (SP)

factors. The standard allocation of the environmental/noise factors as WP is certainly a solution that allows for the most accurate estimate of the factors of interest, as well as the estimate of the 1st order interactions, e.g., the 1st order interaction between a WP factor (for example a noise factor) with a SP (process) factor, in order to perform a robust design (Berni et al., 2020). This structure is also natural in many applications, given the generally high cost of controlling the noise factors in production.

Nevertheless, planning a split-plot design in a RSM context implies that all the variables included in the experimental plan (irrespective of whether WP or SP factors) must be quantitative in nature. In fact, the consideration of a qualitative process variable implies the carrying out of the optimization step conditioned to the levels of the categorical variable involved. To this end, the inclusion of a qualitative variable should be limited (Berni, 2010) or restricted to two levels where they can be treated as quantitative in standard models. Moreover, the presence of measurable noise factors, involved as random effects, is possible when the split-plot design is applied through mixed RS models, or alternatively, through GLMMs.

Additional recent developments in the literature have contributed significantly to the inclusion of the split-plot design in the RSM, showing the equivalence of *Ordinary Least Squares* (OLS) with *Generalized Least Squares* (GLS) for split-plot designs and mixed-RSM (Vining et al., 2005); and improving inference issues (Vining and Kowalski, 2008).

2.1. The split-plot design: theory

When working with a split-plot design, it is essential to proceed with a primary classification between Whole-Plot (WP) factors and Sub-Plot (SP) factors. It is therefore desirable to carefully evaluate the specific definition of the process (industrial process, laboratory experiment) to be analyzed, considering the exact definition of the response (quantitative) variables, Y . Also, it is necessary to define the role of each variable in the study, in order to plan the split-plot design according to the most efficient arrangement for the specific scenario. This step plays a central role, not only in the attribution of factors as whole-units or sub-units, but also considering the subsequent model estimation, in which each variable, according to its nature (qualitative, discrete quantitative or continuous) has a specific role. It is also key to clarify the distinction between fixed and random effects.

In short, a Whole Unit (WU) is defined by runs where WP factors are manipulated, and the run order of all the WUs is randomized. Subsequently, the Sub-Units (SU), defined

through the combination of levels (runs) of the SP factors, are associated to the WUs and randomized separately.

In this study, we consider a split-plot design in a RSM context. More precisely, we are interested in using a second-order polynomial model with random effects. The response surface (polynomial) model with random effects for the single experimental observation y_u ($u = 1, \dots, n$) and J variables $(x_1, \dots, x_j, \dots, x_J)$ has the following structure:

$$y_u = \beta_0 + f(\mathbf{x}_u)\boldsymbol{\beta} + \mathbf{z}_u\boldsymbol{\gamma} + g(\mathbf{x}_u)\boldsymbol{\Delta}\mathbf{z}'_u + \boldsymbol{\varepsilon}_u \quad (1)$$

where β_0 is the intercept; $\boldsymbol{\beta}$ is the column vector $[p \times 1]$ of the unknown parameters for $p \geq J$; $f(\mathbf{x}_u)$ is a linear and independent function for each \mathbf{x}_u , that is, $f(\mathbf{x}_u) = (x_{u1}, \dots, x_{up})$ in relation to the p 2nd order effects related to the J variables. Therefore, \mathbf{F} is the so-called "extended" matrix of dimension $[n \times p]$; $\boldsymbol{\varepsilon}_u$ is the column vector of the error component. For the random effects, $\mathbf{z}_u = (z_{u1}, \dots, z_{ub})$ is the row vector of binary values (0,1) to describe the presence and structure of the block factors; $\boldsymbol{\gamma} = (\gamma_1, \dots, \gamma_b)$ is the column vector of the unknown coefficients relating to the random effects of dimension $[b \times 1]$. The matrix $\boldsymbol{\Delta}$ is the matrix relating to the first order interactions between polynomial effects (fixed) and random effects. The maximum dimension of $\boldsymbol{\Delta}$ is $[p \times b]$ if the interactions of all fixed effects with random effects are included in model (1). Note that this latter matrix contains the coefficients for evaluating the robust design.

Starting from the model formula (1), we now illustrate the second order polynomial model of response surfaces from a split-plot design, where all variables are quantitative. For further details, see Myers et al. (2016).

Let's consider two sets of factors: i) the set Z for the WP factors, and ii) the set X for J SP factors. This notation assumes that the noise factors are WP random variables. Let $\mathbf{Z}: (\mathbf{z}_1, \dots, \mathbf{z}_i, \dots, \mathbf{z}_I)$ be the set of WP random factors/variables and $\mathbf{X}: (\mathbf{x}_{i1}, \dots, \mathbf{x}_{ij}, \dots, \mathbf{x}_{iJ})$ the set of SP variables/factors.² The 2nd order RS mixed model for a split-plot design, defined for the k -th block ($k = 1, \dots, K$), and u -th observation, is as follows:

$$y_{ijk}(Z, X) = \beta_0 + \boldsymbol{\gamma}'_i\mathbf{z}_i + \boldsymbol{\beta}'_j\mathbf{x}_{ij} + \mathbf{z}'_i\boldsymbol{\Gamma}\mathbf{z}_i + \mathbf{x}'_{ij}\mathbf{B}\mathbf{x}_{ij} + \mathbf{z}'_i\boldsymbol{\Delta}\mathbf{x}_{ij} + \psi_{ik} + \varepsilon_{ijk} \quad (2)$$

where, from formula (1), we note the inclusion of the $\boldsymbol{\Gamma}$ array, related to the coefficients for the 1st order interaction and quadratic terms for the WP variables; the \mathbf{B} array, containing 2nd

² Please note that we are referring to a factor/variable considering that the experimental region (χ) is defined by the factor ranges; a finite number of experimental points, forming the experimental design, is then selected by the experimental region. Following, the model estimation is performed within the whole experimental region, by inferring from a discrete set of points, e.g., the experimental points, to a continuous one.

order coefficients for the fixed effects of SP variables; the matrix $\mathbf{\Delta}$, contains coefficients of the 1st order interaction effects between the WP and SP factors. These are important in a context of robust design evaluation. For the error components, ψ_{ik} is the WP error component, where we assume that $\psi_{ik} \sim iid N(0, \sigma_{\psi}^2)$, while ε_{ijk} is the SP error component, where $\varepsilon_{ijk} \sim iid N(0, \sigma_{\varepsilon}^2)$, and $Cov(\psi_{ik}, \varepsilon_{ijk}) = 0$.

In the model formula (2), the assumptions about the error variances are analogous to assuming that the covariance between two observations belonging to the same WU remains constant across all its observations.

The existence of two error components, with corresponding two error variance components, complicates the application of a split-plot within the RSM context. This issue substantially influences both the estimation of the variance components and the model coefficients.

In the case-study illustrated in Section 4, the multi-response case is related to the optimization involving three split-plot models, one for each response, estimated within a RSM context.

3. Optimization methods

This Section includes a short description of both optimization methods considered. The Pareto front approach (Lu et al., 2011; Chapman et al., 2014a; Chapman et al., 2014b) is then detailed within the case-study, with details specific to the application, including a brief introduction of the analytical method (Section 4.2). For further details see (Berni and Gonnelli, 2006; Berni, 2010; Berni and Burbui, 2014).

3.1. The Pareto front approach

The Pareto front approach is a multi-response analytical-qualitative optimization method, which allows the search for optimum to consider subjective priorities and constraints, such as those due to a company's requirements (for example, costs or technical/engineering specifications). It consists of two sequential steps (Chapman et al., 2014a; Myers et al., 2016; Anderson-Cook, 2017), as outlined below.

Let's start by indicating with \mathcal{X} the entire experimental region; within this region a finite set, possibly a grid, of experimental points, is selected and used to define a Pareto-optimal set. A possible solution is called non-inferior (or Pareto-optimal), if and only if, there is no other combination within the set with the values of all the responses at least as good, and the value of at least one response is strictly better; otherwise, it is called inferior or dominated.

The set of non-inferior (or Pareto-optimal) experimental input combinations is called the Pareto-optimal set, and the corresponding set of vectors for the responses under consideration is known as the Pareto front or frontier. Since the inferior solutions are not rational choices conditional on the choice of responses under consideration, they are not considered further and definitively discarded (Zitzler, 1999; Marler and Arora, 2004; Coello Coello et al., 2007).

Therefore, the Pareto front approach can be summarized with the following two steps:

1. An objective step, where the Pareto-optimal set is identified from the initial set of choices, based on the corresponding estimated response values;
2. A subjective step, in which the experimental points belonging to the Pareto-optimal set are examined and then compared. Only experimental points that provides the best combination of responses are considered as the compromise among all the estimated response values (quantitative considerations). This choice is based on evaluation and incorporation of the priorities/preferences of the company.

It must be noted that several optimal experimental points corresponding to input combinations could be selected, by considering the priorities of different teams (decision-makers) involved in the study. Therefore, the best optimal solution takes the quantitative results and the decision-makers' priorities into account. Moreover, graphical methods are a useful tool for discussion and achieving a consensus among all stakeholders (Anderson-Cook and Lu, 2018).

3.2. The analytical methods for a robust process optimization

When dealing with several response variables, it is generally not feasible in practical terms to reach a simultaneous ideal optimum for each of them with a single input combination. To this end, many authors, starting from the methods suggested by Derringer and Suich (1980) and Khuri and Conlon (1981), have proposed methods to synthesize and optimize the responses, such as Ames et al. (1997), Del Castillo et al. (1996), Rajagopal et al. (2005).

In addition, a further issue emerges when considering the multi-response case and the dual response approach. Here, the simultaneous optimization of several variables jointly with the consideration of two statistical models, e.g., location and dispersion models, increases the complexity and dimensionality of the problem (as introduced in Section 1).

In order to solve the latter issue, which could imply a notable computational burden, analytical optimization methods are simplified starting from the dual approach theory and

the concept of a performance measure (Leon et al., 1987). To this end, we consider a multiplicative relationship between the expected value ($E(Y) = \mu$) and the process variance ($Var(Y) = \sigma^2$) of the response variable. The risk function, defined as the expected value of the corresponding loss function, is expressed as follows:

$$R(x, z) = (\mu - \tau)^2 + f(\mu(x))\sigma^2 \quad (3)$$

Moreover, formula (3) makes it possible to define specific objective functions (Berni and Gonnelli, 2006) to optimize several response variables without separately estimating two statistical models for each response.

More recently, split-plot designs and modelling have been optimized by explicitly involving one model only for each response in a robust process optimization context, in which random effects (noise factors) are also evaluated (Berni and Bertocci, 2018; Berni and Nikiforova, 2021).

We begin by defining a general response surface model, Y_t ($t = 1, \dots, T$), for each of the T dependent variables or responses.

The simultaneous optimization may be performed considering the T estimated surfaces, where each estimated model is evaluated as a single function to be included in the objective function to be optimized.

Therefore, by considering formula (3) and the concept of a dual response approach, we can define the following distance between the estimated surface \hat{Y}_t and the corresponding target value τ_t :

$$S_t(C, X) = (\hat{Y}_t(C, X) - \tau_t)^2$$

Here we consider optimization for a response with a desired target, but the approach can be easily adapted for responses where the goal is to achieve a maximum or minimum value. Subsequently, the minimization on the coded experimental region (χ) is performed through the following expression:

$$\min_{\chi} \left\{ \sum_t S_t(C, X) \right\} \quad (4)$$

The objective function in formula (4) is optimized conditional on the whole experimental region (χ) defined by the process variable ranges (and potentially any limiting constraints for other problems), as well as involving the estimated confidence interval for each random coefficient when random noises are present.

In the following section, we compare two optimization methods described above, e.g., the Pareto front approach (Subsection 3.1), and formula (4), where the goal is to improve the accuracy of the measurement process for a Numerical Control machine (N/C machine) used in the orthodontic field, the measurements of which are analyzed for a generic dental implant.

4. The case study: data description and process optimization

In this Section, a multi-response optimization comparison is made, with a short description of the experimental planning and data from which the data were obtained. For further details see Berni (2010).

4.1. Split-plot design and data description

The aim of the study is to improve the accuracy in measurements for a Numerical Control (N/C) machine, jointly with the reduction of the measuring time. The machine uses a feeler pin with a movable bridge framework to facilitate the positioning of the measured piece, which in our case is a dental implant. The machine needs specific environmental conditions to function properly, all ensured previously (see Berni and Gonnelli, 2006).

In Berni (2010), five response variables $T = 5$ were optimized simultaneously considering formula (4) and related to the different positioning of the feeler pin on the dental implant during the process measurement steps. In this paper we focus on the optimization comparison by involving three key response variables.

The responses, considering the dental implant used to set the measurement process, are as follows (with targets in brackets): maximum circle diameter- $crmax$ ($\tau_1: 3.000$), minimum circle diameter- $crmin$ ($\tau_2: 2.790$), and eccentricity- $eccen$ ($\tau_5: 0.000$). There is no problem with correlation among the three dependent variables, since each type of measurement is carried out as a distinct step; moreover, each response variable is independent from the others during the measurement of the piece. In order to reduce the measuring time, it is possible to intervene on the process phase related to the identification of the cone frustum, identified by three circles (Figure 1), at three different distances. In Figure 1, the frustum of cone is shown by highlighting the three circles used to locate it.

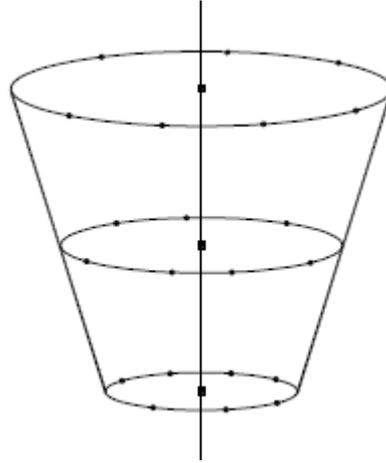


Figure 1: Location of the frustum of cone by three circles and definition of the "circle-point" factor

In the initial setting, the numbers of points are set at (7,7,7), e.g. the NC machine measures 7 points on each circle. A categorical input factor "circle-point-*cp*" is then defined at four levels with each level corresponding to a different number of points measured on each circle: (1) 7,7,7; (2) 7,5,7; (3) 5,7,5; (4) 5,5,5.

Two other variables are involved in the split-plot design: measurement speed-*mspeed* (mm/sec), and drift speed-*dspeed* (mm/sec). Therefore, a split-plot design with three factors is planned: two WP process factors, both at two levels (measurement and drift speeds), only one SP control factor, and the *cp* categorical factor at four levels. The final split-plot has 112 runs with seven replicates.

Standardization of the responses was carried out (Berni, 2010) to compensate for differences in magnitude among responses, even though both responses and WP factors are expressed with the same unit of measurement.

4.2. The Pareto front approach: objective phase

In order to identify the Pareto-optimal set, a series of 1764 combinations of factor levels were identified (*mspeed*, *dspeed* and *cp*), from which, the predicted response values (\widehat{crmax} , \widehat{crmin} and \widehat{eccen}) are estimated using the model form described in formula (2). The set of possible input combinations shown in Figure 2, was formed by constructing a grid of points based on discrete levels of *mspeed* and *dspeed* for each level of the factor *cp*. The fineness of the mesh of each grid is equal to 0.1, since this choice balances between the complexity of calculation and valid coverage of the two-dimensional region, identified by the ranges of *mspeed* and *dspeed* factors. The combinations of the possible solutions are labelled from 1 to 1764 as follows (Chapman et al., 2014a): i) from the first grid on the upper

left to the lower right grid; ii) inside each grid starting from the bottom row and moving from left to right, then starting at the end of each row, from the leftmost point of the next row.

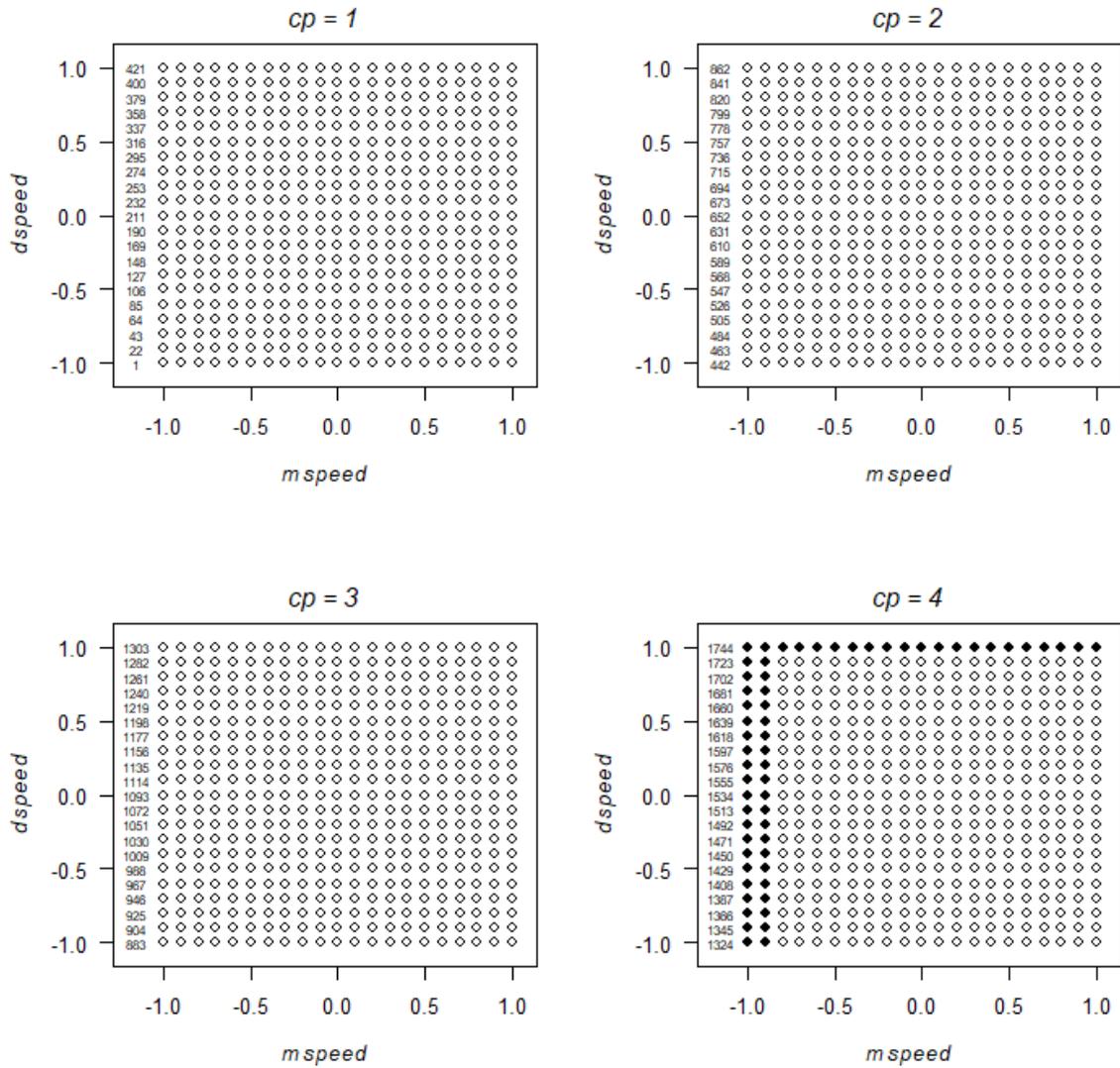


Figure 2: Input grid plot

The obtained Pareto-optimal set consists of 61 combinations, indicated by the solid circles in Figure 2. These combinations all involve $cp = 4$, which requires the smallest number of points. Therefore, irrespective of the choice in the subjective phase, an improvement in the measurement time will always be obtained.

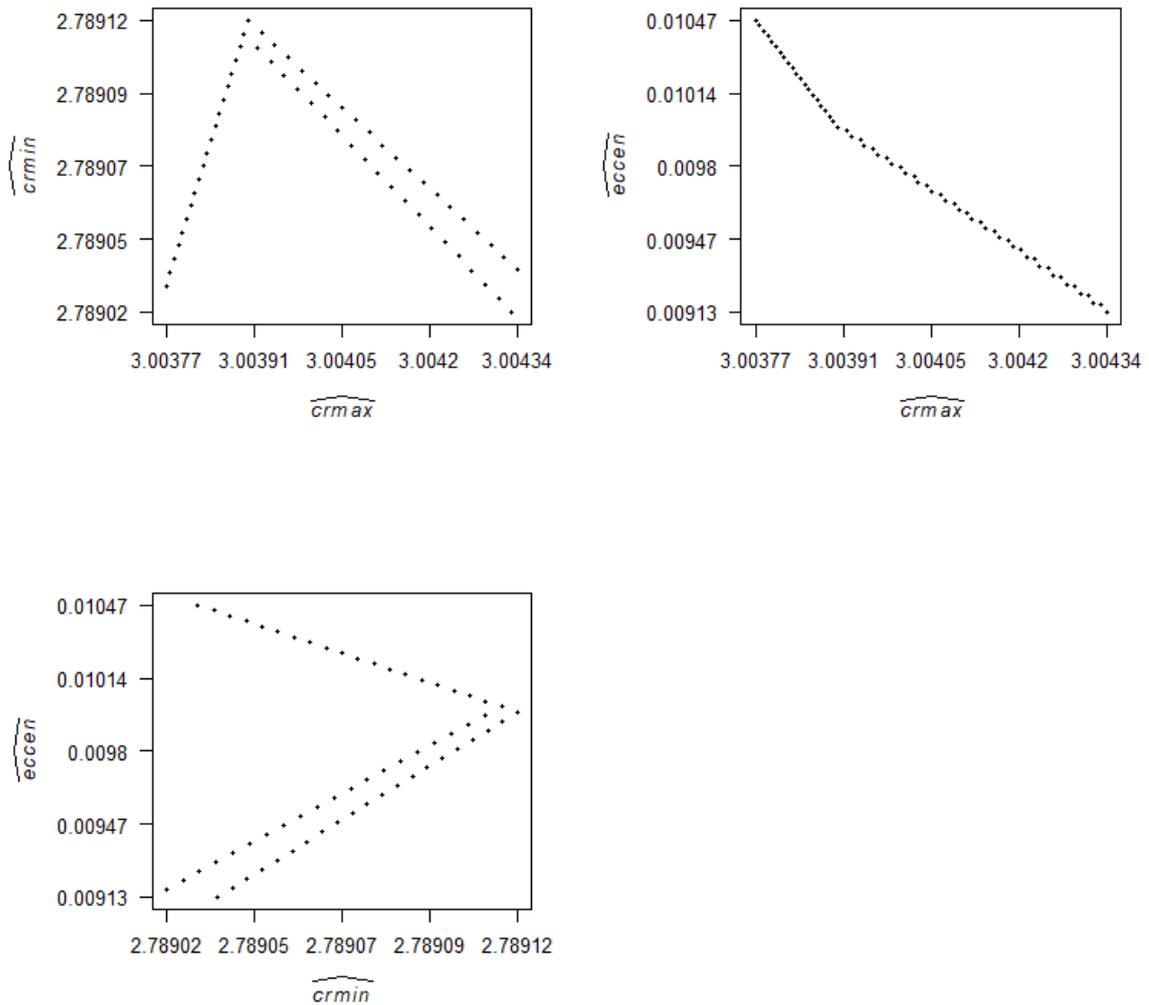


Figure 3: Pairwise scatterplots of the points belonging to the Pareto front

Figure 3 shows the pairwise scatterplots of the points belonging to the Pareto front (Chapman et al., 2014a; Anderson-Cook, 2017). The analysis of this set of points shows that there is a strong trade-off between the maximum circle diameter and eccentricity. The trade-offs between the other two pairs of response variables appear smaller. Finally, by observing the ranges of the predicted responses, we note how all 61 combinations of the Pareto-optimal set lead to values of \widehat{crmax} , \widehat{crmin} and \widehat{eccen} , close to the respective targets.

4.3. The Pareto front approach: subjective phase

In order to compare the 61 combinations of the Pareto-optimal set, the following procedure is carried out (Chapman et al., 2014a; Myers et al., 2016; Anderson-Cook, 2017):

i) the Pareto front values of each predicted response are transformed into desirability values, so that the best value obtained (from the set of solutions comprising the front) for each response is scaled to one, while the worst value is scaled to zero; ii) for each combination (of the Pareto-optimal set), the respective desirability values are combined in a single global desirability function. Since it was considered appropriate to heavily penalize undesirable predicted response values in this work, we choose the standard multiplicative desirability form, based on the geometric mean expression, as follows:

$$D(\mathbf{x}_{\mathcal{P}}, \mathbf{w}) = d_{crmax}(\mathbf{x}_{\mathcal{P}})^{w_{crmax}} \cdot d_{crmin}(\mathbf{x}_{\mathcal{P}})^{w_{crmin}} \cdot d_{eccen}(\mathbf{x}_{\mathcal{P}})^{w_{eccen}}$$

where $\mathbf{x}_{\mathcal{P}}$ is a combination of the Pareto-optimal set; $d_{crmax}(\mathbf{x}_{\mathcal{P}})$, $d_{crmin}(\mathbf{x}_{\mathcal{P}})$, $d_{eccen}(\mathbf{x}_{\mathcal{P}})$ the single desirability values related to the three predicted responses; $\mathbf{w} = (w_{crmax}, w_{crmin}, w_{eccen})'$ a weight vector, with $w_{crmax}, w_{crmin}, w_{eccen} \geq 0$ representing the weights assigned to the three response variables and $w_{crmax} + w_{crmin} + w_{eccen} = 1$.

Figure 4 shows the mixture plot, which identifies the best combination (i.e., the optimum point for achieving the highest value of the global desirability function) for each possible weighting of the response variables. Each point of the mixture plot represents a weight vector (e.g., the left bottom vertex represents $\mathbf{w} = (1,0,0)'$, and the bottom edge represents the weight vectors with $w_{crmax}, w_{crmin} > 0$ and $w_{eccen} = 0$). For further details see Cornell (2002).

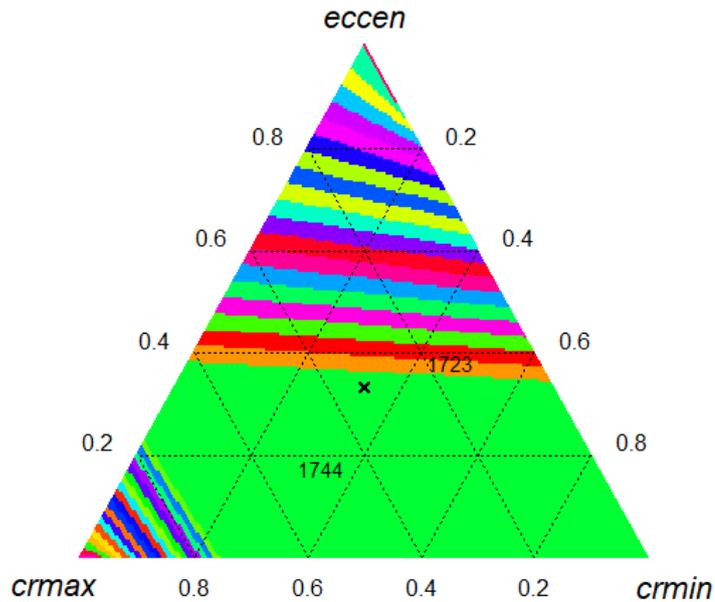


Figure 4: Mixture plot

In this case-study, 41 of the 61 combinations belonging to the Pareto-optimal set appear in the mixture plot (where each colored area identifies a different combination), that is, they are best for at least one weight vector. Assuming that the three response variables are thought to be of equal importance, the weights reflecting company priorities/preferences are those around the centroid of the triangle, indicated in Figure 4 with a black cross, and corresponding to the weight vector $\mathbf{w} = \left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right)'$. The two best points for these weight combinations are 1723 and 1744. In particular, 1744 is better for most of these weights, including the one directly at the centroid of the triangle as well. Table 1 shows the detailed results obtained for these two points, e.g., 1723 and 1744, only differ in the value of *dspeed*, and they provide similar predicted response values.

Combination	Factors			Predicted responses		
	<i>mspeed</i>	<i>dspeed</i>	<i>cp</i>	\widehat{crmax}	\widehat{crmin}	\widehat{eccen}
1723	-1	0.9	4	3.00392	2.78911	0.00994
1744	-1	1	4	3.00390	2.78912	0.00998

Table 1: Factor levels and predicted response values for the combinations 1723 and 1744

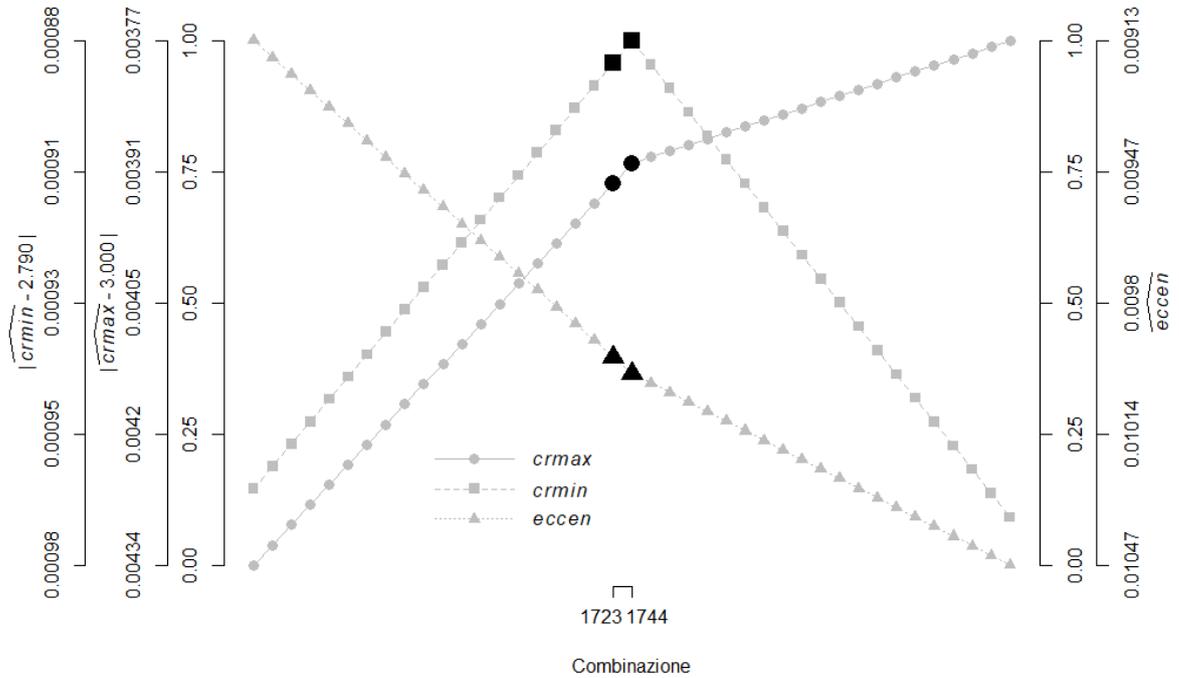


Figure 5: Trade-off plot of the 41 best point combinations for at least one weight combination

Figure 5 contains the trade-off plot which illustrates the desirability values (internal vertical axes) and absolute value differences between the predicted response values and the respective targets (external vertical axes) considering the 41 solutions that are best for at least one weight combination. In Figure 5, the trade-offs between the pairs of responses are similar to those highlighted by the pairwise scatterplots in Figure 3. Moreover, as shown by the mixture plot (Figure 4), it is evident that the point combinations 1723 and 1744 provide an ideal balance among the three responses.

In order to better analyze and compare these two combinations of interest, Figure 6 shows the synthesized efficiency plots (Lu and Anderson-Cook, 2012) which allows comparison of the relative efficiency of individual solutions with the best available across all the possible weight vectors.³ The synthesized efficiency of a point combination (belonging to the Pareto-optimal set) \mathbf{x}_p , with weight vector \mathbf{w} , is defined as follows:

$$\frac{D(\mathbf{x}_p, \mathbf{w})}{\max_{\mathbf{x}_p} [D(\mathbf{x}_p, \mathbf{w})]}$$

The shading, from white to black, represents the transition from high to low values of the synthesized efficiency. Each of the 19 shades of grey, starting from the lightest, corresponds to a decrease in the synthesized efficiency of 0.05.

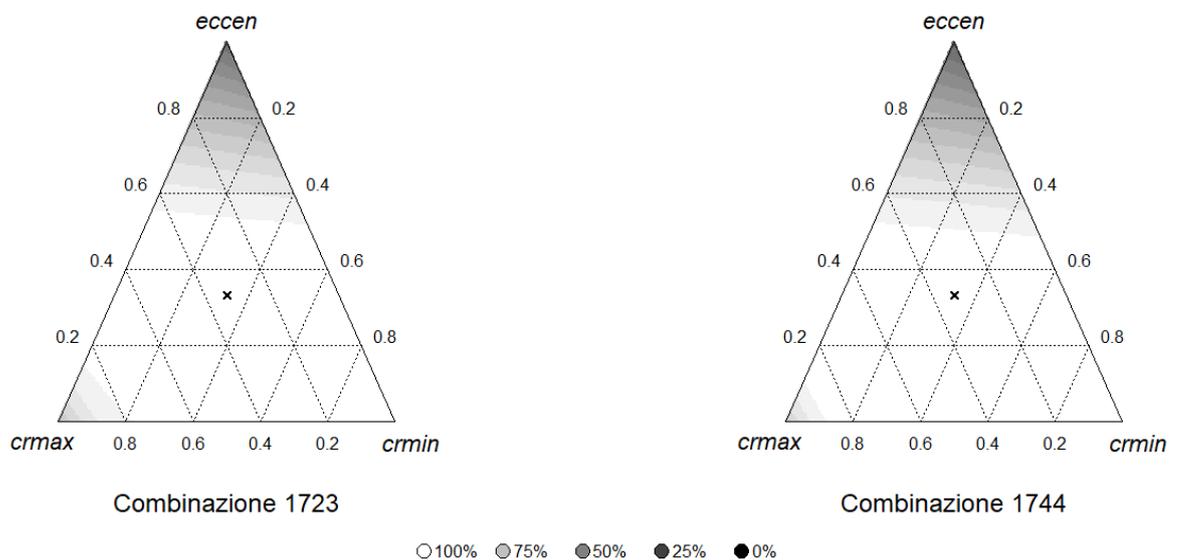


Figure 6: Synthesized efficiency plot for the point combinations 1723 and 1744

³ It should be noted that for the construction of the synthesized efficiency plots (Figure 6) and the mixture plot (Figure 4), a set of 20301 weight combinations has been defined, where adjacent weights related to a same response variable are separated by a distance equal to 0.005.

The large white region characterizing the two graphs, represents approximately 75% and 74% of the total area of the triangles, respectively, and indicates that both points have a synthesized efficiency of at least 0.95 for a substantial number of weight combinations. In particular, the white region around the centroid of the triangle, containing a black cross (Figure 6), shows that both point combinations provide excellent performance at the weighting region, which reflects the company's priorities/preferences.

Moreover, we select the optimal solution as represented by combination 1744, since it is slightly better for a large number of weight combinations, and in particular, for the weighting giving equal importance to the three response variables. However, input combination 1723 provides a similar performance, thus representing a valid competitive alternative.

4.4. Comparison between the Pareto front approach and the analytical optimization method

Table 2 shows the results from both multi-response optimization methods: the Pareto front approach and the analytical method suggested in Berni (2010). By comparing (Table 2) the optimum point combination 1744 and the optimal solution identified in Berni (2010), we can observe how only one process factor, cp , shows the same optimal level; nevertheless, it must be noted that the circle point variable is the main process variable that we are interested in optimizing. Although both combinations provide similar predicted response values, the optimization method used in Berni (2010) allows for obtaining a better value than \widehat{eccen} . This is an important result in view of the relevance that this response variable has in the actual process. The Pareto front constructed does contain similar solutions to those identified by the optimal solution, but corresponded to different weight combinations than those around the centroid. Hence, with a more thorough exploration of the solution set identified with the Pareto front, a similar solution could be selected.

Method	Factors			Predicted responses		
	$mspeed$	$dspeed$	cp	\widehat{crmax}	\widehat{crmin}	\widehat{eccen}
Pareto front	-1	1	4	3.00390	2.78912	0.00998
Analytical	0.710	0.362	4	3.00300	2.78500	0.00100

Table 2: Optimization results: the comparison

It is important to note, however, that although a Pareto front can be constructed for any number of responses of interest, the graphical tools considered here only used three response

variables, unlike the five considered in Berni (2010). For this reason, it was only possible to make a partial comparison between the results obtained through the two different methods. Nevertheless, it is worth noting that the Pareto front approach offers the possibility of using additional graphical tools (Lu et al., 2017), which enable multi-response optimization of more than three response variables.

Moreover, in Berni (2010) the optimization was carried out considering both non-standardized and standardized data, where the latter gave the best optimization results.

5. Discussion and final remarks

By considering the case study, and evaluating the theoretical differences between the two optimization methods applied as well, it is possible to highlight the following main differences.

Undoubtedly, the Pareto front approach offers the advantage of using graphical tools in a simple and intuitive way, enabling straightforward identification of leading solutions with convergence toward the optimal solution among the various company teams involved. The elimination of non-competitive choices streamlines where to focus further discussion. Moreover, a subjective evaluation can also be performed, with the possible achievement of a unanimous decision among different stakeholders. It is possible to compare different identified solutions, and see their relative strengths and weaknesses for each of the responses of interest. Indeed, it allows for accurate comparison among several input combinations of interest. A further advantage is the flexibility in response weighting to handle multiple combinations of business priorities and to examine the impact of these choices on the identified results. The transparent nature of the Pareto front presents the experimenter with different alternatives that can be explored and compared. Nevertheless, this is also possible by performing analytical optimization methods (see Lin and Tu, 1995). In addition, response weighting and analytical methods assign relative importance to each response according to the estimated corresponding weight (Berni, 2010).

A further advantage of analytical methods with respect to the Pareto front approach is the inclusion of random effects, within both the modelling and the optimization steps. Therefore, fixed as well as random effects are wholly involved, and as a result a robust process optimization can be carried out. It would be straightforward to use the above optimization function based on the inclusion of random effects for each of the responses as the basis for constructing the Pareto front.

The aforementioned advantages and disadvantages highlight the significant relevance of both methods, as each has specific strengths and weaknesses that would be relevant for a wide range of empirical situations (real industrial processes, technological contexts) where they can be effectively applied.

References

Ames, A. E., Mattucci, N., Macdonald, S., Szonyi, G., and Hawkins, D. M. (1997). "Quality loss functions for optimization across multiple response surfaces". *Journal of Quality Technology*, 29 (3): 339-346.

Anderson-Cook, C. M. (2017). "Optimizing in a complex world: a statistician's role in decision making". *Quality Engineering*, 29 (1): 27-41.

Anderson-Cook, C. M., and Lu, L. (2018). "Graphics to facilitate informative discussion and team decision making". *Applied Stochastic Models in Business and Industry*, 34 (6): 963-980.

Berni, R. (2010). "Split-plot and robust designs: weighting and optimization in the multiple response case". In: Giovagnoli, A., Atkinson, A. C., Torsney, B., and May, C., eds. *mODa 9 – advances in model-oriented design and analysis: proceedings of the 9th international workshop in model-oriented design and analysis held in Bertinoro, Italy, June 14-18, 2010*. Heidelberg: Physica-Verlag, 25-32.

Berni, R., and Bertocci, F. (2018). "Optimization of gas sensors based on advanced nanomaterials through split-plot designs and GLMMs". *Sensors*, 18 (11): 3858.

Berni, R., Bertocci, F., Nikiforova, N. D., and Vining, G. G. (2020). "A tutorial on randomizing versus not randomizing split-plot experiments". *Quality Engineering*, 32 (1): 25-45.

Berni, R., and Burbui, M. (2014). "Process optimization of a superfinishing machine through experimental design and mixed response surface models". *Quality Engineering*, 26 (4): 404-415.

Berni, R., and Gonnelli, C. (2006). "Planning and optimization of a numerical control machine in a multiple response case". *Quality and Reliability Engineering International*, 22 (5): 517-526.

- Berni, R., and Nikiforova, N. D. (2021-forthcoming). "A joint multiresponse split-plot design modeling and optimization including fixed and random effects". *Austrian Journal of Statistics*, 1-17.
- Bisgaard, S. (2000). "The design and analysis of $2^{k-p} \times 2^{q-r}$ split plot experiments". *Journal of Quality Technology*, 32 (1): 39-56.
- Box, G. E. P., Hunter, W. G., MacGregor, J. F., and Erjavec, J. (1973). "Some problems associated with the analysis of multiresponse data". *Technometrics*, 15 (1): 33-51.
- Box, G. E. P., and Jones, S. (1992). "Split-Plot designs for robust product experimentation". *Journal of Applied Statistics*, 19 (1): 3-26.
- Chapman, J. L., Lu, L., and Anderson-Cook, C. M. (2014a). "Process optimization for multiple responses utilizing the Pareto front approach". *Quality Engineering*, 26 (3): 253-268.
- Chapman, J. L., Lu, L., and Anderson-Cook, C. M. (2014b). "Incorporating response variability and estimation uncertainty into Pareto front optimization". *Computers & Industrial Engineering*, 76: 253-267.
- Chiao, C.-H., and Hamada, M. (2001). "Analyzing experiments with correlated multiple responses". *Journal of Quality Technology*, 33 (4): 451-465.
- Cochran, W. G., and Cox, G. M. (1957). *Experimental designs*. 2^o ed. New York: Wiley.
- Coello Coello, C. A., Lamont, G. B., and Van Veldhuizen, D. A. (2007). *Evolutionary algorithms for solving multi-objective problems*. 2^o ed. New York: Springer, 1-13.
- Copeland, K. A. F., and Nelson, P. R. (1996). "Dual response optimization via direct function minimization". *Journal of Quality Technology*, 28 (3): 331-336.
- Cornell, J. A. (2002). *Experiments with mixtures: designs, models, and the analysis of mixture data*. 3^o ed. New York: Wiley.
- Del Castillo, E., Montgomery, D. C., and McCarville, D. R. (1996). "Modified desirability functions for multiple response optimization". *Journal of Quality Technology*, 28 (3): 337-345.
- Derringer, G., and Suich, R. (1980). "Simultaneous optimization of several response variables". *Journal of Quality Technology*, 12 (4): 214-219.

- Dror, H. A., and Steinberg, D. M. (2006). "Robust experimental design for multivariate generalized linear models". *Technometrics*, 48 (4): 520-529.
- Jones, B., and Nachtsheim, C. J. (2009). "Split-plot designs: what, why, and how". *Journal of Quality Technology*, 41 (4): 340-361.
- Khuri, A. I., and Conlon, M. (1981). "Simultaneous optimization of multiple responses represented by polynomial regression functions". *Technometrics*, 23 (4): 363-375.
- Kowalski, S. M., Parker, P. A., and Vining, G. G. (2007). "Tutorial: industrial split-plot experiments". *Quality Engineering*, 19 (1): 1-15.
- Kowalski, S. M., and Potcner, K. J. (2003). "How to recognize a split-plot experiment". *Quality Progress*, 36 (11): 60-66.
- Lee, Y., and Nelder, J. A. (2003). "Robust design via generalized linear models". *Journal of Quality Technology*, 35 (1): 2-12.
- León, R. V., Shoemaker, A. C., and Kacker, R. N. (1987). "Performance measures independent of adjustment". *Technometrics*, 29 (3): 253-285.
- Lin, D. K. J., and Tu, W. (1995). "Dual response surface optimization". *Journal of Quality Technology*, 27 (1): 34-39.
- Lu, L., and Anderson-Cook, C. M. (2012). "Rethinking the optimal response surface design for a first-order model with two-factor interactions, when protecting against curvature". *Quality Engineering*, 24 (3): 404-422.
- Lu, L., Anderson-Cook, C. M., and Robinson, T. J. (2011). "Optimization of designed experiments based on multiple criteria utilizing a Pareto frontier". *Technometrics*, 53 (4): 353-365.
- Lu, L., Chapman, J. L., and Anderson-Cook, C. M. (2017). "Multiple response optimization for higher dimensions in factors and responses". *Quality and Reliability Engineering International*, 33 (4): 727-744.
- Marler, R. T., and Arora, J. S. (2004). "Survey of multi-objective optimization methods for engineering". *Structural and Multidisciplinary Optimization*, 26 (6): 369-395.
- McCullagh, P., and Nelder, J. A. (1989). *Generalized linear models*. 2^o ed. London: Chapman & Hall.

- Myers, R. H., Khuri, A. I., and Vining, G. G. (1992). "Response surface alternatives to the Taguchi robust parameter design approach". *The American Statistician*, 46 (2): 131-139.
- Myers, R. H., Montgomery, D. C., and Anderson-Cook, C. M. (2016). *Response surface methodology: process and product optimization using designed experiments*. 4^o ed. Hoboken, New Jersey: Wiley.
- Nair, V. N. (1992). "Taguchi's parameter design: a panel discussion". *Technometrics*, 34 (2): 127-161.
- Nelder, J. A., and Lee, Y. (1991). "Generalized linear models for the analysis of Taguchi-type experiments". *Applied Stochastic Models and Data Analysis*, 7 (1): 107-120.
- Rajagopal, R., Del Castillo, E., and Peterson, J. J. (2005). "Model and distribution-robust process optimization with noise factors". *Journal of Quality Technology*, 37 (3): 210-222.
- Robinson, T. J., Wulff, S. S., Montgomery, D. C., and Khuri, A. I. (2006). "Robust parameter design using generalized linear mixed models". *Journal of Quality Technology*, 38 (1): 65-75.
- Tang, L. C., and Xu, K. (2002). "A unified approach for dual response surface optimization". *Journal of Quality Technology*, 34 (4): 437-447.
- Vining, G. G., and Kowalski, S. M. (2008). "Exact inference for response surface designs within a split-plot structure". *Journal of Quality Technology*, 40 (4): 394-406.
- Vining, G. G., Kowalski, S. M., and Montgomery, D. C. (2005). "Response surface designs within a split-plot structure". *Journal of Quality Technology*, 37 (2): 115-129.
- Vining, G. G., and Myers, R. H. (1990). "Combining Taguchi and response surface philosophies: a dual response approach". *Journal of Quality Technology*, 22 (1): 38-45.
- Zitzler, E. (1999). *Evolutionary algorithms for multiobjective optimization: methods and applications* [dissertation]. Zurich: Swiss Federal Institute of Technology Zurich, 5-10.

