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Robust parameter design in embedded high-variability production processes: an alternative approach to mitigating sources of variability

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Many of today's industrial firms seek the continuous and systematic reduction of variability as a primary engineering goal across key production dimensions. Robust parameter design (RPD) is often considered among the most important methods for achieving these ends. Focused on statistical modelling and numerical optimisation strategies, most researchers typically assume processes possess moderate to low variability, which facilitates the use of ordinary least squares (OLS) regression. Realistically, however, industrial processes often exhibit high variability. In such cases, many of the modelling assumptions underpinning OLS methods do not hold. Consequently, the results and recommendations provided to decision-makers using these could generate suboptimal modifications to processes and products. This paper proposes an alternative method for dealing with high process variability. Specifically, using the coefficient of variation to identify influential sources of variability between design points, the proposed method advocates removing these sources and then applying optimal design theory to rebalance the experimental framework. Thereafter, RPD optimisation schemes may be applied to obtain more precise optimal operating conditions with less variability and bias. A numerical example combined with Monte Carlo simulation is used to illustrate the proposed procedure.

Keywords: robust parameter design; optimal design; response surface methodology; coefficient of variation

1. Introduction

1.1 *Introductory remarks*

Contemporary efforts in production engineering and quality control/assurance embrace variability reduction as a primary means to improve product quality in terms of achieving performance targets while reducing defects. In fact, many firms today seek the continuous and systematic reduction of variability as a primary engineering goal across key process and product dimensions. Typically associated with unwanted process conditions, variation may be defined as the difference between a current reality in the context of system performance and a desired end-state. Clearly, nearly all manufacturing and product performance processes possess some degree of variation. Variation occurs in all production processes, even those in which it may appear non-existent. If variation cannot be measured, it is most likely because the measurement systems being used do not possess sufficient capabilities in terms of precision and accuracy. Certainly, some processes will tend to possess more than others, depending on the type of process, what is being measured, and who/what is measuring it. Notwithstanding, irrespective of the degree of variability that exists, managing and reducing it requires that it be traced back to its sources.

In solving this problem, a variety of assumptions are made in order to facilitate the application of ordinary least squares (OLS) regression. These include normality, independence and constant variance (or homoscedasticity) in the residuals. By extension, the validity of these assumptions, namely the last regarding constant variance, also presume moderate to low degrees of inherent process variability or that the process is stable. When these assumptions fail, however, alternative methods to OLS regression become necessary. When high variability is the culprit, the most common approach is the application of weighted least squares (WLS) regression. While effective and time-tested, the precision of results obtained via the WLS method still can be negatively affected when high process variability exists. Moreover, this method is applied in the post-experimentation phase, *after* the development of fitted response surface estimators.

This paper proposes an alternative method for dealing with inherently high process variability in the experimental phase itself. In particular, pursuant to a thorough data analysis to identify sources of variability using the coefficient of variation (CV) as a distinguishing factor between design points, the proposed method advocates removing sources of

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variability and then applying optimal design theory to rebalance the experimental framework. Thereafter, fitted response surfaces are developed and commonly known robust parameter design (RPD) optimisation schemes may be applied to obtain more precise optimal operating conditions with less variability and bias.

1.2 *Literature review*

In the 1980s, Taguchi (1986, 1987) introduced the RPD concept as a customer-focused quality engineering methodology that aims to achieve customer specifications while minimising variability and costs in the results. This methodology has generated a considerable level of interest among researchers and practitioners over the years. However, despite the widely recognised contributions of Taguchi's philosophical approaches to quality engineering, many researchers have scrutinised his methods (see Nair 1992). Among several criticisms of Taguchi's analytical and experimental design approaches, the general consensus was that his methodology merely facilitated process improvement rather than optimisation. Accordingly, many researchers proposed RPD models that investigated a variety of alternative optimisation methodologies more firmly grounded in well-established approaches to experimental design, most notably dual response methods and response surface methodology (RSM), which predate Taguchi's methods by more than three decades. In the RPD context, the dual response approach uses separate response function estimators for the process mean $\hat{\mu}(x)$ and standard deviation $\hat{\sigma}(x)$ as the basis for determining the optimal operating conditions (or factor settings) that would minimise variability while achieving a specified target threshold. The numerous optimisation schemes developed over the years use these functions in a variety of ways to achieve optimal operating conditions; Table 1 depicts some of the more commonly applied approaches found in the literature.

Initial efforts by Vining and Myers (1990) focused on a priority-based scheme which constrained results to strict adherence to desired targets in the spirit of Taguchi's philosophy. However, subsequent research by Cho (1994) and Lin and Tu (1995) demonstrated that allowing for some bias in process targets could facilitate even further reductions in variability, which led to their mean square error (MSE)-based schemes. This sparked a debate regarding the amount of bias that could

Table 1. Common optimisation schemes applied in contemporary RPD research.

	Quality characteristic type		
Reference	S-type	N-type	L-type
Vining and Myers (1990)	Minimise $\hat{\mu}$ Subject to: $\hat{\sigma} = \tau_\sigma$	Minimise $\hat{\sigma}$ Subject to: $\hat{\mu} = \tau_\mu$	Minimize $\hat{\mu}$ Subject to: $\hat{\sigma} = \tau_\sigma$
Cho (1994), Lin and Tu (1995)	Min $(\omega\hat{\mu}^2 + (1-\omega)\hat{\sigma}^2)$	Min $(\omega(\hat{\mu} - \tau_\mu)^2 + (1-\omega)\hat{\sigma}^2)$	Min $(-\omega\hat{\mu}^2 + (1-\omega)\hat{\sigma}^2)$
Copeland and Nelson (1996)	Minimise $\hat{\mu}$ Subject to: $\hat{\sigma} \leq U_\sigma$	Minimise $\hat{\sigma}$ Subject to: $(\hat{\mu} - \tau_\mu)^2 \leq \Delta^2$	Minimize $\hat{\mu}$ Subject to: $\hat{\sigma} \leq U_\sigma$
Kim and Lin (1998)	$z = \frac{\hat{y}-L}{U-L}$	Maximise λ Subject to $d_j(Z) \leq \lambda, \quad j = \mu, \sigma$ With $d_j(z) = \begin{cases} \frac{\exp(t)-\exp(t\lvert z\rvert)}{\exp(t)-1}, & t \neq 0 \\ 1-\lvert z\rvert, & t = 0 \end{cases}$ $z = \frac{\hat{y}-\tau}{\tau-L}$	$z = \frac{U-\hat{y}}{U-L}$
Tang and Xu (2002)		Minimise $(\delta_\mu^2 + \delta_\sigma^2)$ Subject to $\hat{\mu} - \omega_\mu\delta_\mu = \tau_\mu$ and $\hat{\sigma} - \omega_\sigma\delta_\sigma = \tau_\sigma$	
Kim and Cho (2002)		Minimise $\omega_\mu^-(g_\mu^-)^2 + \omega_\mu^+(g_\mu^+)^2 + \omega_\sigma(\tau_\sigma - g_\sigma^- - g_\sigma^+)^2$ Subject to $\hat{\mu} + g_\mu^- - g_\mu^+$ and $\hat{\sigma} + g_\sigma^- - g_\sigma^+ = \tau_\sigma$ with $g_\mu^- * g_\mu^+ = 0, \quad g_\sigma^- * g_\sigma^+ = 0$, and $g_\mu^-, g_\sigma^+, g_\sigma^-, g_\sigma^+ \geq 0$	
Shaibu and Cho (2009)	Min $(\hat{\mu} + (\hat{\sigma} - \tau_\sigma)^2)$	Min $((\hat{\mu} - \tau_\mu)^2 + (\hat{\sigma} - \tau_\sigma)^2)$	Min $(-\hat{\mu} + (\hat{\sigma} - \tau_\sigma)^2)$
Costa (2010)		Minimise $\left(\frac{\lvert\hat{\mu}(\mathbf{x})-\tau_\mu\rvert}{U_\mu - L_\mu}\right)^{\omega_\mu} + \left(\frac{\lvert\hat{\sigma}(\mathbf{x})-\tau_\sigma\rvert}{U_\sigma - L_\sigma}\right)^{\omega_\sigma}$	

or should be allowed, leading Copeland and Nelson (1996) to propose a model which constrained the degree of allowable bias to some fixed level, Δ. Others, still, explored the concept of specifying allowable biases in both the process and variability targets, incorporating weighting schemes in some instances to distinguish relative priorities between the two.

Numerous researchers have developed extensions of these models, contributing to the breadth of knowledge in the field. Many of these, including Kim and Lin (1998, 2006), Tang and Xu (2002), Kim and Cho (2002), and Koksoy and Yalcinoz (2008), are extensively delineated in Robinson, Borror, and Myers (2004), Costa (2010), Truong and Shin (2012), Shin and Cho (2009), Shin et al. (2011), Kovach and Cho (2007b, 2008), Shaibu, Cho, and Kovach (2009) and Kovach, Cho, and Antony (2009).

The vast majority of research in the literature, including the various works listed above, uses OLS regression as a basis for model development and optimisation. In many cases, this is because the same data-sets are used to facilitate comparisons between alternative approaches. As such, the same assumptions initially made on a particular data-set tend to carry through the other research efforts that utilise it. However, a number of researchers have explored situations in which certain assumptions fail to hold, most notably, the assumption of constant variance in the residuals. While some researchers, such as Lee and Nelder (2003), have examined the use of generalised linear models in such situations, the most common alternative has been the WLS approach. Cho and Park (2005) used a WLS approach in RPD applications involving unbalanced data-sets in which the number replicates between design points vary, which in turn can induce non-constant variance in the residuals. They suggested the use of a weighting scheme based on the number of replicates at a particular design point to overcome this shortfall, which proved to outperform the OLS approach typically applied in such situations. Similarly, Goethals and Cho (2011) utilised the WLS approach in the context of the optimal process target problem, applying an iterative reweighting scheme to overcome the effects of heteroscedasticity. Chen, Yang, and Hsia (2008) used WLS regression to develop response surface estimates for demand product mix in a semiconductor manufacturing study. In particular, they apply a time-based dynamic weighting scheme to account for disparate demand emphases across time periods and thereby obtain more accurate estimates of the optimal product mix. In a tangential engineering field, Li and Korakiantis (2011) used a non-linear WLS approach to accurately estimate the health of gas-turbine engines.

1.3 *Motivating concept*

In the traditional RPD research, it is usually assumed that moderate variability in system responses, as well as normality, homoscedasticity and independence among the residuals are valid within a set of observational data to support the application of OLS regression in obtaining unbiased, minimum variance estimates. While this may greatly simplify a problem, it is often the case that such conditions do not hold in many industrial settings. In fact, virtually every facet of a manufacturing process (materials, work methods, machinery, measurement, human interaction, etc.) possesses inherent variability and in many cases the associated levels can be comparatively high. In turn, this can introduce non-constant variance in the residuals of system outputs. The reality of such conditions can complicate the search for optimal solutions using the OLS approach and highlights the need to consider alternative approaches.

To motivate this concept, consider a well-known experiment involving a printing press that has served as a basis of comparison for many of the optimisation schemes discussed in Section 2. Introduced by Box and Draper (1987), the experiment concerns a printing machine's index in applying colouring inks to package labels, which is a normally distributed N-type quality characteristic of interest, Y. Three factors are known to influence Y: the speed (X_1), pressure (X_2) and distance (X_3) settings for the machine. The desired target value for the machine's index is $\tau = 500$. Table 2 displays the experimental framework for this study, along with the calculations for the mean and standard deviation at each design point.

Using this framework, previous researchers developed second-order response surface designs for the mean and standard deviation and then applied their particular optimisation scheme to identify optimal solutions $\mathbf{x}^* = (X_1^*, X_2^*, X_3^*)$. However, as Myers and Montgomery (1995) note, these solutions are, in fact, simply estimates and subsequent implementations of the experiment could very well yield a different set of optimal coordinates. As an example, suppose this particular experiment is repeated 500 times via Monte Carlo simulation, using the vectors for the mean and standard deviation in Table 2 as the basis for generating random variates. Additionally, the *MSE*-based optimisation scheme proposed by Cho (1994) and Lin and Tu (1995) is used in each instance to determine $\mathbf{x}^*$. Figure 1(a) shows the set of all 500 optimal points $\mathbf{x}^*$ identified in the simulation. The corresponding figures in (b)–(d) show the relative positions of these solutions as they relate to each cross-section of factors. Global solutions at each iterate are obtained via a random search technique coupled with a large search-point array.

From the various plots in Figure 1, it is clear that the experimental region is confining the potential solution space. Thus, if the experimental region is expanded fourfold to $-4 \leqslant X_i \geqslant 4$ and the simulation is repeated, the extent of the optimal operating region for this example is more readily observed (Figure 2). Although this presents an extrapolated

Table 2. Experimental design for the printing press study.

Run	Coded units: Speed X_1	Pressure X_2	Distance X_3	Labelling index Y (3 replications): y_1	y_2	y_3	Mean $\bar{y}$	Standard deviation s
1	−1	−1	−1	34	10	28	24.00	12.490
2	0	−1	−1	115	116	130	120.33	8.386
3	1	−1	−1	192	186	263	213.67	42.829
4	−1	0	−1	82	88	88	86.00	3.464
5	0	0	−1	44	188	188	140.00	83.138
6	1	0	−1	322	350	350	340.67	16.166
7	−1	1	−1	141	110	86	112.33	27.574
8	0	1	−1	259	251	259	256.33	4.619
9	1	1	−1	290	280	245	271.67	23.629
10	−1	−1	0	81	81	81	81.00	0.000
11	0	−1	0	90	122	93	101.67	17.673
12	1	−1	0	319	376	376	357.00	32.909
13	−1	0	0	180	180	154	171.33	15.011
14	0	0	0	372	372	372	372.00	0.000
15	1	0	0	541	568	396	501.67	92.500
16	−1	1	0	288	192	312	264.00	63.498
17	0	1	0	432	336	513	427.00	88.606
18	1	1	0	713	725	754	730.67	21.079
19	−1	−1	1	364	99	199	220.67	133.822
20	0	−1	1	232	221	266	239.67	23.459
21	1	−1	1	408	415	443	422.00	18.520
22	−1	0	1	182	233	182	199.00	29.445
23	0	0	1	507	515	434	485.33	44.636
24	1	0	1	846	535	640	673.67	158.210
25	−1	1	1	236	126	168	176.67	55.510
26	0	1	1	660	440	403	501.00	138.935
27	1	1	1	878	991	1161	1010.00	142.454

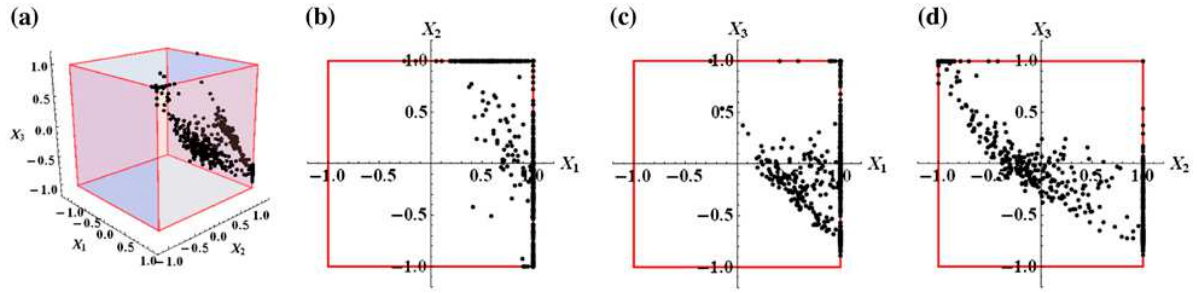


Figure 1. Identification of $\mathbf{x}^*$, printing press study, $-1 \leqslant X_i \leqslant 1$ (500 iterations).

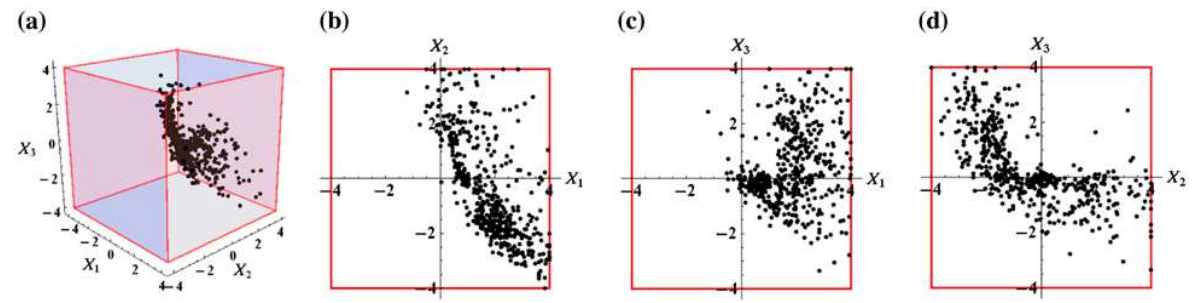


Figure 2. Identification of $\mathbf{x}^*$, printing press study, $-4 \leqslant X_i \leqslant 4$ (500 iterations).

view of the design space, it facilitates a clearer illustration of what is occurring and more effectively portrays the imprecision among the generated solutions.

These results demonstrate a weakness in the design of the RPD problem for processes that possess inherently high variability. In short, because the number of replications at each design point is typically low, repeating the experiment under identical conditions can yield a set optimal coordinates that span the full expanse of the factor space, or more. This indicates considerable imprecision in the estimated functions used to generate the factor settings and further suggests that, because of the high variability, the obtained results are very likely questionable.

Additional replications could be performed at each design point to mitigate issues with high variability but constraints on time and other resources typically preclude it. As such, alternative approaches must be considered to more directly address the sources of variability. Certainly, time, costs and a variety of other resource constraints will impact the experimental approaches employed, but this should be weighed against the need for elevated levels of precision. In short, if our model is imprecise in estimating the appropriate response surface, then optimising that model is going to yield equally imprecise results as they relate to the true optimal factor settings. Accordingly, the results and recommendations provided to decision-makers could generate suboptimal modifications to processes and products. This paper proposes an alternative technique that uses the CV to identify and extract sources of variability and then use optimal design to restructure the experimental approach in order to obtain more precise RPD solutions. In section two, the methodology for the proposed approach is outlined. Thereafter, a numerical example and simulation are used to illustrate potential benefits.

2. Methodology development

2.1 *Experimentation and analysis*

Experimentation and analysis begin with the specification of response variables, factors or predictors influencing the responses, and a region of interest for a designed experiment. Suppose the objective is to identify the optimal factor settings $\mathbf{x}^* = (X_1^*, X_2^*, \ldots, X_k^*)$ that support achieving a mean process performance with minimal deviation from a desired target and with minimum variability in the result. Pursuant to this, consider an experimental framework whereby a quality characteristic, Y, is influenced by a set of control factors $X_1, X_2, \ldots, X_k$. The experiment consists of n design points, or runs, each of which contains m replicates for the observed response. Let y_{qj} denote the jth response at the qth design point, where $q = 1, \ldots, n$ and $j = 1, \ldots, m$. Table 3 portrays the framework for such an experiment.

The replicates at each design point are then used to obtain parameter estimates for the mean and standard deviation using the following formulas:

$$\bar{y}_q = \frac{\sum_{j=1}^{m} y_{qj}}{m_q}, \quad s_q = \sqrt{\frac{\sum_{j=1}^{m} \left(y_{qj} - \bar{y}_q\right)^2}{m_q - 1}} \tag{1}$$

Prior to the final estimation of response surface functions for the process mean and variability, a comprehensive data analysis of both the responses and the residuals must be performed to ascertain the underlying conditions in the data. This includes an investigation of normality and variability in the process responses, as well as the verification of the assumptions of normality, constant variance, and independence in the residuals. These may be investigated via an assortment of graphical and statistical methods, which may include those briefly discussed in (1)–(3) below:

(1) To assess deviations from normality, researchers often use either the Kolmogorov-Smirnov test for large samples (>2000), or the Shapiro-Wilk test for small or medium-sized samples. Generally, in RPD experimentation the obtained sample sizes fall in the latter category. Thus, for the Shapiro-Wilk test, when the p observations made

Table 3. Experimental RSM framework.

Design point	X_1 X_2 .... X_k	Replications	$\bar{y}$	s
1	Control factor settings	y_{11} ... y_{1m}	$\bar{y}_1$	s_1
⋮		⋮ ⋮	⋮	⋮
q		y_{q1} ... y_{qm}	$\bar{y}_q$	s_q
⋮		⋮ ⋮	⋮	⋮
n		y_{n1}...y_{nm}	$\bar{y}_n$	s_n

on quality characteristic are sorted in ascending order, the alternative hypotheses $H_0 : Y \in N(\mu, \sigma^2)$ and $H_1 : Y \notin N(\mu, \sigma^2)$ are evaluated using the W statistic given by:

$$W^* = \left[\frac{b}{s\sqrt{p-1}}\right]^2, \quad \text{where } b = \sum_{l=1}^{\kappa} a_{p-l+1}\left[y_{(p-l+1)} - y_l\right] \tag{2}$$

Different from most statistical tests, since the critical region lies in the small tail of the distribution, if $W^* > W_\alpha$ then H_0 is concluded (that is, sufficient evidence exists to suggest the observations follow a normal distribution).

(2) A trademark of high variability data is that their sample standard deviation is in general quite large, implying a 'largely uninformative' sample mean that fails to adequately describe the location of the bulk of the observed values. Willinger, Alderson, and Lun (2004) associated high variability with situations in which a set of observations assume values that vary over orders of magnitude, with most observations taking values that are relatively close together, with a few extreme observations attaining values that deviate considerably from this first group with non-negligible probabilities, and with intermediate-sized observations occurring with appreciable frequencies. Using this concept, a highly variable process is classified as one in which the range of variability in the responses is noticeably large and where one or more of the responses lies more than three standard deviations ($+/-3\sigma$) from the mean response.

(3) The investigation of non-constant variance typically involves the use of graphical measures, such as a plot of the residuals against the fitted values, as well as objective hypothesis testing using either the Brown-Forsythe test, which is more robust to departures from normality in the data, or the Breusch-Pagan test. The Breusch-Pagan test assumes independence and normality among the residuals, but further assumes a relationship for the error variance σ_q^2 among the k regression coefficients and $k-1$ predictor variables that takes the form $\log_e \sigma_q^2 = \gamma_0 + \gamma_1 X_{q1} + \cdots + \gamma_{k-1} X_{q,k-1}$, and implies that the error variance fluctuates up or down with $\mathbf{x}$, based on the sign of the associated coefficients. Since constant error variance corresponds to the instance in which each of the coefficients contained in response function equals 0, the alternative hypotheses $H_0 : \gamma_1 = \gamma_2 = \cdots = \gamma_{k-1} = 0$ vs. H_1 : not all $\gamma_i = 0$ are tested using the statistic:

$$\chi^2_{\mathrm{BP}} = \frac{\mathrm{SSR}^*}{2} \div \left(\frac{\mathrm{SSE}}{Nm}\right)^2 \tag{3}$$

in which Nm denotes the total number of experimental observations, SSR^* is the regression sum of squares obtained by regressing the squared residuals, e_j^2, against one or more of the predictor variables, and SSE is the error sum of squares obtained for the full regression model. Comparing this statistic to the chi-square distribution with $k-1$ degrees of freedom, if $\chi^2_{\mathrm{BP}} > \chi^2_{(1-\alpha),k-1}$ H_0 is rejected and it is concluded that sufficient evidence exists to suggest non-constant variance. In processes with inherently high variability or even asymmetry in the responses, the assumption of constant variance in the residuals would most likely not hold and would thereby necessitate the use of remedial measures or alternative approaches to OLS regression for the development of fitted response surface functions.

2.2 *Identifying and overcoming sources of variability*

Pursuant to an analysis of the responses and residual errors, the effort to reduce the influences of system variation relies on the identification and mitigation of those influences at their sources. This section describes two approaches to achieving this. First, the WLS method provides a means for strictly mitigating sources of variability through a priority-based weighting scheme. The second consists of the proposed alternative which uses the CV as a way to identify and eliminate the most influential sources of variability and thereby attain greater degrees of precision. The key differences between these two approaches lie in the manner in which they deal with sources of variability, which are described in the following subsections.

2.2.1 *The WLS approach*

Traditionally, when heteroscedastic conditions prevail, investigators use one of two alternative approaches to obtaining improved estimators for the mean and standard deviation response surface functions. These include either a transformation of the response variable Y, which essentially induces constant variance by equalising the error variation across all predictor variables, or through the application of a WLS approach in the estimation process to mitigate the effects of unequal error deviations. While either method may work well in a broad variety of applications, the WLS approach seems to be the most common choice, as it avoids the possibility of an inappropriate regression relationship which can result from transformations of Y.

Since the error variance is rarely known, two approaches for developing estimates of the variance σ_j^2 are considered. First, it can be shown that $\sigma_j^2 = E[\varepsilon_j^2]$. Letting $E[\varepsilon_j^2] = e_j^2$, wherein e_j^2 denotes the squared residual for the jth design point, it may then be said that e_j^2 is an unbiased estimator of σ_j^2. As Kutner et al. (2005) point out, these relationships facilitate an estimate of the variance function by first fitting the regression model using ordinary unweighted least squares and then regressing the squared residuals against the appropriate factors, or predictor variables. Pursuant to estimating the standard deviation function, shown in Equation (2), this resulting variance function $\hat{s}_j$ is then used to obtain fitted values, for each of the N design points, which in turn facilitate the estimation of the weights for each point, j, as follows:

$$w_j = 1/(\hat{s}_j)^2 \tag{4}$$

Using the estimated weights, the weight matrix may be constructed as:

$$\underset{\mathbf{N}\times\mathbf{N}}{\mathbf{W}} = \begin{bmatrix} w_1 & 0 & \cdots & 0 \\ 0 & w_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & w_N \end{bmatrix}$$

Standard regression procedures are then applied to the weighted regression models. Notably, for a regression model with k parameters, the WLS estimators of the regression coefficients $\mathbf{b}_w = (b_{1w}, b_{2w}, \ldots, b_{kw})^T$, whereby $\mathbf{b}_w = (\mathbf{X}_w^T\mathbf{X}_w)^{-1}\mathbf{X}_w^T\mathbf{Y}_w$, may be obtained via the weight matrix, $\mathbf{W}$ as follows:

$$\begin{aligned} \hat{\boldsymbol{\beta}}_{\mathbf{w}} = \mathbf{b}_w &= [\mathbf{W}^{1/2}\mathbf{X})^T\mathbf{W}^{1/2}\mathbf{X}]^{-1}(\mathbf{W}^{1/2}\mathbf{X})^T\mathbf{W}^{1/2}\mathbf{Y} \\ &= (\mathbf{X}^T\mathbf{W}^{1/2}\mathbf{W}^{1/2}\mathbf{X})^{-1}\mathbf{X}^T\mathbf{W}^{1/2}\mathbf{W}^{1/2}\mathbf{Y} \\ &= (\mathbf{X}^T\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^T\mathbf{W}\mathbf{Y} \end{aligned} \tag{5}$$

Obviously, the elimination or reduction of the influences of variability is achieved by assigning the largest weight to those terms with the smallest error variance. The second approach involves cases in which, given sufficient replication at each experimental design point, the sample variances or sample standard deviations of the observations at each design point may be used to estimate the error deviations. These, in turn, allow for the calculation of estimates for the various weights, w_j, using the ratio in Equation (4). The key to this approach is determining how many replications at each design point are sufficient. It is worth noting that either approach for estimating the weights can be particularly helpful in cases where the error variances differ significantly; that is, in highly variable processes. However, when the differences are relatively modest, the value of using these approximation methods in the WLS approach diminishes.

The iteration in the WLS approach occurs through a comparison between the standard errors of the WLS coefficients to the OLS coefficients. If the regression coefficients obtained using this method are significantly different than those obtained using ordinary least squares regression, the model may be reweighted using a subsequent re-estimation of the variance. This process continues in an iterative fashion, whereby revised weights are recomputed and then used to ensure convergence and the reduction of model error. Pursuant to this approach, fitted response functions are developed for the mean, and standard deviation. In particular, using the mean response $\bar{y}$ and standard deviation s, the general form of the estimated response functions for the process mean and standard deviation with k parameters or $k-1$ predictor variables changes from the formulations in Equation (2) with the inclusion of $\mathbf{W}$, as given by:

$$\begin{aligned} \hat{\mu}(\mathbf{x})_{\mathrm{WLS}} &= \mathbf{X}\hat{\beta}_\mu \quad \text{where} \quad \hat{\beta}_\mu = (\mathbf{X}^T\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^T\mathbf{W}\bar{\mathbf{y}} \\ \text{and } \hat{\sigma}(\mathbf{x})_{\mathrm{WLS}} &= \mathbf{X}\hat{\beta}_\sigma \quad \text{where} \quad \hat{\beta}_\sigma = (\mathbf{X}^T\mathbf{W}\mathbf{X})^{-1}\mathbf{X}^T\mathbf{W}\mathbf{s} \end{aligned} \tag{6}$$

and where $\mathbf{X}$, $\bar{\mathbf{y}}$, and $\mathbf{s}$ are defined precisely the same as in Equation (2).

2.2.2 *The proposed CV technique*

Whereas the WLS method addresses variability *after* response surface models have been fitted via priority-based weighting, an alternative approach to eliminating variability can be applied in the experimental phase itself using the CV to scope the design space and then applying optimal designs to rebalance the experiment. Obviously, this component in the proposed methodology implies either a priori knowledge of process conditions or that some experimentation has been performed and it has been determined that (1) the process under study possesses elevated levels of inherent variability, (2) the assumption of homoscedasticity fails to hold and, consequently, (3) the estimated model is a poor fit. Thus, invoking this particular approach further implies that we would revisit the experiment in order to redefine the experimental parameters and the associated design space to reduce variability and achieve greater precision.

The CV for a quality characteristic aims to describe the dispersion of the characteristic in a way that does not depend on its measurement unit. That is, it describes data variability in terms of the relative sizes of the squared residuals and outcome values. The CV for the qth design point is determined using the following ratio:

$$\mathrm{CV}_q = \frac{s_q}{\bar{y}_q} \tag{7}$$

Using this ratio, a higher CV indicates greater dispersion in the response. Conversely, a lower CV corresponds to smaller residuals relative to the predicted value, suggesting a sufficient relationship exists between the estimated and true responses. Unfortunately, no definitive threshold exists for the CV that indicates elevated or high variation, as it depends on the process and responses under examination. Nevertheless, it can be used to identify sources of variation that unduly influence or exert leverage upon the response based on order-of-magnitude comparisons between the various CV computed at each design point. Once identified, these select points may be removed from consideration. However, this will very likely result in a non-standard experimental design, which raises the need for alternative design strategies, such as optimal design.

The need to consider optimal design arises either when certain conditions render the use of traditional experimental approaches inappropriate. These usually include instances where time, resource limitations or physical restrictions constrain the experimental region. In this situation, however, the identification and elimination of sources of process variability equates to the imposition of constraints on the design space in the interest of obtaining enhanced precision in the response surface models and ultimately the optimisation results.

The objective for any optimal design is to determine the set of design points from among a list of candidate points that best satisfy the selected criterion. Most often, the optimality criterion used is a function of the variance of the estimated model parameters. Moreover, due to the iterative nature and the complexity involved, these designs typically require the use of sophisticated computer algorithms. Traditional optimality criteria involve invariants of the information matrix ($\mathbf{X}^T\mathbf{X}$), where $\mathbf{X}$ is the design matrix and $\mathbf{X}^T$ is its transposed form. Ultimately, one of the chief advantages afforded by optimal design is that it provides the researcher with the flexibility to design a tailor-made experiment in an objective way. While an assortment of optimal designs exists for consideration, the objective of this paper is not to discuss the full range of alternatives. Atkinson and Donev (1992), Pukelsheim (1995), Montgomery et al. (2002), as well as Kovach and Cho (2007a) provide considerable detail regarding optimal design theory applications. Nevertheless, in the interests of not confining the methodology to a singular design approach, *D*-, *A*- and *G*-optimal designs are examined.

The *D*-optimal design criterion stands out as the most widely used in the literature, in large part due to its availability in various commonly used software packages, although some environments, such as *R*, have begun to include several others, including the *A*-, *G*- and *I*-criteria. *D*-optimal designs are particularly useful when precision is the primary factor in model estimation. The goal of *D*-optimality is to improve the experimental design through the careful selection of candidate points, which is done using the *D*-criterion. The *D*-criterion is based on the ellipsoidal joint confidence region for the parameters in the standard regression model. This region is defined by the set of coefficient vectors $\hat{\boldsymbol{\beta}}$, which satisfies

$$\frac{(\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta})^T \mathbf{X}^T \mathbf{X} (\widehat{\boldsymbol{\beta}} - \boldsymbol{\beta})}{p\mathrm{MSE}} \leq F(1-\alpha; p, N-p) \tag{8}$$

where $\mathbf{X}$ denotes the design matrix. Among others, two properties that make *D*-optimal designs appealing to analysts involve their ability to minimise both the generalised variance of the estimated parameters $\widehat{\boldsymbol{\beta}}$ and the volume of the ellipsoidal confidence region. Using the notation described in Section 2.2.2, we can determine the variance of the estimates in $\widehat{\boldsymbol{\beta}}$ through

$$V(\widehat{\boldsymbol{\beta}}) = \sigma^2(\mathbf{X}^T\mathbf{X})^{-1} \tag{9}$$

Simple deduction shows that the variance of $\widehat{\boldsymbol{\beta}}$ depends on the generalised variance $(\mathbf{X}^T\mathbf{X})^{-1}$. The larger this value, the poorer the estimation of $\widehat{\boldsymbol{\beta}}$. Consequently it becomes equally clear that a large value for $|\mathbf{X}^T\mathbf{X}|$ will serve to minimise $(\mathbf{X}'\mathbf{X})^{-1}$ and thereby minimise $V(\widehat{\boldsymbol{\beta}})$. Thus, the objective of the *D*-criterion is to maximise the determinant of the information matrix.

Unlike the *D*-optimal design, *A*-optimal designs do not consider the covariances among regression coefficients, focusing instead on the individual variances of the coefficients themselves. Albeit, the overarching goal remains focused on minimising the variance of estimators. *A*-optimal designs achieve this by minimising the trace of the inverse of the information matrix, whereby the trace of an $N \times N$ square matrix, call it $\mathbf{M}$, is defined to be the sum of the elements on the diagonal of $\mathbf{M}$. That is,

$$\underset{\mathbf{N}\times\mathbf{N}}{\text{trace}}(\mathbf{M}) = m_{11} + m_{22} + \ldots + m_{NN} = \sum_{j=1}^{N} m_{jj} \tag{10}$$

Thus, the *A*-criterion used is shown by Minimise trace$(\mathbf{X}^T\mathbf{X})^{-1}$, which once again is associated with the generalised variance. The result is the minimisation of the average variance of the regression coefficient estimates.

Whereas *D*- and *A*-optimal designs employ invariants of the information matrix in their optimality criteria, *G*-optimal designs (along with *I*- and *V*-optimal designs) focus on the variance of predictions. Considering the mean response, we can express the variance of predictions, $Var\,[\hat{\mu}(\mathbf{x})]$ as:

$$Var\,[\hat{\mu}(\mathbf{x})] = \text{MSE}\ [\mathbf{X}_\mathbf{m}^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}_\mathbf{m}]$$

Where the vector $\mathbf{X}_\mathbf{m}^T = [\,1 \quad X_{m1} \quad \cdots \quad X_{m,p-1}\,]$ represents the location within the design space where a prediction is being made. Typically, the prediction variance is scaled as shown in Equation (11) to facilitate comparison between various designs.

$$\frac{NVar[\hat{\mu}(\mathbf{x})]}{\text{MSE}} = N\mathbf{X}_\mathbf{m}^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}_\mathbf{m} \tag{11}$$

In contrast to *D*- and *A*-optimality criteria that comprise a single value, the *G*-optimality criterion depends on the location $\mathbf{X}_\mathbf{m}$ at which predictions are being made. Specifically, this criterion seeks to minimise the maximum entry in the main diagonal of the $(N \times N)$ hat matrix, $\mathbf{H} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$. The generalised effect is to minimise the maximum variance of the predicted values.

The objective for any optimal design is to determine the set of design points from among a list of candidate points that best satisfy the selected criterion. Most often, the optimality criterion used is a function of the variance of the estimated model parameters. Moreover, due to the iterative nature and the complexity involved, these designs typically require the use of sophisticated computer algorithms. A variety of methods exist for determining the best set of candidate points. Our approach uses the Federov exchange method. A general exchange comprises the simultaneous addition and removal of a pair of a design point, shown as follows:

$$(\mathbf{X}_\mathbf{new}^T\mathbf{X}_\mathbf{new}) = (\mathbf{X}_\mathbf{old}^T\mathbf{X}_\mathbf{old}) - (X_iX_i^T) + (X_jX_j^T)$$

where X_i and X_j denote the point being considered for removal and the point being considered for inclusion respectively.

In contrast, the method developed by Federov (1972) incorporates the interaction of the variance functions of the candidate pair into the calculation of the new determinant such that

$$(\mathbf{X}_\mathbf{new}^T\mathbf{X}_\mathbf{new}) = (\mathbf{X}_\mathbf{old}^T\mathbf{X}_\mathbf{old})(1 + \Delta(X_i, X_j)$$

Essentially, the algorithm iteratively examines the list of candidate points, seeking to replace an existing point with another one that yields a higher determinant. Thus, at each iterate, the goal is to generate a new vector of included design points that will increase the determinant of the information matrix and ultimately generate the best design.

At each stage, one of the design points is exchanged with another design point so that the ratio of the new determinant (containing the new design point) to the previous determinant is maximised. When the ratio falls below some tolerance level, the previous design is taken as the optimal design.

In *R*, the optFederov() function from the AlgDesign Package (Wheeler 2004) applies Federov's exchange algorithm to compute 'an exact or approximate algorithmic design' for each of the aforementioned criteria. Thereafter, a best-subsets regression is performed to determine the best, or most appropriate mix of predictors for the refined experimental design. This may be performed in R using the leaps() function from the Leaps Package (Lumley 2009). In short, this function executes an exhaustive search for the best subsets of predictors using an efficient branch-and-bound algorithm. Models therein are compared using four well-known criteria, including the adjusted coefficient of determination $R^2_{a,p}$, Mallow's C_p, the prediction sum of squares (PRESS_p), and the mean square error (MSE_p). Table 4 summarises these criteria.

Experimental designs, such as those heretofore described, are viable alternatives for a variety of situations in which standard experimental approaches do not apply or cannot achieve adequate precision. Generally, they provide an efficient and cost-effective way to select design points for experimentation. We should note, however, that the use of optimal designs should not serve as a direct substitute for standard experimental approaches, but rather as an alternative approach when standard methods are inappropriate or otherwise insufficient.

2.3 *Determination of approved models and optimisation*

Considering the framework delineated in Section 2.1 for an industrial process involving a nominal-the-best (*N*-type) quality characteristic as the response of interest, we assume that the levels of x_i for $i = 1, 2, \ldots, k$ are both quantitative and continuous, and can be controlled by the experimenter. Fitted response functions are developed for the process mean and standard deviation using the techniques described in Section 2.2. In particular, assuming second-order polynomials for the response functions in each case, the general form of the estimated response functions for the process mean and standard deviation with k parameters or $k-1$ predictor variables appears as:

$$\hat{\mu}(\mathbf{x}) = \hat{\beta}_0 + \mathbf{x}^T \widehat{\mathbf{b}}_\mu + \mathbf{x}^T \widehat{\mathbf{B}}_\mu \mathbf{x} + \varepsilon_\mu \tag{12}$$

$$\text{and } \hat{s}(\mathbf{x}) = \hat{\gamma}_0 + \mathbf{x}^T \widehat{\mathbf{b}}_\sigma + \mathbf{x}^T \widehat{\mathbf{B}}_\sigma \mathbf{x} + \varepsilon_\sigma \tag{13}$$

$$\text{where } \underset{\mathbf{1}\times\mathbf{k}}{\mathbf{x}} = \begin{bmatrix} X_1 \\ X_2 \\ \vdots \\ X_{n,k-1} \end{bmatrix}, \underset{\mathbf{k}\times\mathbf{1}}{\hat{\mathbf{b}}} = \begin{bmatrix} \beta_1 \\ \beta_2 \\ \vdots \\ \beta_k \end{bmatrix}, \text{ and } \underset{\mathbf{k}\times\mathbf{k}}{\hat{\mathbf{B}}} = \begin{bmatrix} \beta_{11} & \beta_{12}/2 & \cdots & \beta_{1k}/2 \\ & \beta_{22} & \cdots & \beta_{2k}/2 \\ & & \ddots & \vdots \\ sym. & & & \beta_{kk} \end{bmatrix}$$

and where β_0 (and γ_0), $\hat{\mathbf{b}}_{\boldsymbol{\mu}}$ (and $\hat{\mathbf{b}}_\sigma$) and $\hat{\mathbf{B}}_\mu$ (and $\hat{\mathbf{B}}_\sigma$) reflect the estimates of the intercept, linear and second-order coefficients, respectively. The term ε_μ and ε_σ correspond to the residual error for the mean and standard deviation,

Table 4. Evaluation criteria for the model with p parameters.

Measure (with Formula)	Description/Interpretation
$R^2_{a,p} = 1 - \left(\frac{N-1}{N-v}\right)\frac{\text{SSE}_p}{\text{SSTO}}$	High criterion values are sought. Here, the number of parameters is taken into account through the corresponding degrees of freedom. Thus, this measure is not influenced by an increase in predictor variables
$C_p = \frac{\text{SSE}_p}{MSE(X_1,\ldots,X_{p-1})} - (n-2p)$	Mallow's criterion is concerned with the total MSE of the n fitted values for the subset regression model. The objective is to identify subsets for which C_p is small (low total MSE) but is near p (which indicates low bias)
$\text{PRESS}_p = \sum_{j=1}^{N} \left(\frac{e_j}{1-h_{jj}}\right)^2$	Here, e_j represents the jth residual and h_{jj} represents the jth diagonal element of the hat matrix $\mathbf{H}$. For models with large h_{jj}, the prediction sum of squares will be large, resulting in more influential points within a regression model. Models with smaller PRESS_p values contain less overall prediction error in their estimation
$\text{MSE}_p = \frac{\text{SSE}_p}{N-p}$	Measures the average of the square of the error for a model with p parameters. Low values are sought

respectively. An MSE-based optimisation scheme is used on either a spherical region of interest (in the case of a central composite design) such that $\mathbf{x}'\mathbf{x} \leq \rho^2$, where ρ defines the spherical experimental region, and $\mathbf{x} \in$ the domain of the control factors, Ω; or a cuboidal region of interest bounded by $(-1,1)$ (in the case of factorial design).

3. Numerical example – printing press study revisited

Using the methodology advanced in Section 2, this section investigates the application of the CV technique as an alternative to the traditional WLS approach for solving RPD problems. Specifically, the printing press study introduced in Section 3 is revisited in two parts to facilitate comparison between the proposed technique and traditional approaches. In the first part, we examine the three methods in the context of the original experiment and draw inferences from the performances of each. In the second, we employ Monte Carlo simulation to more fully investigate performance trends and precision; observations are made and conclusions drawn regarding the simulation results.

3.1 *Initial data analysis*

Pursuant to a thorough analysis of the original data associated with the print press experiment, two observations emerge. First, based on the criteria established in Section 2.1, the time-sequence plot in Figure 3(a) shows that the process qualifies as highly variable since one or more observations exceeds the +/− 3σ threshold. Second, as the residual plots for both first- and second-order models in Figure 3(b) and (c) show, regression of the residuals against the fitted line suggests evidence of non-constant variance. After regressing the absolute values of the residuals against each of the predictor variables for the fitted line separately, the evidence for non-constant variance becomes more conclusive for each of the primary factors (see Figure 4).

To confirm the variability trends observed in the residual plots, the Breusch-Pagan hypothesis test is applied. In the first-order model, the calculated statistic (1) tests H_0: $\gamma_1 = \gamma_2 = \gamma_3 = 0$ vs. H_1: Not all $\gamma = 0$, whereas in the second-order model (2), the hypotheses are extended for $p = 10$ parameters.

$$(1)\ \chi^2_{BP} = \frac{SSR^*}{2} \div \left(\frac{SSE}{Nm}\right)^2 = \frac{7.95e{+}09}{2} \div \left(\frac{1{,}012{,}557}{27(3)}\right)^2 = 25.45 \qquad (2)\ \chi^2_{BP} = \frac{SSR^*}{2} \div \left(\frac{SSE}{Nm}\right)^2 = \frac{2.28e{+}09}{2} \div \left(\frac{539{,}518}{81}\right)^2 = 25.72$$

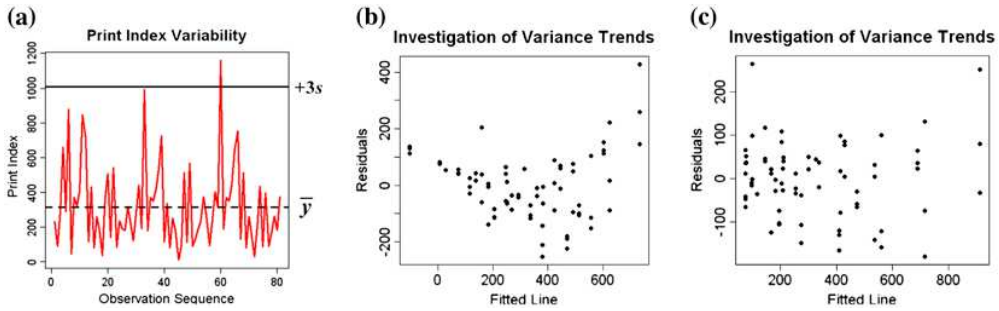


Figure 3. Investigation of assumptions on (a) variability in the responses and (b)–(c) constant error variance for first and second order models, respectively.

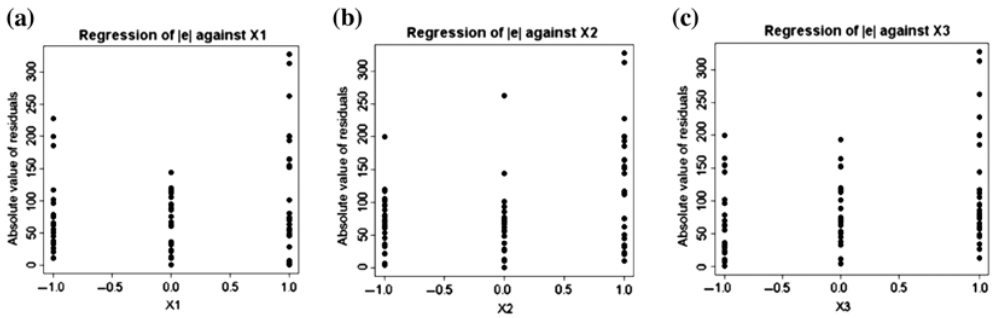


Figure 4. Regression of squared residuals against (a) X_1, (b) X_2, and (c) X_3.

Since $25.447 > \chi^2$ (.95, 3) = 7.81 and $25.720 > \chi^2$ (.95, 9) = 16.92 for the first- and second-order models, respectively, we conclude H_1; that is, the error variance is not constant. The results of these tests reinforce the inferences drawn from the graphical analysis and further suggest the need for remedial measures in the development of fitted functions. Such remedial actions are performed using both the usual WLS approach and the proposed CV technique, which are described in the ensuing paragraphs.

3.2 *Comparison of methods via a single iteration of the original experiment*

The initial comparison of the three methods (OLS, WLS and the proposed CV technique) was performed using the original data for the printing press experiment shown in Table 2. Applying the OLS regression method first yields the following second-order response surface models, which are commensurate with the models obtained in previous research:

$$\begin{aligned}\hat{\mu}(x)_{\text{OLS}} &= 327.63 + 177.01x_1 + 109.42x_2 + 131.47x_3 + 32.01x_1^2 - 22.39x_2^2 \\ &\quad -29.06x_3^2 + 66.03x_1x_2 + 75.46x_1x_3 + 43.58x_2x_3 \\ \hat{\sigma}(x)_{\text{OLS}} &= 34.884 + 11.529x_1 + 15.327x_2 + 29.191x_3 + 4.206x_1^2 - 1.318x_2^2 \\ &\quad +16.776x_3^2 + 7.724x_1x_2 + 5.115x_1x_3 + 14.083x_2x_3\end{aligned}$$

As with previous research using this particular data-set, these models were developed under the premise that underlying assumptions regarding variability and the residual errors held.

The development of second-order fitted response surface functions for the mean and standard deviation was performed using an iteratively reweighted least squares regression programme constructed in R. At each iterate in the WLS procedure, the standard error for each regression coefficient is observed and compared to the standard error obtained in the previous trial. Once the estimated coefficients stabilise, the iterative process ceases and the fitted function obtained in the last trial is selected. This process is iterated up to 50 times to ensure convergence, which occurs when the difference between standard error for each of the estimated coefficients is less than 0.05 when compared to the corresponding errors obtained in the previous iterate. Table 5 depicts the results of this process for the mean response surface function, which converged after 11 iterations; the analogous process for the standard deviation converged after 23 iterations.

The application of the WLS procedures resulted in the following estimated response surface functions for the mean and standard deviation for each method, respectively:

$$\begin{aligned}\hat{\mu}(x)_{\text{WLS}} &= 317.09 + 171.23x_1 + 132.43x_2 + 125.67x_3 + 25.27x_1^2 - 11.43x_2^2 \\ &\quad -11.76x_3^2 + 37.63x_1x_2 + 46.69x_1x_3 + 60.66x_2x_3 \\ \hat{\sigma}(x)_{\text{WLS}} &= 45.014 + 21.461x_1 + 25.435x_2 + 34.658x_3 - 5.041x_1^2 - 19.516x_2^2 \\ &\quad +22.875x_3^2 - 21.45x_1x_2 + 21.177x_1x_3 + 27.421x_2x_3\end{aligned}$$

As expected, a comparison of the fitted response surface models developed using the WLS procedure to those obtained via OLS regression shows clear improvements in the precision of the models for both the mean and standard

Table 5. Standard errors for mean regression coefficients in each iterate of the WLS procedure.

Iteration	$s(b_{0w})$	$s(b_{1w})$	$s(b_{2w})$	$s(b_{3w})$	$s(b_{4w})$	$s(b_{5w})$	$s(b_{6w})$	$s(b_{7w})$	$s(b_{8w})$	$s(b_{9w})$
1	22.646	13.099	17.355	14.210	22.274	20.926	21.880	23.649	22.351	24.224
2	21.578	13.341	14.767	15.296	20.580	20.743	21.657	20.571	22.450	21.863
3	23.927	13.777	14.306	15.576	21.939	19.933	23.026	18.404	20.352	19.151
4	23.382	12.729	14.307	15.506	21.472	19.999	22.257	17.083	18.996	19.152
5	22.791	11.793	14.215	15.046	21.400	19.086	21.588	17.247	18.684	18.733
6	22.726	11.502	14.200	14.827	21.413	18.860	21.391	17.350	18.401	18.623
7	22.773	11.374	14.150	14.669	21.412	18.756	21.301	17.364	18.212	18.486
8	22.830	11.307	14.117	14.575	21.426	18.714	21.241	17.399	18.080	18.418
9	22.849	11.260	14.092	14.511	21.429	18.673	21.204	17.412	18.001	18.366
10	22.862	11.229	14.075	14.472	21.432	18.649	21.179	17.423	17.948	18.335
11	22.868	11.209	14.063	14.447	21.433	18.631	21.163	17.428	17.914	18.315

deviation. In particular, as shown in Table 6, a significant reduction in the error for each of the coefficients is observed when comparing the mean and standard deviation response models obtained through the WLS approach against those calculated using traditional OLS regression.

The application of the proposed CV technique begins with the identification of potential sources of variability or instability in the process. Per the plot in Figure 3(a), a handful of responses either approach or exceed the 3σ-threshold used to identify a high-variability process. Computing the CV for each design point (see Figure 5) reveals three likely sources of variability at design points 1, 5 and 19. The box plot in Figure 5 provides a more visual portrayal of these points, indicating clearly the extent to which they deviate from the rest of the data. The corresponding violin plot illustrates the influence these points exert on the rest of the data, further indicating the degree to which they infuse asymmetry into process outputs.

Per the methodology outlined in Section 2, these three points are then removed from the experiment, which results in a non-standard experimental region. Optimal design theory is then applied using the optFederov() function in R to rebalance the design while retaining 27 design points. This yields the design in Table 7, including the points retained from the original experiment, the points to be replicated (highlighted), and the values for each of the optimal design criteria. An additional output in *R* is the lower bound on *D*-efficiency, which is determined by $D_e \geq e^{(1-1/G_e)}$, where G_e denotes the *G*-efficiency, which is an available standard of optimal design quality since the theoretical optimum value of the *G*-criterion is known.

Interestingly, as Table 7 shows, this procedure results in the extraction of three additional points from the original experiment, namely design points 11, 13 and 18. Thus the optimal design consists of 21 experimental points, six of which are replicated twice to achieve the 27 runs desired. Figure 6 depicts the new experimental region for the experiment after removing the identified sources of variability.

Thereafter, a best-subsets regression procedure is performed using the leaps() function in *R*, which yields the results shown in Table 8. Using the evaluation criteria listed in Table 4, the preferred model excludes the pure quadratic effect for x_1^2, resulting in $k=9$ parameters for the modified experimental design (Model 15 in Table 8).

Applying the OLS regression procedure to the new experimental design yields the following response surface functions for the mean and standard deviation, respectively:

$$\begin{aligned}\hat{\mu}(x)_{\mathrm{CV}} &= 371.53 + 182.17x_1 + 103.74x_2 + 104.06x_3 - 46.22x_2^2 \\ &\quad -45.71x_3^2 + 50.07x_1x_2 + 114.26x_1x_3 + 72.24x_2x_3 \\ \hat{\sigma}(x)_{\mathrm{CV}} &= 50.39 + 20.63x_1 + 27.67x_2 + 19.06x_3 - 5.38x_2^2 - 9.60x_3^2 \\ &\quad -2.67x_1x_2 + 13.48x_1x_3 + 23.49x_2x_3\end{aligned}$$

Using the estimated response surface functions obtained via the OLS, WLS and proposed CV methods, a non-linear optimisation scheme using the MSE-based model of Cho/Lin and Tu is employed in *R* to identify the optimal operating conditions for which total MSE and bias are minimised. Table 9 contains the consolidated results for each of the three methods. These include comparisons of the standard errors for each of the coefficients; overall model performance based on the PRESS_p, $R^2_{p,adj}$, and MSE_p for each; and the optimisation results in terms of the total *MSE* and bias for the optimal operating conditions, shown in Table 9(a)–(c), respectively.

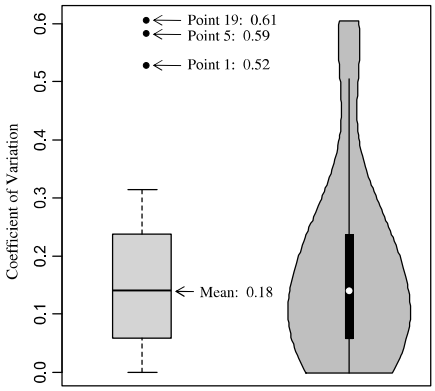
It is immediately clear from the results in Table 9 that both the WLS and CV methods exhibit significant improvements over the traditional OLS approach. Between the two, the performances are comparable, with each outperforming the other based on certain evaluation criteria. In Table 9(a), the standard errors for the WLS and CV mean response surface models are equally split, whereas for the standard deviation model, the CV technique clearly outperforms the WLS alternative. If we examine the overall model evaluation criteria in Table 9(b), the CV technique demonstrates much better predictive capability in terms of the PRESS_p criterion.

However, based on the $R^2_{p,adj}$, and MSE_p criteria, which essentially provide equivalent information, the model produced by the CV technique contains a greater degree of overall error suggesting a slightly poorer fit. As for the optimisation performance, the WLS and CV approaches yield a virtual tie for both total MSE and bias in the optimisation results. Thus, the results indicate that in some respects, the proposed CV technique is, at the very least comparable to the more traditional WLS approach, but in some ways potentially superior in terms of the precision it achieves.

Nevertheless, analysing the actual optimal operating conditions obtained using each method raises questions regarding precision. Figure 7 shows the relative proximity of the (X_1^*, X_2^*, X_3^*) point obtained for each method, and the disparities between them are obvious. However, recalling the variability in the simulated results from the pilot study plotted in Figures 1 and 2, it is practically impossible to determine from these results which method is more reliable and precise.

Table 6. Comparison of mean and standard deviation response models obtained via the OLS, WLS methods.

		Standard errors of regression coefficients									
		$s(b_0)$	$s(b_1)$	$s(b_2)$	$s(b_3)$	$s(b_4)$	$s(b_5)$	$s(b_6)$	$s(b_7)$	$s(b_8)$	$s(b_9)$
Mean	OLS	38.753	17.939	17.939	17.939	31.071	31.071	31.071	21.971	21.971	21.971
	WLS	22.868	11.209	14.063	14.447	21.433	18.631	21.163	17.428	17.914	18.315
Error reduction (%)		47.03	43.91	29.63	27.70	38.08	46.17	38.86	28.79	26.80	25.17
Standard deviation	OLS	22.312	10.329	10.329	10.329	17.890	17.890	17.890	12.650	12.650	12.650
	WLS	17.870	9.514	9.569	10.080	14.432	13.804	13.772	11.484	12.409	12.826
Error reduction (%)		58.61	52.39	52.12	49.56	58.30	60.12	60.21	53.08	49.30	47.60



Design Point	Mean	Standard Deviation	CV	Design Point	Mean	Standard Deviation	CV
1	24	12.49	0.52	15	501.7	92.5	0.18
2	120.3	8.39	0.07	16	264	63.5	0.24
3	213.7	42.8	0.20	17	427	88.61	0.21
4	86	3.46	0.04	18	730.7	21.08	0.03
5	136.7	80.41	0.59	19	220.7	133.8	0.61
6	340.7	16.17	0.05	20	239.7	23.46	0.10
7	112.3	27.57	0.25	21	422	18.52	0.04
8	256.3	4.62	0.02	22	199	29.45	0.15
9	271.7	23.63	0.09	23	485.3	44.64	0.09
10	81	0	0.00	24	673.7	158.2	0.23
11	101.7	17.67	0.17	25	176.7	55.51	0.31
12	357	32.91	0.09	26	501	138.9	0.28
13	171.3	15.01	0.09	27	1010	142.5	0.14
14	372	0	0.00				

Figure 5. Box plot, violin plot, and table of CV values for the printing press study.

Table 7. Optimal design results generated by the optFederov() function in *R*.

	# Times to replicate	X_1	X_2	X_3	Criterion	Value
1	1	0	−1	−1		
2	1	1	−1	−1	*D*-	0.458
3	1	−1	0	−1	*A*-	3.708
4	1	1	0	−1	*G*-	0.998
5	2	−1	1	−1	*I*-	9.709
6	1	0	1	−1	Lower bound on *D*-efficiency	0.998
7	2	1	1	−1		
8	2	−1	−1	0		
9	1	1	−1	0		
10	1	0	0	0		
11	1	1	0	0		
12	1	−1	1	0		
13	1	0	1	0		
14	1	0	−1	1		
15	2	1	−1	1		
16	1	−1	0	1		
17	1	0	0	1		
18	1	1	0	1		
19	2	−1	1	1		
20	1	0	1	1		
21	2	1	1	1		

Hence, while the comparisons to this point demonstrate comparable or improved results using the CV technique, the real question is one of precision. That is, is it reasonable to expect a greater degree of precision in the results obtained via the CV technique compared to the other two? Monte Carlo simulation is used to examine this question.

3.3 *Comparison of methods via Monte Carlo simulation*

As the results in Figures 1 and 2 showed from the pilot study, simulation of the printing press experiment revealed considerable imprecision in the optimisation results obtained for the 500 runs. Thus, by extension, it was presumed that the two alternative methods would likewise possess some degree of imprecision in the results. The questions were how much and to what extent did one method outperform the others? To this end, the overarching purpose of the simulation was to facilitate an investigation of performance trends between the three methods to determine whether better and more precise solutions could be expected via the proposed CV technique in the presence of high system variability.

Two simulations were constructed in *R*, one for the OLS and WLS approaches and the other for the proposed CV technique, which required a unique approach to the former based on the aspects of optimal design and best-subsets regression used in the procedure. In each iterate of the simulation, fresh observations are generated using the values for

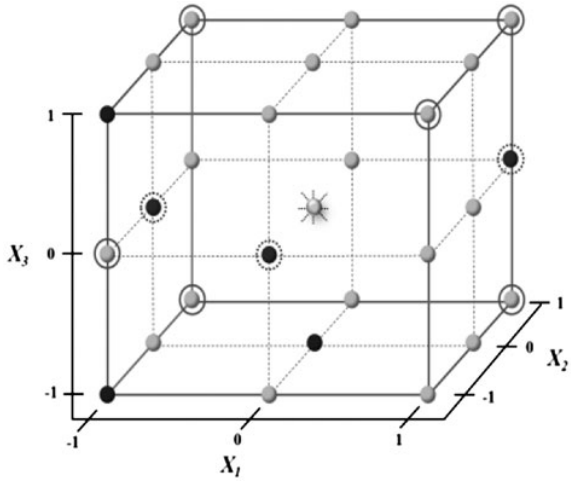


Figure 6. Optimal experimental design generated in *R*, where (●) denotes points extracted based on their CV, (◉) denotes additional points omitted through the optimal design process, and (◎) denotes replicated points in the new design space.

the mean and standard deviation at each design point in Table 2 to generate normal random variables consistent with the original experiment. These data are then used to obtain estimates for the sample mean and standard deviation at each design point, which in turn are used to perform the appropriate regression procedure to obtain fitted response surface functions for the mean and standard deviation. Thereafter, the fitted functions are used in the MSE-based optimisation framework to determine the optimal operating conditions, results at each iterate are recorded, and output is generated to facilitate consolidation, averaging and plotting for analysis.

Two trials of the simulation were performed in which both the number of observations generated per design point and the number of iterations executed were varied. In the interest of remaining consistent with the original experiment, the first trial involved three simulated observations per design point. The experiment was iterated 1000 times, yielding the results shown in Table 10, which reflect average values across all 1000 iterations.

As the results from the first simulation trial show, the CV technique performs at least comparable to, but in several ways better than the WLS approach when examined in the context of coefficient errors and overall model error and predictive capabilities. However, the optimisation results in Table 10(c) demonstrate nearly 50% reductions in both the *MSE* and bias for the optimal process mean when using the CV technique. Furthermore, comparing the plots in Figure 8 illustrate clear gains in precision using the CV technique. Specifically, as (X_1^*, X_2^*, X_3^*) are plotted for each of the 1,000 iterations of the simulation, a much tighter grouping of the results is observed in the plots corresponding to the CV technique (Figure 8(c)). By comparison, the plots associated with the OLS and WLS methods (Figure 8(a) and (b), respectively) continue to reflect results that span a considerable portion of the design space.

In the second simulation trial, the number of observations per design point is increased to 25 in order to examine the effects of added replication on the simulation results. Additionally, the number of iterations is increased to 2000. These modifications yielded the results in Table 11.

As with the results in Trial 1, both alternatives drastically outperform the traditional OLS approach, but between the two the CV technique once again performs at the level of or slightly better than the WLS approach, at least in the context of predicting process responses. In terms of the optimisation results, however, the gap between the two methods closes considerably, with the CV technique yielding, on average, the result with the least variability, but the WLS technique on average delivering slightly less bias.

Whereas the gap between the WLS and CV techniques regarding the optimisation results appears to close with greater replication at each design point, the opposite is observed to occur in terms of the precision in the results. As the plots in Figure 9(a)–(c) show, the x^* obtained via the CV technique continue to consolidate even more tightly in the (+, –, +) quadrant of the experimental region. Thus, while the average optimisation results between the two appear nearly equal, the precision achieved by the CV technique clearly exceeds the improvements attained through the WLS approach.

4. Summary of findings

Whereas the WLS approach affords some flexibility in iteratively down-weighting sources of variability, it does not eliminate them altogether. The proposed CV technique, on the other hand, does. And as the results of the numerical

Table 8. Results of the best-subsets regression procedure performed in *R*.

Model	x_1	x_2	x_3	x_1^2	x_2^2	x_3^2	x_1x_2	x_1x_3	x_2x_3	$R^2_{p,adj}$	C_p	PRESS_p	MSE_p
1	X									39.9%	230.14	995,279	34066.90
2			X							22.8%	302.26	1279200.6	43773.53
3	X		X							62.4%	131.04	654308.6	21313.93
4	X							X		50.3%	180.03	883,956	28181.29
5	X	X	X							75.4%	76.18	468233.1	13922.96
6	X		X					X		68.9%	101.56	554024.7	17635.95
7	X	X	X					X		84.0%	42.23	322833.1	9058.63
8	X	X	X				X			77.8%	65.19	451590.9	12569.76
9	X	X	X					X	X	89.7%	21.48	215416.1	5844.10
10	X	X	X				X	X		87.7%	28.57	267707.2	6980.80
11	X	X	X				X	X	X	93.1%	10.31	145201.3	3922.04
12	X	X	X			X		X	X	90.7%	18.50	194087.4	5298.24
13	X	X	X		X		X	X	X	93.7%	9.05	143,351	3550.65
14	X	X	X			X	X	X	X	93.6%	9.38	138457.8	3608.01
15	X	X	X		X	X	X	X	X	94.3%	8.16	138,370	3207.90
16	X	X	X	X	X		X	X	X	93.5%	10.87	155,710	3714.19
17	X	X	X	X	X	X	X	X	X	94.1%	10.00	149750.9	3364.48

Table 9. Comparison of the consolidated results for the OLS, WLS and proposed CV methods based on a single iteration of the original printing press experiment.

		Standard errors of regression coefficients									
(a)		$s(b_0)$	$s(b_1)$	$s(b_2)$	$s(b_3)$	$s(b_4)$	$s(b_5)$	$s(b_6)$	$s(b_7)$	$s(b_8)$	$s(b_9)$
Mean	OLS	38.753	17.939	17.939	17.939	31.071	31.071	31.071	21.971	21.971	21.971
	WLS	22.868	11.209	14.063	14.447	21.433	18.631	21.163	17.428	17.914	18.315
	CV	28.237	13.546	13.728	13.834	–	25.179	26.259	15.488	15.437	16.004
Standard Deviation	OLS	22.312	10.329	10.329	10.329	17.890	17.890	17.890	12.650	12.650	12.650
	WLS	17.870	9.514	9.569	10.080	14.432	13.804	13.772	11.484	12.409	12.826
	CV	13.856	6.647	6.736	6.788	–	12.355	12.885	7.600	7.575	7.853

(b)	Process mean			Process standard deviation		
	OLS-*m*	WLS-*m*	CV-*m*	OLS-*s*	WLS-*s*	CV-*s*
Avg. $PRESS_p$	337,730.1	243,597.9	138,370	93,049.95	99,770.42	28,900.63
Avg. $R^2_{p,adj}$	0.888	0.990	0.943	0.165	0.736	0.625
Avg. MSE_p	5792.602	0.725	3207.904	1920.224	0.948	772.423

(c)		OLS	WLS	CV
Optimisation results	Avg. MSE	406.349	1.73E-19	1.03E-16
	Avg. bias	2.386	1.24E-10	8.61E-09

OOCs obtained using each method (single run)

OLS	1.20	-0.32	-0.08
WLS	1.15	-0.12	-0.14
CV	1.41	1.55	-0.62

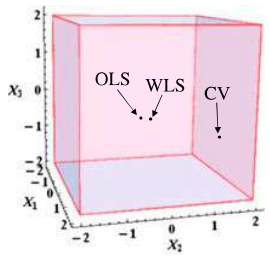


Figure 7. Comparison of optimal operating conditions obtained via the OLS, WLS and proposed CV methods using a single run of the original experimental data.

example and simulations suggest, removing sources of variability followed by a restructuring of the experimental design through a combination of optimal designs and best-subsets regression can have three significant positive impacts:

(i) First, it tends to produce a model with a much greater degree of predictive capability regarding system outputs or responses (Y_i). In each aspect of the numerical example, the proposed technique resulted in a $PRESS_p$ that was up 46% less than the WLS approach for the mean response model, and up to 70% less for the standard deviation.

(ii) Second, the CV technique tends to generate the best RPD solutions in terms of minimal MSE and bias in the optimisation results. Although the gap between the WLS and proposed CV approaches closes with the introduction of additional replication, it would still be fair to suggest the CV technique would be preferred due to the added costs that would be incurred to achieve such increases in experimental replication.

(iii) Finally, after 3000 iterations of the experiment, it is clear that the CV technique is more precise. That is, judging by the plots shown for the CV method in Figures 8(c) and 9(c) relative to the corresponding plots for the OLS and WLS methods in each, there is a considerable enhancement in the degree of precision attained using the proposed method. This translates to a greater degree of certainty that the generated results are indeed optimal.

The results of the numerical example and associated simulations demonstrate that both the WLS method and proposed CV technique provide viable alternatives to traditional OLS regression approaches when inherently high variability permeates process operations. Although this represents but a single simulation study based on a particular set of data, it is the examined conditions that make the work extendable. In short, the results can be generalised to practically any situation in which high variability influences process operations and outputs, which in turn causes various

Table 10. Comparison of consolidated results for trial 1 (1000 iterations; 3 observations per design point) for (a) coefficient errors, (b) model performance and (c) optimisation results.

		Standard errors of regression coefficients									
(a)		$s(b_0)$	$s(b_1)$	$s(b_2)$	$s(b_3)$	$s(b_4)$	$s(b_5)$	$s(b_6)$	$s(b_7)$	$s(b_8)$	$s(b_9)$
Mean	OLS	43.17	19.98	19.98	19.98	34.61	34.61	34.61	24.47	24.47	24.47
	WLS	26.27	15.82	16.17	17.41	23.44	24.31	24.32	21.24	22.69	22.01
	CV	33.67	16.15	16.37	16.49	–	30.02	31.31	18.47	18.40	19.08
Error reduction (%)	OLS → WLS	39.15	20.82	19.09	12.88	32.29	29.76	29.75	13.22	7.31	10.08
	OLS → CV	22.02	19.18	18.09	17.46	–	13.27	9.55	24.55	24.80	22.04
Standard deviation	OLS	24.63	11.40	11.40	11.40	19.75	19.75	19.75	13.96	13.96	13.96
	WLS	17.19	9.37	9.03	10.04	14.17	14.82	14.10	11.27	12.04	11.62
	CV	18.57	8.91	9.03	9.10	–	16.56	17.27	10.19	10.15	10.53
Error reduction (%)	OLS → WLS	60.19	53.10	54.80	49.78	59.05	57.19	59.26	53.93	50.80	52.54
	OLS → CV	56.98	55.42	54.82	54.47	–	52.16	50.11	58.38	58.52	56.99

(b)	Process mean			Process standard deviation		
	OLS-*m*	WLS-*m*	CV-*m*	OLS-*s*	WLS-*s*	CV-*s*
Avg. PRESS	407,375.30	323,176.10	194,641.40	116,673.80	106,025.60	56,619.01
Avg. R^2_{adj}	0.86	0.94	0.92	0.11	0.41	0.40
Avg. MSE_p	7311.70	0.94	4689.57	2462.60	1.00	1498.16

(c)		OLS	WLS	CV
Optimisation results	Avg. MSE	220.63	143.35	74.94
	Avg. bias	0.91	0.63	0.37

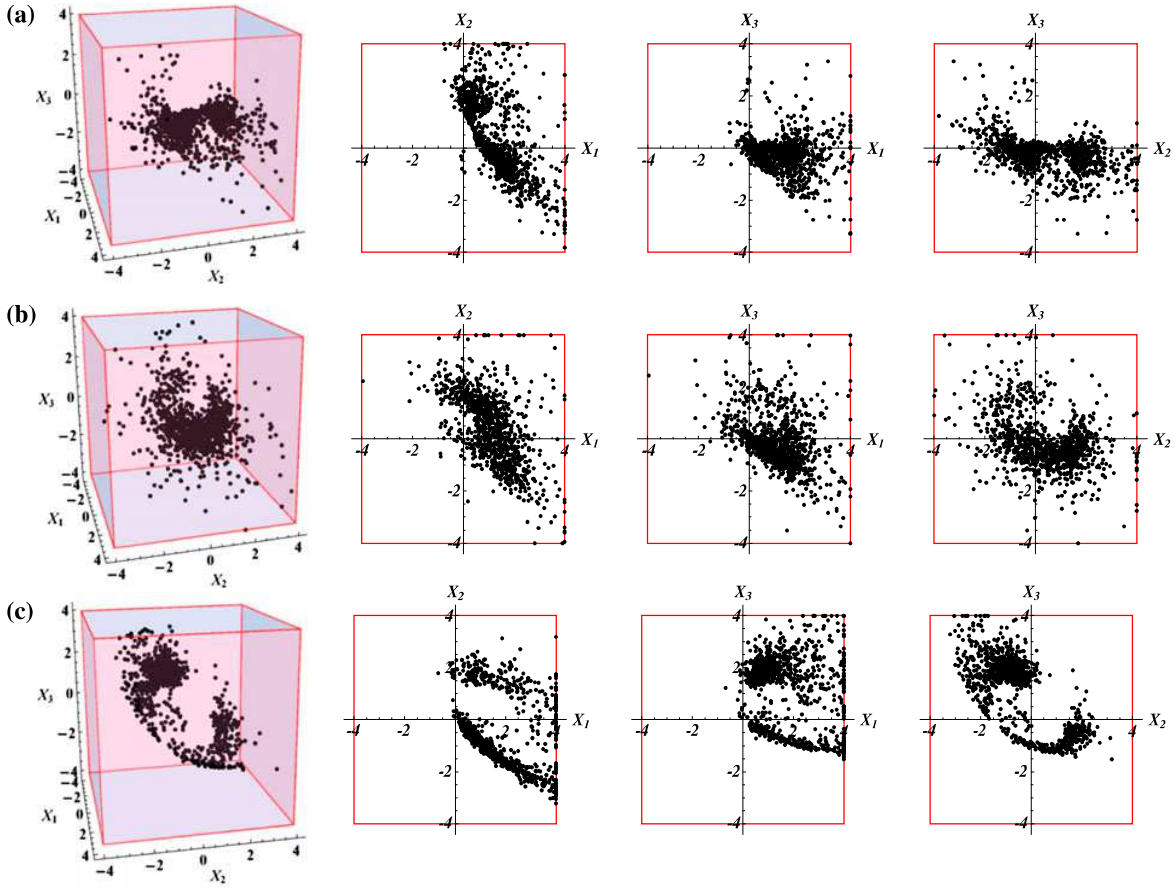


Figure 8. Identification of $\mathbf{x}^*$ for simulation trial 1, $-4 \leqslant X_i \leqslant 4$; (a) $\mathbf{x}^*$ for OLS method, (b) $\mathbf{x}^*$ for WLS method, (c) $\mathbf{x}^*$ for CV technique.

Table 11. Comparison of consolidated results for trial 2 (2000 iterations; 25 observations per design point) for (a) coefficient errors, (b) model performance and (c) optimisation results.

(a)		Standard errors of regression coefficients									
		$s(b_0)$	$s(b_1)$	$s(b_2)$	$s(b_3)$	$s(b_4)$	$s(b_5)$	$s(b_6)$	$s(b_7)$	$s(b_8)$	$s(b_9)$
Mean	OLS	39.28	18.18	18.18	18.18	31.50	31.50	31.50	22.27	22.27	22.27
	WLS	24.56	13.49	14.11	15.45	21.70	21.46	22.20	18.30	20.36	19.20
	CV	28.93	13.88	14.06	14.17	–	25.79	26.90	15.87	15.81	16.40
Error reduction (%)	OLS → WLS	43.11	32.49	29.39	22.69	37.31	38.01	35.86	25.22	16.80	21.57
	OLS → CV	33.00	30.56	29.63	29.09	–	25.48	22.29	35.18	35.39	33.01
Standard deviation	OLS	22.57	10.45	10.45	10.45	18.09	18.09	18.09	12.79	12.79	12.79
	WLS	17.36	9.78	9.88	10.50	14.58	14.04	14.18	12.20	12.67	12.88
	CV	14.44	6.93	7.02	7.08	–	12.88	13.43	7.92	7.89	8.19
Error reduction (%)	OLS → WLS	59.78	51.08	50.54	47.47	57.89	59.43	59.04	50.13	48.22	47.38
	OLS → CV	66.55	65.33	64.87	64.59	–	62.80	61.20	67.64	67.74	66.56

(b)	Process mean			Process standard deviation		
	OLS-*m*	WLS-*m*	CV-*m*	OLS-*s*	WLS-*s*	CV-*s*
Avg. PRESS	345,490.00	268,920.00	144,710.00	95,499.00	102,320.00	31,709.00
Avg. R^2_{adj}	0.89	0.96	0.94	0.16	0.70	0.60
Avg. MSE_p	5966.70	0.77	3377.30	1975.90	1.04	851.62

(c)		OLS	WLS	CV
Optimisation results	Avg. MSE	515.76	32.21	31.56
	Avg. bias	1.61	0.14	0.17

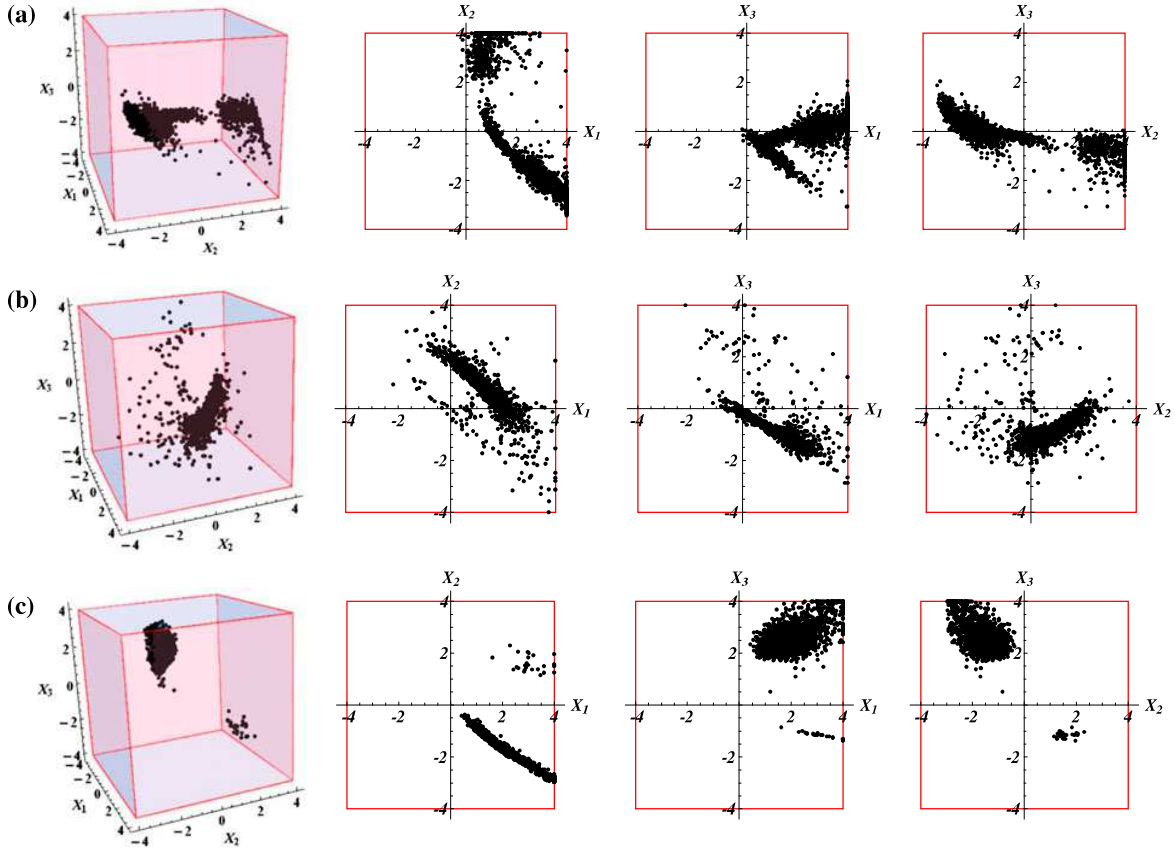


Figure 9. Identification of $\mathbf{x}^*$ for simulation trial 2, $-4 \leqslant X_i \leqslant 4$; (a) $\mathbf{x}^*$ for OLS method, (b) $\mathbf{x}^*$ for WLS method, (c) $\mathbf{x}^*$ for CV technique.

common assumptions to fail. By identifying and eliminating those sources of variability, the proposed method facilitates achieving greater degrees of precision in the array of potential optimal settings that can result.

5. Concluding remarks

This work has focused on robust parameter design in processes possessing elevated degrees of variability. The presence of such conditions can invalidate several of the assumptions that underpin the application of ordinary least squares regression. This paper demonstrates that the application of traditional approaches under such conditions can lead to imprecise estimates that likely will yield imprecise and potentially suboptimal solutions. To overcome this, an alternative technique is proposed in which engineers identify and then remove influential sources of variability using the CV and then apply optimal design techniques to restructure and balance the experiment in order to obtain more precise estimators and ultimately determine the true optimal operating conditions. Numerical illustration via Monte Carlo simulation was used to illustrate some potential advantages of the proposed approach. These benefits include flexibility provided to the experimenter and decision-maker regarding the disposition of influential sources of variability, as well as the improved quality of the optimisation results obtained. While the results of the proposed method demonstrate improvements, there appears to be room for yet greater improvements in the overall degree of precision achieved. Thus, future extensions to this method might explore the incorporation of higher-order modelling, or perhaps alternative experimental designs that would facilitate increased replication. This would ultimately help analysts to develop recommendations that offer decision-makers a greater degree of flexibility and control in the decision process.

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