

A Computational Algorithm for Selecting Robust Designs in Safety and Quality Critical Processes

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Abstract

This article considers robust designs for safety and quality critical processes. In critical processes, the choice of control settings should ensure that the product quality remains near the target for each and every value of the noise variable. This objective is realized by using a min-max approach which minimizes the maximum possible deviation (caused by noise) of the estimated response from the target value. An algorithm for computing such control settings based on entropic regularization is discussed. The proposed method is used on automobile crash test data to select maximally safe designs for the interior rim of cars. A second example on the design of drug granulation parameters to produce uniformly sized granules is also included.

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1 Introduction

In this article, we propose a min-max approach to address the issue of robust parameter designs for safety and quality critical processes. In any production process, there are two types of inputs: some easy-to-manipulate control factors and some difficult-to-control noise factors. The noise factors

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are the sources of uncontrollable variations in the process response. However for some products (henceforth called safety or quality critical), each and every sample (e.g. drugs or safety equipment) must meet some pre-specified quality standard to be usable. Otherwise, even though the majority of the produce is usable, the few sub-quality samples might lead to loss of life or fatal accidents. Hence during the production of such articles, one has to choose the control settings for which the product quality remains near the target for *all* settings of the noise factors. This objective is realized here, by choosing control settings which minimizes the maximum possible deviation (caused by noise) of the estimated response from the target value. A numerical algorithm is proposed to solve the resulting continuous min-max optimization.

Some instances of critical processes are the production processes in the automobile, drug or defense industries. Consider a drug manufacturing process, where *every* batch (lot or package) of the manufactured drug, irrespective of the uncontrollable noise factors, should be near the target quality. Otherwise, some samples of the drug may prove fatal once released in the market. Suppose, the quality of a manufactured drug is quantified by the percentage of impurities it may safely contain. Then the production process should ensure that this percentage is never exceeded no matter what value the noise factors may take during a particular run of the manufacturing process. This is also the case in the manufacturing of military equipments and also certain safety devices (e.g. in the air/automobile industry), where certain safety standards must be guaranteed for each and every product. Failure to adhere to the standards may result in loss of life.

Traditional robust parameter design algorithms however may not be appropriate for such safety or quality critical processes mentioned above. Two main approaches are available in the literature for solving the robust parameter design problem: the Taguchi method and the response surface approach. Several papers by Taguchi and Wu (1985), Kacker (1985), Nair (1992) discuss Taguchi's methodology in details. The response surface approach to robust parameter design can further be categorized into the dual and single model approaches. Several authors like Vining and Myers (1990) Del Castillo and Montgomery (1993), Lin and Tu (1995), Del Castillo et al. (1997), Fan (2000), discussed the dual response surface approach. The single model approach was introduced by Welch et al. (1990) and later used by Myers et al. (1992). Most traditional approaches (e.g. see Vining and Myers (1990), Myers et al. (1992) and the references therein) have developed algorithms to choose the control factors so as to achieve the dual objective of keeping the process mean near some pre-assigned

target and simultaneously minimizing the process variance. However, choosing the control factors merely to minimize variance may not be safe enough in safety and quality critical processes discussed in above applications. For example, in a sensitive process like airbag manufacture for automobiles it is necessary for the chosen levels of control variables to guarantee that product quality is close to the pre-specified safety standards for *all* values of the noise variable. Minimizing variance may not be enough in this situation since it gives no guarantee that the airbags produced will meet the required safety standard for each and every value of the noise. Even if there is a single value of the noise, for which the control variables give rise to a product quality which deviates from the target, it may result in injury or even death. Hence, for these and other applications we seek to re-formulate the robust parameter design paradigm using a min-max strategy. To keep the product quality near the pre-specified target or standard for all values of noise, we minimize the worst deviation (maximum possible deviation due to noise) of the estimated product quality from the target. Such a procedure leads to the control settings for which the estimated product quality always stays near the target whatever be the value of the noise. Though the min-max formulation is rather new in the area of robust parameter designs, it has been used earlier in the construction of optimal designs (Mukherjee and Huda (1985), Sitter (1992) and Dette et al. (2003)). Here, the optimality criterion, for example the D-optimality criterion, is maximized over the parameter space while being minimized with respect to the set of all designs.

For introducing the min-max formulation, the response surface approach proposed by Myers et al. (1992) seems well suited. The response, y , is modeled as a function of the control and noise variables. Due to the easy to manipulate nature of the control variables, they are considered as fixed effects, while noise variables are considered to be random. However, for the sake of experimentation and estimating the response, the noise factors are considered to be fixed, while in the process they are taken to be random. To model y we use the full single response model for the response,

$$y(\mathbf{x}, \mathbf{z}) = \beta_0 + g^T(\mathbf{x})\beta + h^T(\mathbf{z})\gamma + g^T(\mathbf{x})\Delta h(\mathbf{z}) + \varepsilon, \quad (1.1)$$

where $\mathbf{x} = (x_1, \dots, x_k)^T$ and $\mathbf{z} = (z_1, \dots, z_l)^T$ are the vectors of control and noise variables, respectively; $\mathbf{x} \in R_x$ and $\mathbf{z} \in R_z$ where both R_x and R_z are closed and bounded (compact) sets. The experimental region, R , is the Cartesian product of the sets R_x and R_z , i.e., $R = R_x \times R_z$. Also, $g(\mathbf{x})$ is a known vector function of \mathbf{x} containing polynomial terms and interactions of the control variables; $h(\mathbf{z})$

is a known vector function of \mathbf{z} containing polynomial terms and interactions of the noise variables; β and γ are the coefficients of the control and noise variables, respectively; Δ contains the coefficients of the interaction effects between the control and the noise variables and $\varepsilon \sim N(0, \sigma^2)$ is the error term. The estimated process response is,

$$\hat{y}(\mathbf{x}, \mathbf{z}) = \hat{\beta}_0 + g^T(\mathbf{x})\hat{\beta} + h^T(\mathbf{z})\hat{\gamma} + g^T(\mathbf{x})\hat{\Delta}h(\mathbf{z}). \quad (1.2)$$

where $\hat{\beta}_0, \hat{\beta}, \hat{\gamma}, \hat{\Delta}$ are the parameter estimates.

2 Preliminary Notion

As stated in the Introduction, our goal is to choose the control factor vector \mathbf{x} so as to keep the estimated response \hat{y} of formula (1.2) near the target for all values of $\mathbf{z} \in R_z$. In other words we would like to minimize the worst deviation of the estimated response from the target: let the target response be T ; Then for any choice \mathbf{x} of the control factor, the worst possible deviation of the estimated response from the target is

$$\sup_{\mathbf{z} \in R_z} \|T - \hat{y}(\mathbf{x}, \mathbf{z})\| \quad (2.1)$$

where $\|\cdot\|$ is some appropriately defined error criterion. However this worst deviation is still a function of the control variable \mathbf{x} . Hence we would like to choose a $\mathbf{x} \in R_x$ (say $\mathbf{x}^* \in R_x$) which minimizes $\sup_{\mathbf{z} \in R_z} \|T - \hat{g}(\mathbf{x}, \mathbf{z})\|$ i.e.

$$\sup_{\mathbf{z} \in R_z} \|T - \hat{g}(\mathbf{x}^*, \mathbf{z})\| = \inf_{\mathbf{x} \in R_x} \sup_{\mathbf{z} \in R_z} \|T - \hat{g}(\mathbf{x}, \mathbf{z})\| \quad (2.2)$$

It may be noted, that unlike most traditional approaches, the control settings \mathbf{x}^* may be decided without making any assumptions on the distribution of the noise variables, nor on the expectation or the variance-covariance structure of the noise variables. The only assumption we make is that R_z is known. This seems to be a valid assumption, since in production processes the experimenter usually has a fair idea about the range of the noise variable.

The min-max optimization implied in (2.2) is clearly appropriate for the safety or quality critical production examples mentioned. However, the resulting numerical optimization for finding \mathbf{x}^* is hard in general. For example, (2.2) is not solvable by conventional gradient based optimization techniques

due to the non-differentiability of the max function ($\sup_{\mathbf{z} \in R_z} \|T - \hat{y}(\mathbf{x}, \mathbf{z})\|$) (Polak (1994)). Finite or discrete versions of this min-max optimization, where the sets R_x and/or R_z are finite, or variants where the function $\|T - \hat{y}(\mathbf{x}, \mathbf{z})\|$ is convex and concave in \mathbf{x} and \mathbf{z} respectively, have been studied by numerous authors in the numerical optimization literature (Polyak (1988), Rustem and Nguyen (1998), Kiwiel (1987), Sasai (1974) and Zakovic et al. (2000)), and can be solved efficiently by a number of available algorithms. However, in (2.2) above, the sets R_x and R_z are compact subsets of Euclidean spaces and the function $\|T - \hat{y}(\mathbf{x}, \mathbf{z})\|$ is a multivariate polynomial which is not necessarily convex-concave in \mathbf{x} and \mathbf{z} . This general problem is computationally difficult, only recently some papers have addressed special cases of the generalization (Parpas et al. (2009), Rustem et al. (2008)). In this work, we outline a method for the computation of the optimal control setting \mathbf{x}^* of (2.2), based on the iterative entropic regularization algorithm proposed in Sheu and Lin (2004). This algorithm is guaranteed to find the solution to (2.2), if a series of subproblems with smooth but non-convex optimizations, can be solved approximately. Sheu and Lin (2004) do not point out any method for solving these subproblems. For solving these intermediate optimization problems, we combine the above algorithm with a global multilevel coordinate search algorithm developed in Huyer and Neumaier (1999). It is shown that this combination of algorithms solves (2.2) satisfactorily for the practical examples considered.

The remainder of the article is organized as follows. In Section 3 we describe the problem formulation in details. The algorithm used to compute the min-max solution is defined in Section 4. Section 5 presents numerical examples to illustrate the proposed min-max methodology. The first example considers the designing of the interior rim of a car in such a way as to reduce the risk of fatal head injury to the passenger in case of an accident. In the second numerical example, control factors are chosen for a drug granulation process used for the manufacture of tablets in the pharmaceutical industries. As discussed above, the min-max optimization of (2.2) is especially appropriate for these examples. In Section 5 we also compare our method with the variance minimizing method of Myers et al. (1992). The comparisons show that the min-max approach is better suited for application to critical processes than the traditional variance minimizing methods. Concluding remarks are given in Section 6.

3 The Min-max Problem Formulation

In a production process, Taguchi identified that an experimenter may be interested in choosing the control setting with one of the following objectives:

1. The response achieving a given target T ,
2. Minimizing the response,
3. Maximizing the response.

Associated with these goals are numerous error/performance criteria (e.g. see Taguchi (1986), Vining and Myers (1990), Myers et al. (1992), Lin and Tu (1995), Copeland and Nelson (1996)). Since deviation on either side of T is undesirable, we use the squared distance between the estimated response and the specified target T as our performance criterion, also known as the estimated squared error loss (denoted by M below):

$$M(\mathbf{x}, \mathbf{z}) = (T - \hat{y}(\mathbf{x}, \mathbf{z}))^2. \quad (3.1)$$

Myers et al. (1992) used the expected value of $M(\mathbf{x}, \mathbf{z})$, taken with respect to \mathbf{z} , assuming that the noise variables are uncorrelated with expectation zero and variance unity. In this article however, we do not make any such assumptions on the distribution, expectation or variance of \mathbf{z} ; consequently our performance criterion is given by (3.1).

Using this definition of error, we would like to translate the goals outlined by Taguchi into a min-max setting.

3.1 Target is specified

We assume that the experimenter is trying to realize goal (1) mentioned above: namely he is interested to keep $\hat{y}(\mathbf{x}, \mathbf{z})$ near the target T . In this endeavor, we recall that the noise variable \mathbf{z} is a random quantity in the process and takes an unknown value in the pre-specified set R_z during a particular ‘run’ of the process. For a particular value of the control factor \mathbf{x} and a particular realization of the noise factor \mathbf{z} , the estimated response from (1.2) is $\hat{y}(\mathbf{x}, \mathbf{z})$. Given any choice of the control variable \mathbf{x} , the worst possible scenario for the experimenter who is trying to realize goal (1), occurs, when the noise variable maximizes the deviation of the estimated response from the target value i.e. when \mathbf{z} satisfies: $\mathbf{z} = \arg \sup_{\mathbf{z} \in R_z} (T - \hat{y}(\mathbf{x}, \mathbf{z}))^2$, if it exists. Let $M^*(\mathbf{x}) = \sup_{\mathbf{z} \in R_z} (T - \hat{y}(\mathbf{x}, \mathbf{z}))^2$. Now,

$M^*(\mathbf{x})$ is still a function of the control factor \mathbf{x} . From the point of view of achieving goal (1), the best choice of the control factor would be the one which minimizes the worst deviation $M^*(\mathbf{x})$ with respect to \mathbf{x} . Let this best choice of the control factor, if it exists, be $\mathbf{x}^* \in R_x$. Hence, \mathbf{x}^* should satisfy $M^*(\mathbf{x}^*) = \inf_{\mathbf{x} \in R_x} M^*(\mathbf{x})$. By hypothesis, the sets R_x and R_z are compact; and clearly the function $M(\mathbf{x}, \mathbf{z})$ is continuous in both \mathbf{x} and \mathbf{z} . Using standard arguments (e.g., see Evans and Gariepy (1992)) it can be shown that there exists $\mathbf{x}^* \in R_x$ and $\mathbf{z}^* \in R_z$ which satisfies:

$$M(\mathbf{x}^*, \mathbf{z}^*) = \min_{\mathbf{x} \in R_x} \max_{\mathbf{z} \in R_z} (T - \hat{y}(\mathbf{x}, \mathbf{z}))^2 \quad (3.2)$$

By such a choice of the control factor i.e. $\mathbf{x} = \mathbf{x}^*$, the experimenter guarantees the following:

1. That the predicted response never deviates from the specified target T by more than $M(\mathbf{x}^*, \mathbf{z}^*)$, whatever be the actual value realized by the noise variables in a particular process run. In other words $(T - \hat{y}(\mathbf{x}^*, \mathbf{z}))^2 \leq M(\mathbf{x}^*, \mathbf{z}^*)$ for all $\mathbf{z} \in R_z$.
2. This choice of the control factor minimizes the worst deviation. Hence, for any other choice of the control factor $\mathbf{x} = \mathbf{x}_1$, the maximum deviation due to noise can be worse. Equivalently, for any $\mathbf{x}_1 \in R_x$ there exists $\mathbf{z}_1 \in R_z$ for which: $M(\mathbf{x}^*, \mathbf{z}^*) \leq (T - \hat{y}(\mathbf{x}_1, \mathbf{z}_1))^2$.

An important fact to note here is that, unlike most previous works in this area, no assumptions are made about the distribution, expectation, variance-covariance structure of \mathbf{z} .

It should be noted, however, that claims (1) and (2) above are valid for the actual process only if we assume that the model used to fit the process response and the estimated response is accurate over the experimental region.

Unacceptable worst deviation

The design paradigm outlined above, guarantees that the worst deviation of the predicted response from the target is never more than $M(\mathbf{x}^*, \mathbf{z}^*)$. However, from the strict quality control requirements of safety or quality critical processes, it may turn out that this deviation of $M(\mathbf{x}^*, \mathbf{z}^*)$ is not acceptable. In that case, one may try to choose the control factors outside the previously considered design region R_x . Since the linear model (1.2) is only valid over the experimental region $R_x \times R_z$ a re-estimation of the model over a different experimental region may then be required. However, it is not apparent a priori that where exactly the experimental region should be chosen from the entire set of possible

control and noise settings, so that the min-max deviation $M(\mathbf{x}^*, \mathbf{z}^*)$ is minimized. Hence an iterative search may be the only solution in this approach. However, if even this method fails to lower the min-max deviation below acceptable limits, the process may have to be modified (if economically or physically possible) to reduce the range of variation of the uncontrollable noise factors.

3.2 Smaller/Larger is better

For designs where Taguchi's second objective is applicable, our min-max design philosophy, necessitates the control factors to minimize the maximum (with respect to the noise factors) estimated response. That is, we need to find the value of \mathbf{x} which minimizes $\max_{\mathbf{z} \in R_z} \hat{y}(\mathbf{x}, \mathbf{z})$. Again since R_x and R_z are compact by assumption and the estimated response $\hat{y}(\mathbf{x}, \mathbf{z})$ is continuous in both \mathbf{x} and \mathbf{z} , there exists $\mathbf{x}^* \in R_x$ and $\mathbf{z}^* \in R_z$ which satisfy:

$$\hat{y}(\mathbf{x}^*, \mathbf{z}^*) = \min_{\mathbf{x} \in R_x} \max_{\mathbf{z} \in R_z} \hat{y}(\mathbf{x}, \mathbf{z}), \quad (3.3)$$

Similarly for Taguchi's "larger is better" paradigm, our approach chooses a control factor \mathbf{x} which maximizes the minimum (with respect to \mathbf{z}) $\hat{y}(\mathbf{x}, \mathbf{z})$. Consequently, the problem is to find \mathbf{x} which maximizes $\min_{\mathbf{z} \in R_z} \hat{y}(\mathbf{x}, \mathbf{z})$. Under the assumptions made on R_x , R_z and $\hat{y}(\mathbf{x}, \mathbf{z})$, there exists $\mathbf{x}^* \in R_x$ and $\mathbf{z}^* \in R_z$ which satisfy:

$$\hat{y}(\mathbf{x}^*, \mathbf{z}^*) = \max_{\mathbf{x} \in R_x} \min_{\mathbf{z} \in R_z} \hat{y}(\mathbf{x}, \mathbf{z}), \quad (3.4)$$

Clearly, the optimal solution \mathbf{x}^* to the equation (3.4) may equivalently be calculated by considering a min-max problem, simply by considering $-\hat{y}(\mathbf{x}, \mathbf{z})$ instead of $\hat{y}(\mathbf{x}, \mathbf{z})$.

4 Computing the Min-max Using the IER-MCS Algorithm

Some of the difficulties in computing a solution to (3.2) were mentioned in Section 2. In this section, we propose to use a method of outer approximation first proposed in Polak (1994) and modified using an entropic regularization in Sheu and Lin (2004). We follow the authors of the latter paper in calling this algorithm as Iterative entropic regularization (or IER). This method has been shown to have guaranteed convergence properties to the min-max solution. However, in using this method one needs to solve a sequence of (possibly non-convex) maximization and/or minimization problems. The

convergence of the min-max algorithm is based on the successful solution of these intermediate maximization and/or minimization problems. Clearly, in our case the error criterion $M(\mathbf{x}, \mathbf{z})$ is frequently non-convex in \mathbf{x} or \mathbf{z} . This makes the solution of the intermediate optimization problems difficult. For this purpose we propose to use a proven global optimization algorithm based on multilevel coordinate search (MCS) (Huyer and Neumaier (1999) and Jones et al. (1993)). This method, in turn, is guaranteed to converge if the optimized function is continuous in the neighborhood of the global optimum. We show that this combination, which we name as IER-MCS, performs consistently in finding the min-max optimization posed in (3.2) above. First we briefly describe the IER algorithm to make this presentation self-contained.

Iterative Entropic Regularization:

Let us rewrite (3.2) simply as: Find $(\mathbf{x}^*, \mathbf{z}^*) \in R_x \times R_z$ such that $M(\mathbf{x}^*, \mathbf{z}^*) = \min_{\mathbf{x} \in R_x} \max_{\mathbf{z} \in R_z} M(\mathbf{x}, \mathbf{z})$ where $M(\mathbf{x}, \mathbf{z})$ is defined as in (3.1). Further recall that $M^*(\mathbf{x}) = \max_{\mathbf{z} \in R_z} M(\mathbf{x}, \mathbf{z})$.

Next approximate R_z by a finite subset $R_z^m := \{\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_m\}$ of m points. Correspondingly $M^*(\mathbf{x})$ is approximated by $M_m^*(\mathbf{x}) = \max_{\mathbf{z} \in R_z^m} M(\mathbf{x}, \mathbf{z})$. However this approximate function is still not differentiable and hence we use the following smoothed version using entropic regularization (Polak (1994) and Sheu and Lin (2004)):

$$M_{m,p}^*(\mathbf{x}) = (1/p) \log \left\{ \sum_{\mathbf{z} \in R_z^m} \exp \{pM(\mathbf{x}, \mathbf{z})\} \right\}$$

where $p > 0$. Then the algorithm can be written as follows:

1. Select $\mathbf{z}_1 \in R_z$ and let $R_z^1 := \{\mathbf{z}_1\}; m = k = 1$. Choose $\delta \in (0, 1)$, and $p > 0$.
2. Find $\mathbf{x}_{m,p} \in R_x$ satisfying $M_{m,p}^*(\mathbf{x}_{m,p}) \leq \min_{\mathbf{x} \in R_x} M_{m,p}^*(\mathbf{x}) + \delta^k$. Increase the iteration count k by one.
3. If (i) $M^*(\mathbf{x}_{m,p}) \leq M_{m,p}^*(\mathbf{x}_{m,p})$ and (ii) $\delta^k + \log(m)/p$ is below a desired tolerance, then stop. If (i) is violated then choose any $\mathbf{z}_{m+1} = \arg \max_{\mathbf{z} \in R_z} M(\mathbf{x}_{m,p}, \mathbf{z})$, set $R_z^{m+1} = R_z^m \cup \{\mathbf{z}_{m+1}\}$, increase m by one, select $p \geq (\log(m))^2$ and go to step 2. If (ii) is violated increase p by a constant factor and go to step 2.

This algorithm is guaranteed to converge to the global solution at step 3 with at most a $(\delta^k +$

$\log(m)/p$ error; or it produces an infinite sequence of solutions $\mathbf{x}_m \in R_z(m \rightarrow \infty)$, any cluster point of which is a global solution.

However, the successful implementation of this algorithm needs the correct computation of the minimum of $M_{m,p}^*(\mathbf{x})$ in step 2. Clearly, if $M(\mathbf{x}, \mathbf{z})$ is not convex in \mathbf{z} , for each value of \mathbf{x} , the smoothed version $M_{m,p}^*(\mathbf{x})$ also may turn out to be non-convex. Hence, one needs to solve a non-convex optimization problem every time step 2 needs to be executed. Moreover for checking condition (i) of step 3 one needs to compute $M^*(\mathbf{x}_{m,p})$, which is again a (possibly non-convex) maximization problem over R_z . For these purposes, we use the global optimization algorithm based on multilevel coordinate search proposed in Huyer and Neumaier (1999) and Jones et al. (1993). Briefly, this method uses a modified branch and bound scheme to find the global minimizer by combining global search with a fast local search. This algorithm is guaranteed to converge given that the function to be optimized is continuous in the neighborhood of the global minimum. For details about the performance of this algorithm in benchmark optimization problems and about related convergence properties, the reader is referred to Huyer and Neumaier (1999). In this article we use the MCS algorithm to solve the non-convex optimization sub-steps of step (2) and (3)(i).

5 Numerical Examples

In this section, we illustrate our proposed min-max approach using four numerical examples. The first two examples are based on data from sensitive processes, crash test and granulation of drug. While, the third and fourth examples are based on data sets frequently used in literature. We also provide a comparison of the results obtained by the min-max approach and the method proposed in Myers et al. (1992).

5.1 Example 1: Automobile crash test

In this example we consider a data set taken from Rai et al. (2005) studying the effect of four factors on the head injury criteria (HIC) measured during automobile crash tests. The objective of the experiment is to design the interior rim of a car in such a way as to reduce the risk of fatal head injury to the passenger in case of an accident. The critical interior rim dimensions known to affect HIC values are wall thickness, draft angle and rib pitch (see Rai et al. (2005) for a complete description). These

parameters can be chosen easily and hence are considered as control factors. Similarly, the angle at which the head collides with the rim during the accident is known to affect the HIC value substantially. However, this angle of head impact is completely unpredictable and is hence treated as noise variable. It should be noted that the bounds on the control factors are clearly known, being imposed by the engineering, manufacturing and assembly guidelines while the angle of impact is bounded by the 45 and 90 degrees due to the geometry of possible head collisions. (Rai et al. (2005)). A dummy equivalent of HIC denoted by HIC(d) is used as the response variable in the following model. It should be emphasized, that the min-max paradigm is ideally suited for this example, since the design should guarantee that the HIC value remains low for *all* possible angles of head impact.

To summarize, there are three control variables: x_1 (wall thickness measured in mm), x_2 (draft angle), x_3 (rib height measured in mm), and one noise variable: z_1 (angle of head impact). A list of factors and their levels is given in Table 1. Each factor is present at two levels. Here, $R_x = \{-1 \leq x_i \leq 1; i = 1, 2, 3\}$ and $R_z = \{-1 \leq z_1 \leq 1\}$. The goal is to determine the settings of the control variables for which the head injury criteria is minimized, for all values of the angle of head impact, z_1 .

Table 1: Factors and levels (Example 5.1)

Factors	-1	1
Wall thickness (x_1)	2.4 mm	3.5 mm
Draft angle (x_2)	5 degrees	10 degrees
Rib height (x_3)	12.5 mm	21 mm
Angle of impact (z_1)	45 degrees	90 degrees

The fitted response $\hat{y}(\mathbf{x}, z_1)$, is

$$741.57 - 121.74x_1 - 118.07x_2 - 28.33x_3 - 103.64z_1 + 121.96x_1x_2 + 53.97x_1z_1 + 40.31x_2z_1 + 10.08x_3z_1. \quad (5.1)$$

The analysis of variance results are given in Table 3. We also fitted a model with the interaction terms, x_1x_3 , x_2x_3 , zx_1x_2 , zx_1x_3 and zx_2x_3 included. However, the corresponding p-values for these interaction terms were greater than 0.55. There was also no improvement in the adjusted $R^2(= 0.9265)$, $F(= 26.21)$ value and the $F(= 0.2189)$ value for the lack of fit test. Studentized residuals corresponding to the fitted model (5.1) all lie between -2 and 2, with approximate mean 0 and variance 1. Various

Table 2: Design and response values (Example 5.1)

x_1	x_2	x_3	z_1	y	x_1	x_2	x_3	z_1	y
-1	-1	-1	-1	1362	1	-1	-1	-1	968
-1	-1	1	1	677	1	-1	1	1	510
-1	-1	1	-1	750	1	-1	1	-1	511
-1	-1	1	1	734	1	-1	1	1	501
-1	1	-1	1	584	1	1	-1	1	499
-1	1	-1	-1	742	1	1	-1	-1	584
-1	1	-1	1	731	1	1	-1	1	499
-1	1	1	-1	636	1	1	1	-1	581
-1	1	1	1	608	1	1	1	1	578
-1	1	1	-1	716	1	1	1	-1	680
1	-1	-1	-1	857					

Table 3: Analysis of variance (Ex 5.1)

Source	df	SS	MS	F	p-value	R^2	adjusted- R^2
Model	8	764063	95508	36.2185	<0.0001	0.9602	0.9337
Residuals	12	31644	2637				
Lack of fit	5	4913	983	0.2573	0.9229		
Pure error	7	26730	3819				
variable				partial t			p-value
x_1				-10.058			<0.0001
x_2				-9.755			<0.0001
x_3				-2.207			0.0475
z_1				-8.876			<0.0001
x_1x_2				9.012			<0.0001
x_1z_1				4.623			0.0006
x_2z_1				3.452			0.0048
x_3z_1				0.891			0.3907

diagnostic measures showed that there were no outliers or influential points. Normal probability and residual plots were used to confirm that normality and constant variance assumptions on the residuals were satisfied.

Since our objective is to minimize the response (i.e., $T = 0$) for all values of z_1 , \mathbf{x}^* is the value of \mathbf{x} which satisfies

$$\max_{\{-1 \leq z_1 \leq 1\}} \hat{y}(\mathbf{x}^*, z_1) = \min_{\{-1 \leq x_i \leq 1; i=1, 2, 3\}} \max_{\{-1 \leq z_1 \leq 1\}} \hat{y}(\mathbf{x}, z_1).$$

Using the IER-MCS algorithm (see Section 4) implemented in Matlab, we obtain $\mathbf{x}^* = (x_1 = 1, x_2 = 1, x_3 = 1)$.

We, next compare our results with those of Myers et al. (1992). The performance criterion of

Myers et al. (1992) is,

$$E_{z_1}(\hat{y}(\mathbf{x}, z_1) - T)^2 = (E_{z_1}\hat{y}(\mathbf{x}, z_1) - T)^2 + \text{Var}_{z_1}\hat{y}(\mathbf{x}, z_1), \quad (5.2)$$

where $T = 0$, $E_{z_1}\hat{y}(\mathbf{x}, z_1) = 741.57 - 121.74x_1 - 118.07x_2 - 28.33x_3 + 121.96x_1x_2$ and $\text{Var}_{z_1}\hat{y}(\mathbf{x}, z_1) = (-103.64 + 53.97x_1 + 40.31x_2 + 10.08x_3)^2 + (51.35)^2$, making the assumptions that $E(z_1) = 0$ and $\text{Var}(z_1) = 1$. The value of \mathbf{x} which minimizes (5.2), denoted by \mathbf{x}_{MKV} , is $\mathbf{x}_{\text{MKV}} = (x_1 = 1, x_2 = -0.4299, x_3 = 1)$. Figure 5.1 shows a comparison of $M(\mathbf{x}^*, z_1)$ and $M(\mathbf{x}_{\text{MKV}}, z_1)$ against values of z_1

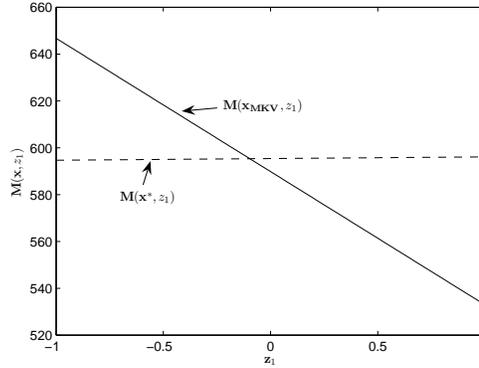


Figure 5.1: Comparison of $M(\mathbf{x}^*, z_1)$ and $M(\mathbf{x}_{\text{MKV}}, z_1)$ against $z_1 \in [-1, 1]$.

in $[-1, 1]$. From the figure we see that the worst (maximum) value of the head injury criteria when $\mathbf{x} = \mathbf{x}^*$ is 596.11 at $z_1 = 1$ (i.e., angle of head impact is 90 degrees). While, the worst (maximum) value of the head injury criteria at \mathbf{x}_{MKV} is 646.74 at $z = -1$. Also we note that for values of z_1 in the interval $[-1, -0.10]$, $M(\mathbf{x}^*, z_1) < M(\mathbf{x}_{\text{MKV}}, z_1)$. This implies that choosing $\mathbf{x} = \mathbf{x}_{\text{MKV}}$ results in a worse deviation due to noise in the interval $[-1, -0.10]$ than selecting $\mathbf{x} = \mathbf{x}^*$. Thus, we see that for quite a wide interval of values of the angle of impact the min-max settings of the control variables give a lower HIC than the settings of Myers et al. (1992).

It should, however, be noted that it may not always be possible to meet the required quality standards using this methodology. For example, if in the current example, the product requires a guaranteed quality quantified as $\hat{y}(\mathbf{x}, z_1) < 500$, then evidently, our methodology fails to give satisfactory results. In such a case any of the alternatives suggested in Section 3.1 (unacceptable worst deviation) may be used to meet the required quality standards.

5.2 Example 2: Granulation of drugs

We consider here a data set based on drug granulation in a 10 l high shear mixer from Vojnovic et al. (1996). The response studied is the percentage in weight of granules smaller than $200 \mu m$. The objective of this experiment is to maintain an uniform granule size of 200μ . This will be achieved by minimizing the number of granules smaller than $200 \mu m$ in size. Note that the experimenter is not concerned with granule sizes larger than $200 \mu m$, since larger granules are removed automatically during the prior filtration process. The control factors known to affecting the response y are moisture level (%) and massing time (minute). In previous studies (Vojnovic et al. (1993) and Ogawa et al. (1994)) found that the impeller speed (measured in rpm) is also an important factor affecting y . However, due to the difficult to control nature of impeller speed they considered it as a noise variable. Each factor and the levels (coded and uncoded) between which they vary are listed in Table 4. As explained in Section 1 it is critical that all the granules are of size $200 \mu m$, otherwise the tablets formed may contain varying concentrations of the active ingredient. Using our min-max methodology in this situation, we are able to find the control settings which guarantee that the response is minimized for all values of the impeller speed.

Table 4: Control and noise variables with their levels (Ex 5.2)

Factors	-1	0	1
Moisture level (x_1)	20%	30%	40%
Massing time (x_2)	3 mins	5 mins	7 mins
Impeller speed (z_1)	100 rpm	200 rpm	300 rpm

Table 5 shows the design points and the response values. The center point is replicated five times. In this example, $R_x = \{-1 \leq x_i \leq 1; i = 1, 2\}$ and $R_z = \{-1 \leq z_1 \leq 1\}$. We started with fitting a second order model to y , however the error variance was not constant. The Box-Cox procedure in SAS 9.1.3 suggested a square root transformation on the response. Thus, we fit the following model to $y^* = \sqrt{y}$,

$$\hat{y}^*(\mathbf{x}, z_1) = 3.82 - 2.49x_1 - 0.91x_2 - 1.41z_1 - 0.07x_1^2 + 0.27x_2^2 + 0.44z_1^2 + 0.34x_1x_2 - 0.65x_1z_1 - 1.03x_2z_1. \quad (5.3)$$

The analysis of variance results are shown in Table 6. Here also, normal probability and residual plots

Table 5: Design and response values (Ex 5.2)

X_1	X_2	Z_1	x_1	x_2	z_1	y	X_1	X_2	Z_1	x_1	x_2	z_1	y
40	5.5	225	1	0.25	0.25	0.47	30	6.5	125	0	0.75	-0.75	27.17
20	4.5	175	-1	-0.25	-0.25	43.82	22.5	5	275	-0.75	0	0.75	27.58
32.5	7	225	0.25	1	0.25	3.68	30	3.5	275	0	-0.75	0.75	19.27
27.5	3	175	-0.25	-1	-0.25	34.6	30	5	200	0	0	0	14.24
37.5	3.5	200	0.75	-0.75	0	6.18	30	5	200	0	0	0	14.65
22.5	6.5	200	-0.75	0.75	0	25	30	5	200	0	0	0	16.23
32.5	5.5	300	0.25	0.25	1	2.63	30	5	200	0	0	0	13.87
27.5	4.5	100	-0.25	-0.25	-1	37.65	30	5	200	0	0	0	14.04
37.5	5	125	0.75	0	-0.75	12.56							

$$x_i = \frac{2X_i - [\max(X_i) + \min(X_i)]}{[\max(X_i) - \min(X_i)]}; \quad i = 1, 2; \quad z_1 = \frac{2Z_1 - [\max(Z_1) + \min(Z_1)]}{\max(Z_1) - \min(Z_1)}.$$

showed that the normality and constant variance assumptions on the residuals were satisfied. Since our interest is in minimizing y , \mathbf{x}^* is the value of \mathbf{x} satisfying,

$$\max_{\{-1 \leq z_1 \leq 1\}} \hat{y}^*(\mathbf{x}^*, z_1).$$

Using the IER-MCS algorithm we obtain, $\mathbf{x}^* = (x_1 = 1, x_2 = -0.86004)$. The worst (minimum) value of the response when $\mathbf{x} = \mathbf{x}^*$ is 3.56. We do not compare our results with those of Myers et al. (1992) for this particular problem. In their paper, Myers et al. (1992) discussed the methodology of obtaining robust design for models with linear terms in the noise variable. However, the fitted model in this example involves a quadratic term in the noise variable. To compute the performance criterion (5.2) of Myers et al. (1992) we require some assumptions on the fourth order moment of z_1 , $E(z_1^4)$. The min-max strategy proposed in this paper however does not need to make any such assumptions on the moments of the noise variable. To apply our method we need to know only the interval in which the noise variable lies in, as illustrated in this example.

5.3 Example 3: Filtration rate of a chemical compound

We consider a data set taken from Robinson et al. (2004) [Table 1] which studies the effect of four factors on the rate of filtration of a chemical product (y). There are three control variables: x_1 (pressure), x_2 (concentration of formaldehyde), x_3 (stirring rate) and one noise variable: z_1 (temperature). Each factor is present at two levels. A 2^4 factorial design was used to get the response values. Here,

Table 6: Analysis of variance (Ex 5.2)

Source	df	SS	MS	F	p-value	R^2	adjusted- R^2
Model	9	42.735	4.748	284.4266	<0.0001	0.9973	0.9938
Residuals	7	0.117	0.017				
Lack of fit	3	0.057	0.019	1.2531	0.402		
Pure error	4	0.060	0.015				
variable				partial t		p-value	
x_1				-40.935		<0.0001	
x_2				-14.861		<0.0001	
z_1				-23.076		<0.0001	
x_1^2				-0.749		0.4782	
x_2^2				2.908		0.0227	
z_1^2				4.793		0.0020	
x_1z_1				-4.494		0.0028	
x_2z_1				-7.098		0.0002	
x_1x_2				2.330		0.0526	

$R_x = \{-1 \leq x_i \leq 1; i = 1, 2, 3\}$ and $R_z = \{-1 \leq z_1 \leq 1\}$. The goal is to determine the settings of the control variables for which y reaches a target of 75, for all settings of z_1 .

Using the same fitted model as in Robinson et al. (2004) for the response,

$$\hat{y}(\mathbf{x}, z_1) = 70.06 + 10.81z_1 + 4.94x_2 + 7.31x_3 - 9.06x_2z_1 + 8.31x_3z_1,$$

where $\mathbf{x} = (x_2, x_3)$. The corresponding analysis of variance results are shown in Table 7. Our per-

Table 7: Analysis of variance (Ex 5.3)

Source	df	SS	MS	F	p-value	R^2	adjusted- R^2
Model	5	5535.8	1107.2	56.7412	<0.0001	0.966	0.9489
Residuals	10	195.1	19.5				
Lack of fit	2	15.6	7.8	0.3482	0.7162		
Pure error	8	179.5	22.4				
variable				partial t		p-value	
x_2				6.622		<0.0001	
x_3				4.471		0.00120	
z_1				9.791		<0.0001	
x_2z_1				-4.494		0.0028	
x_3z_1				-8.206		<0.0001	

formance criterion is $M(\mathbf{x}, z_1) = (\hat{y}(\mathbf{x}, z_1) - 75)^2$. Following the min-max strategy we find, $\mathbf{x}^* =$

$(x_2 = 1, x_3 = -0.21)$. We, compare our results with those of Myers et al. (1992), where $\mathbf{x}_{\text{MKV}} = (x_2 = 1, x_3 = -0.1211)$. Figure 5.2 shows a comparison of $M(\mathbf{x}^*, z_1)$ and $M(\mathbf{x}_{\text{MKV}}, z_1)$ against val-

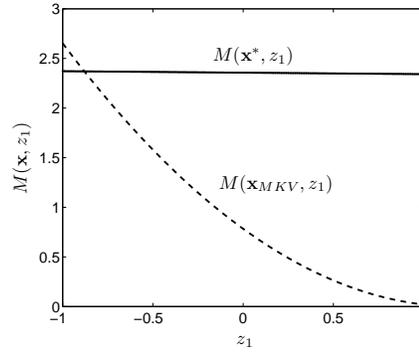


Figure 5.2: Comparison of $M(\mathbf{x}^*, z_1)$ and $M(\mathbf{x}_{\text{MKV}}, z_1)$ against $z_1 \in [-1, 1]$.

ues of z_1 in $[-1, 1]$. We note from Figure 5.2 that for values of z_1 in the interval $[-1, -0.879]$, $M(\mathbf{x}^*, z_1) < M(\mathbf{x}_{\text{MKV}}, z_1)$.

5.4 Example 4

The data set is taken from (Myers et al., 1992) [Table 1]. There are two control variables (x_1 and x_2) and two noise variables (z_1 and z_2). Each factor is at two levels, -1 and 1 . A 2^4 factorial design in the control and noise variables, with five center runs was used. Interest here is to determine the settings of $\mathbf{x} = (x_1, x_2)'$ which maximizes the worst (minimum with respect to $\mathbf{z} = (z_1, z_2)'$ in R_z) response.

Using the same fitted model for the response as in Myers et al. (1992),

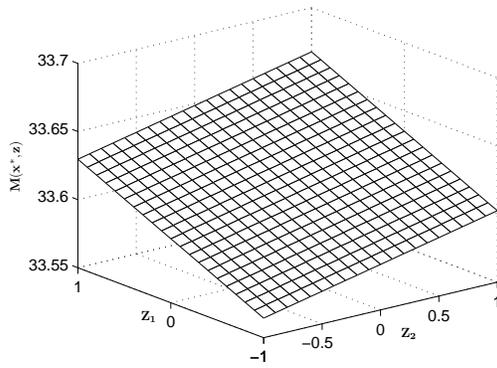
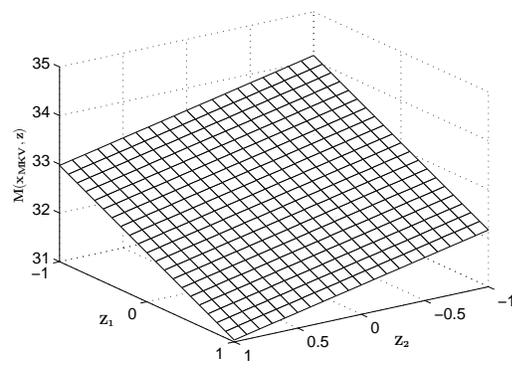
$$\hat{y}(\mathbf{x}, \mathbf{z}) = 24.472 + 6.89x_1 - 9.11x_2 + 4.94z_1 + 3.52x_1x_2 + 3.23x_1z_1 + 1.88x_1z_2. \quad (5.4)$$

The corresponding analysis of variance results are shown in Table 8. As in Section 3.2, \mathbf{x}^* is the setting of the control factors which satisfies, $\max_{\{-1 \leq x_i \leq 1; i=1,2\}} \min_{\{-1 \leq z_i \leq 1; i=1,2\}} \hat{y}(\mathbf{x}, \mathbf{z})$. Using the IER-MCS algorithm we obtain, $\mathbf{x}^* = (x_1 = 0.0101, x_2 = -1)$. The approach by Myers et al. (1992) yields $\mathbf{x}_{\text{MKV}} = (x_1 = -0.3, x_2 = 1)$. The variation in the values of the responses $\hat{y}(\mathbf{x}^*, \mathbf{z})$ and $\hat{y}(\mathbf{x}_{\text{MKV}}, \mathbf{z})$ over different values of the noise variables in R_z is shown in Figure 5.3a and Figure 5.3b, respectively. From the figures it may be observed that the worst (minimum) value of $\hat{y}(\mathbf{x}^*, \mathbf{z}) = 33.56$ which occurs at $(z_1 = -1, z_2 = -1)$ while the worst value of $\hat{y}(\mathbf{x}_{\text{MKV}}, \mathbf{z}) = 31$ for $(z_1 = +1, z_2 = +1)$.

Table 8: Analysis of variance (Ex 5.4)

Source	df	SS	MS	F	p-value	R^2	adjusted- R^2
Model	6	2868.03	478.01	81.8816	<0.0001	0.9723	0.9604
Residuals	14	81.73	5.84				
Lack of fit	10	54.46	5.45	0.7987	0.6495		
Pure error	4	27.27	6.82				

variable	partial t	p-value
x_1	11.345	<0.0001
x_2	-15.005	<0.0001
z_1	8.099	<0.0001
x_1z_1	5.430	<0.0001
x_2z_2	3.054	0.00858
x_1x_2	5.746	<0.0001

(a) $M(\mathbf{x}^*, \mathbf{z})$ versus \mathbf{z} (b) $M(\mathbf{x}_{MKV}, \mathbf{z})$ versus \mathbf{z} Figure 5.3: Comparison of $M(\mathbf{x}^*, \mathbf{z})$ and $M(\mathbf{x}_{MKV}, \mathbf{z})$ over $\{-1 \leq z_i \leq 1, i = 1, 2\}$

6 Concluding Remarks

In certain processes where it is very important to keep the estimated response near the target for all values of the noise, the min-max approach is the only technique which guarantees that the quality of each and every product is better than some guaranteed worst quality. However, determining the min-max setting in most general situations is difficult using conventional optimization techniques. To overcome this difficulty, a computational method for the optimal control setting, based on the iterative entropic regularization algorithm coupled with a global multilevel coordinate search, is proposed. The algorithm is shown to provide satisfactory solutions to the numerical examples considered. Additionally, it is shown using the numerical examples, that variance minimizing methods may sometimes fail to keep the estimated response near the target for all settings of the noise variable for sensitive processes, thus giving rise to a worse guaranteed quality. The proposed min-max method can be used

in various industries like drug manufacturing, defence, auto industry to deliver robust products. The methodology works without requiring any assumptions on the distributional properties of the noise variables. Furthermore, the above described min-max formulation can also be extended to include cases where the noise variable is categorical or quantitative in nature.

As in all model-based approaches, the value of the min-max control settings depends on the model chosen to fit the process response and any misspecification in the model may lead to a change in the optimal settings. However, we do not take into account the implications of model misspecification in this paper and leave it for future research. One possible method to tackle this problem of model misspecification may be to use non-parametric or semi-parametric techniques to model the response as suggested by Pickle et al. (2008).

The R and Matlab codes used to compute the optimum control settings for this article are available on request from the first author.

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