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A multivariate robust parameter optimization approach based on Principal Component Analysis with combined arrays ☆

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ABSTRACT

Today's modern industries have found a wide array of applications for optimization methods based on modeling with Robust Parameter Designs (RPD). Methods of carrying out RPD have thus multiplied. However, little attention has been given to the multiobjective optimization of correlated multiple responses using response surface with combined arrays. Considering this gap, this paper presents a multiobjective hybrid approach combining response surface methodology (RSM) with Principal Component Analysis (PCA) to study a multi-response dataset with an embedded noise factor, using a DOE combined array. How this approach differs from the most common approaches to RPD is that it derives the mean and variance equations using the propagation of error principle (POE). This comes from a control-noise response surface equation written with the most significant principal component scores that can be used to replace the original correlated dataset. Besides the dimensional reduction, this multiobjective programming approach has the benefit of considering the correlation among the multiple responses while generating convex Pareto frontiers to mean square error (MSE) functions. To demonstrate the procedure of the proposed approach, we used a bivariate case of AISI 52100 hardened steel turning employing wiper mixed ceramic tools. Theoretical and experimental results are convergent and confirm the effectiveness of the proposed approach.

1. Introduction

In recent years, considerable attention has been given to Robust Parameter Design (RPD). Initially proposed by Taguchi (1986), RPD is an approach that determines the optimal settings of process variables, combining designed experiments (mainly orthogonal arrays – OA) with some kind of optimization algorithm. RPD aims to make processes less sensitive to the action of noise variables, to improve variability control, and to refine bias correction (the difference between a process mean and a target value; Ardakani & Noorossana, 2008; Quesada & Del Castillo, 2004; Shin, Samanlioglu, Cho, & Wiecek, 2011). Originally developed from a crossed-array – a combination of an inner array formed by control variables and an outer orthogonal array consisting of noise factors – this methodology remains controversial mainly due to its various mathematical flaws and statistical inconsistencies (Nair, 1992). Nevertheless, few researchers disagree on the idea that optimizing the process mean and variance, simultaneously, can achieve quality assurance (Shin et al., 2011).

The main drawback of this controversial approach is related to the inability of a crossed-array to measure the interaction between control and noise variables (Quesada & Del Castillo, 2004). To overcome this, Shoemaker, Tsui, and Wu (1991), Box and Jones (1992), Myers, Khuri, and Vining (1992), Welch, Yu, Kang, and Stokes (1990) and Lucas (1991) studied combined array, as an alternative approach to the crossed array, which contains the settings of both the control and noise factors. Central composite design (CCD), proposed by Box and Wilson (1951), with combined array was studied by Myers et al. (1992). The CCD generates the mean and variance equation from the propagation of the error principle. Quesada and Del Castillo (2004) attribute the first formulations involving the use of RSM for RPD to Box and Jones (1992) and Vining and Myers (1990).

The general scheme of an RPD–RSM problem consists of performing an experimental design with the noise factors considered as control variables and of eliminating from the design the axial points related to the noise factors. Doing so, one can use the ordinary least squares algorithm to fit the polynomial surface for $f(\mathbf{x},\mathbf{z})$ and thus obtain its partial derivatives. This procedure leads to

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the mean and variance equations for a single response, considering the noise-control factor interactions.

To obtain a product's quality, however, most industrial applications call for more than one response to be simultaneously optimized (Kazemzadeh, Bashiri, Atkinson, & Noorossana, 2008). Yet few studies have been devoted to the RPD concept for multiple responses (Paiva et al., 2012; Quesada & Del Castillo, 2004), when these responses are correlated (Govindaluri & Cho, 2007; Paiva, Paiva, Ferreira, Balestrassi, & Costa, 2009). Even in the works involving multivariate approaches, the noise-control interactions are generally neglected and the mean and variance equations come from crossed arrays or design replicates (Govindaluri & Cho, 2007; Jeong, Kim, & Chang, 2005; Kovach & Cho, 2009; Lee & Park, 2006; Paiva et al., 2012; Shaibu & Cho, 2009; Shin et al., 2011; Tang & Xu, 2002). The presence of correlation in the multiple responses causes the model's instability, over-fitting, and errors in the regression coefficients, which can substantially modify the optimization results (Box, Hunter, MacGregor, & Erjavec, 1973; Bratchell, 1989; Khuri & Conlon, 1981; Wu, 2005; Yuan, Wang, Yu, & Fang, 2008). Dual Response Surface (DRS) derived from $f(\mathbf{x},\mathbf{z})$ may be an alternative in modeling the interaction between control and noise variables. DRS is a class of RSM problems in which the mean and variance equations are obtained defining a response surface for the mean $\hat{y}(\mathbf{x})$ and another for the variance $\hat{\sigma}^2(\mathbf{x})$, using replicates, crossed or combined arrays. The correlation, however, can substantially influence the values of the $f(\mathbf{x},\mathbf{z})$ regression coefficients (β_i). Such influence consequently impairs the quality of the Dual Response Surface (DRS) derived from $f(\mathbf{x},\mathbf{z})$. One may deal with this impeding correlation influence by employing Principal Components Analysis (PCA).

Considering correlation structure among response variables, this paper presents a multiobjective hybrid approach of RPD combining RSM and PCA. This multivariate approach rotates the reference axes of correlated random variables to form new axes of random and uncorrelated variables. A multi-response dataset with an embedded noise factor is investigated by using a DOE-combined array. The RSM-PCA approach proposed here differs from the most commonly proposed RPD approaches in that the mean and variance equations of principal component scores are obtained from a control-noise response surface equation, based on propagation of error principle (POE). Besides reducing dimensions, this multiobjective programming approach presents two other advantages: (i) it considers the correlation among the multiple responses; and (ii) it generates convex Pareto frontiers to mean square error (MSE) functions. This latter characteristic plays a crucial role in optimization theory because the convex sets allow attainment of optimality. Moreover, the weighted approach of principal components have already been utilized by some authors (Gomes, Paiva, Costa, Balestrassi, & Paiva, 2013; Paiva, Costa, Paiva, Balestrassi, & Ferreira, 2010; Peruchi, Balestrassi, Paiva, Ferreira, & Carmelossi, 2013) assessing multivariate processes.

To illustrate the proposal, the study used a bivariate case of AISI 52100 hardened steel turning employing wiper mixed ceramic tools. Theoretical and experimental results are convergent and confirm the adequacy of the paper's proposal.

2. Robust optimization of quality characteristics

DRS is, as noted earlier, a class of RSM problems. In DRS, the mean and variance equations are obtained – using replicates, crossed, or combined arrays – so as to define one response surface to the mean $\hat{y}(\mathbf{x})$ and another to the variance $\hat{\sigma}^2(\mathbf{x})$. These functions, usually written as an OLS second-order model, may be optimized simultaneously considering different schemes (Del Castillo, Fan, & Semple, 1999; Kazemzadeh et al., 2008). Vining and Myers (1990) established an optimization figure considering $Min_{x\in\Omega}\hat{\sigma}^2(\mathbf{x})$, subject to the constraint of $\hat{y}(\mathbf{x}) = T$, where T is the target for $\hat{y}(\mathbf{x})$; using a Lagrangean multiplier approach, it evaluated only one quality characteristic. Shin and Cho (2005) presented a bias-specified robust design method formulating a nonlinear optimization program that minimized process variability subject to customer-specified constraints on the process bias, such as $|\hat{y}(\mathbf{x}) - T| \leqslant \varepsilon$.

In several works, however, the most common choice is the combination of mean, variance, and target, using the minimization of the mean square error (MSE). The MSE is an objective function subjected only to the experimental region constraint, such as $Min_{x\in\Omega}\,[\hat{y}(\mathbf{x}) - T]^2 + \hat{\sigma}^2$ (Cho & Park, 2005; Kazemzadeh et al., 2008; Kovach & Cho, 2009; Lee & Park, 2006; Lin & Tu, 1995; Paiva et al., 2012; Shin et al., 2011; Steenackers & Guillaume, 2008). Supposing that mean and variance can have different degrees of importance, the MSE objective function can also be weighted, as $MSE_w = \omega_1 \cdot (\hat{y}(\mathbf{x}) - T)^2 + \omega_2 \cdot \hat{\sigma}^2(\mathbf{x})$, where the weights ω_1 and ω_2 are pre-specified positive constants (Box & Jones, 1992; Kazemzadeh et al., 2008; Lin & Tu, 1995; Tang & Xu, 2002). Still, these weights can be experimented with using different convex combinations, i.e., $\omega_1 + \omega_2 = 1$, with $\omega_1 > 0$ and $\omega_2 > 0$, generating a set of non-inferior solutions for multiple objective optimization (Tang & Xu, 2002).

Note, however, that the examples above treat only one quality optimization. Analogously, when there are several quality characteristics to optimize, the MSE criterion can be extended to multiobjective problems using some kind of agglutination's operator, for instance, a weighted sum, as suggested by Busacca, Marseguerra, and Zio (2001) and Yang and Sen (1996). In this case, MSE becomes $MSE_T = \sum_{i=1}^{p}\left[(\hat{y}_i - T_i)^2 + \hat{\sigma}_i^2\right]$. Nevertheless, if different degrees of importance (w_i) are desired for each MSE_i, the weighted global objective function can be written as proposed by Köksoy and Yalçınoz (2006) and Köksoy (2006):

$$MSE_T = \sum_{i=1}^{p} w_i \cdot MSE_i = \sum_{i=1}^{p} w_i \cdot \left[(\hat{y}_i - T_i)^2 + \hat{\sigma}_i^2\right] \tag{1}$$

The aforementioned ideas may then be combined, and a mean square error approach for the multiobjective problem involving DRS models would be written as:

$$MSE_T = \sum_{i=1}^{p} w_i \left[\omega \cdot (\hat{y}_i - T_i)^2 + (1-\omega) \cdot \hat{\sigma}_i^2\right] \tag{2}$$

In this expression, ω is the weight to prioritize either mean or variance and w_i is the same weight described in Eq. (1). As a matter of comparison, Eq. (2) is referred to as "Weighted Sum" (WSum).

None of the aforementioned formulations takes into account the correlation structure that may be present in the matrix of responses. Again, such correlation structure may significantly jeopardize the optimization results. Considering the correlation among responses and the bias criteria, Vining (1998) presented the minimization of a multivariate expected loss function as a multiobjective function:

$$Min\ E\ [L[\hat{y}(\mathbf{x}), \boldsymbol{\theta}]] = [E[\hat{y}(\mathbf{x})] - \boldsymbol{\theta}]^T \mathbf{C}[E[\hat{y}(\mathbf{x})] - \boldsymbol{\theta}] + trace[\mathbf{C}\sum_{\hat{y}}(\mathbf{x})] \tag{3}$$

where $\mathbf{x}$ represents a vector of controllable design variables, $\hat{y}(\mathbf{x})$ is the vector of estimated response, $\mathbf{C}$ is a $p \times p$ positive defined matrix of costs (or weights) associated with the losses incurred when $\hat{y}(\mathbf{x})$ deviates from their respective targets $\boldsymbol{\theta}$, and $\Sigma_{\hat{y}}$ is the estimated variance–covariance matrix. Likewise, Chiao and Hamada (2001) proposed a multivariate integration approach as a correlated multi-response optimization method. Using a specified region of responses, the optimal solution does not take into consideration the targets. This formulation is written as:

$$\begin{aligned} &Max\ P(Y \in S) = \frac{1}{\sqrt{|\sum|(2\pi)^m}}\left[\int_{a_1}^{b_1}\int_{a_2}^{b_2}\cdots\int_{a_m}^{b_m} e^{-\frac{1}{2}(Y-\mu)^T\sum^{-1}(Y-\mu)}dY\right] \\ &subject\ to:\ \mathbf{x^T x} \leqslant \rho^2 \end{aligned} \tag{4}$$

where Y is the vector of multiple responses, S is the specified region for all responses formed by the lower bounds a_i and upper bounds b_i, $\sum$ is an $m \times m$ symmetric positive definite variance–covariance matrix and $\mathbf{x}^{\mathrm{T}}\mathbf{x} \leqslant \rho^2$ denotes a constraint for the experimental region. Govindaluri and Cho (2007) presented a proposal for multi-objective robust designs by applying the concept of Lp metrics (Ardakani & Noorossana, 2008) to several correlated characteristics with $f_i(\mathbf{x}) = MSE_i(\mathbf{x})$. The authors stated the objective functions and constraints as:

$$\begin{aligned} &Min\ \beta \\ &subject\ to:\ g_i(\mathbf{x}) = w_i \cdot \left(\frac{MSE_i(\mathbf{x}) - MSE_i^I(\mathbf{x})}{MSE_i^{\max}(\mathbf{x}) - MSE_i^I(\mathbf{x})} \right) \leqslant \beta \\ &\qquad \mathbf{x}^{\mathrm{T}}\mathbf{x} \leqslant \rho^2 \\ &\qquad \beta \geqslant 0 \\ &\qquad i = 1, 2, \ldots, p \end{aligned} \tag{5}$$

$$\text{with}: MSE_i(\mathbf{x}) = (\hat{y}_i(\mathbf{x}) - T_i)^2 + \hat{\sigma}_i^2(\mathbf{x}) + \sum_{j=1}^{i-1} \frac{\hat{\sigma}_i(\mathbf{x})}{\hat{\sigma}_i(\mathbf{x}) + \hat{\sigma}_j(\mathbf{x})} \cdot [\hat{\sigma}_{ij}(\mathbf{x}) + (\hat{y}_i(\mathbf{x}) - T_i) \cdot (\hat{y}_j(\mathbf{x}) - T_j)] \tag{6}$$

In this formulation, w_i is the weight associated to each constraint $g_i(\mathbf{x})$ referring to the scaled $\mathrm{MSE}_i(\mathbf{x})$ functions. $MSE_i^I(\mathbf{x})$ corresponds to the individual optimization of each $MSE_i(\mathbf{x})$ (utopia value), only constrained to the experimental region. The denominator in Eq. (5), $MSE_i^{\max}(\mathbf{x}) - MSE_i^I(\mathbf{x})$, stands for the normalization of multiple responses, using $MSE_i^{\max}(\mathbf{x})$ as the maximum value of the payoff matrix (matrix formed by all solutions observed in the individual optimizations). The set of constraints $g_i(\mathbf{x}) \geqslant 0$ can represent any desired restriction, but it is generally used to designate the experimental region. It is straightforward that this proposal establishes the empirical models for the mean, variance, and covariance in terms of design factors, but it is commonly done using crossed arrays. For sake of comparison, this model is used in this work and is referred to as "Beta" approach.

3. Principal Component Analysis on multiobjective optimization

A common concern with multiobjective MSE optimization is related to the convexity of the Pareto frontiers generated using weighted sums. According to Shin et al. (2011), in most RPD applications, a second-order polynomial model is adequate to accommodate the curvature of the process mean and variance functions, thus mean-squared robust design models would contain fourth-order terms. Consequently, the associated Pareto frontier might be non-convex and non-supported efficient solutions could be generated. It is important to state that a decision vector $\mathbf{x}^* \in S$ is Pareto optimal if no other $\mathbf{x} \in S$ exists such that $f_i(\mathbf{x}) \leqslant f_i(\mathbf{x}^*)$ for all $i = 1,2,\ldots,k$.

Suppose now that the multiple objective functions $f_1(\mathbf{x}), f_2(\mathbf{x}),\ldots,f_p(\mathbf{x})$ are correlated response surfaces written as a random vector $Y^T = [Y_1, Y_2,\ldots, Y_p]$. Assuming that Σ is the variance–covariance matrix associated with this vector, then Σ can be factorized in pairs of eigenvalues–eigenvectors $(\lambda_i, e_i),\ldots \geqslant (\lambda_p, e_p)$, where $\lambda_1 \geqslant \lambda_2 \geqslant \ldots \geqslant \lambda_p \geqslant 0$, such as the ith principal component may be stated as $PC_i = e_i^T Y = e_{1i}Y_1 + e_{2i}Y_2 + \ldots + e_{pi}Y_p$, with $i = 1,2,\ldots,p$ (Johnson & Wichern, 2002). This uncorrelated linear combination can be calculated using the PCA approach, based on variance–covariance matrix. In similar manner, the correlation matrix considers $[Z]$ the standardized data matrix and $[E]$ the eigenvectors matrix of multivariate set, then each principal component score can be obtained as $PC_i = [Z]^T[E]$ (Paiva et al., 2009). Bear upon these scores, the DOE analysis can be performed (Liao, 2006).

Bratchell (1989) was the first researcher to employ a second-order response surface model to adequately represent the original set of responses in a small number of latent variables. His work, however, did not contemplate the computation of specification limits and targets of each response represented in the plane of principal components. To fill this gap, Paiva et al. (2009) proposed the Multivariate Mean Square Error (MMSE) method, an approach capable of computing the response's targets and respective deviations for the second-order models of principal component scores. Once modeled, the objective functions may be aggregated using a geometric mean, which in turn often leads to continuous Pareto frontiers. In general, the number of equations obtained to replace the original set is smaller than the initial amount, obviously depending on the strength of the variance–covariance structure. By associating an experimental region constraint, the MMSE optimization can be written as (Lopes et al., 2013; Paiva et al., 2009):

$$\begin{aligned} &Min\ MMSE_T = \left[\prod_{i=1}^{m}(MMSE_i|\lambda_i \geqslant 1)\right]^{\left(\frac{1}{m}\right)} = \left\{\prod_{i=1}^{m}[(PC_i - \zeta_{PC_i})^2 + \lambda_i|\lambda_i \geqslant 1]\right\}^{\left(\frac{1}{m}\right)}, \quad m \leqslant p \\ &subject\ to: \mathbf{x}^{\mathrm{T}}\mathbf{x} \leqslant \rho^2 \end{aligned} \tag{7}$$

$$\text{with}: MMSE_i = (PC_i - \zeta_{PC_i})^2 + \lambda_i \tag{8}$$

$$\zeta_{PC_i} = e_i^T[Z(Y_p|\zeta_{Y_p})] = \sum_{i=1}^{p}\sum_{j=1}^{q} e_{ij}[Z(Y_p|\zeta_{Y_p})] \quad i = 1,2,\ldots,p;\ j = 1,2,\ldots,q \tag{9}$$

where m is the number of MMSE functions according to the significant principal components, PC_i is the fitted second-order polynomial, ζ_{PC_i} is the target value of the ith principal component (that must keep a straightforward relation with the targets of the original data set), $\mathbf{x}^{\mathrm{T}}\mathbf{x} \leqslant \rho^2$ is the experimental region constraint, e_i represents the eigenvector set associated to the ith principal component, and ζ_{Y_p} represents the target for each of the p original responses.

PCA generally reduces the problem dimension according to the strength of variance–covariance structure among the responses and, eventually, it is possible to consider principal components with $\lambda < 1$, since the total explanation achieves 80% (Johnson & Wichern, 2002).

The next section will present, in consideration of what has just been discussed, a multivariate multiobjective optimization method for DRS problems. The method uses the POE derivations of mean and variance response surfaces built with the dataset of a central composite design (CCD), in the form of a combined array.

4. Multivariate robust parameter optimization for combined arrays

Taguchi proposed that a reasonable route to robust optimization would be to do the following: summarize the data from a crossed array experiment with the mean of each observation in the inner array across all runs in the outer array being combined in the signal-to-noise ratio. However, Montgomery (2009) emphasized that one cannot estimate interactions between control and noise parameters since sample means and variances are, in a crossed array structure, computed over the same levels of the noise variables. Hence, the key component to solving robust design problems are the interactions among controllable and noise factors. The general response surface model involving control and noise variables, organized in a combined array, may be written as:

$$y(\mathbf{x}, \mathbf{z}) = \beta_0 + \sum_{i=1}^{k}\beta_i x_i + \sum_{i=1}^{k}\beta_{ii}x_i^2 + \sum_{i<j}\sum \beta_{ij}x_i x_j + \sum_{i=1}^{r}\gamma_i z_i + \sum_{i=1}^{k}\sum_{j=1}^{r}\delta_{ij}x_i z_j + \varepsilon \tag{10}$$

Assume independent noise variables with zero mean and known variances σ_z^2. Furthermore, consider that noise variables and the random error are uncorrelated. With these assumptions, the mean and variance models can be written as (Montgomery, 2009; Myers, Montgomery, & Anderson-Cook, 2009):

$$E_z[y(\mathbf{x},\mathbf{z})] = f(\mathbf{x}) \tag{11}$$

$$V_z[y(\mathbf{x},\mathbf{z})] = \sum_{i=1}^{r}\left[\frac{\partial y(\mathbf{x},\mathbf{z})}{\partial z_i}\right]^2 \sigma_{z_i}^2 + \sigma^2 \tag{12}$$

where k and r are the number of control and noise variables, respectively. Now, suppose the original observations of the multiple responses Y_p, measured with the combined array, can, as discussed in the previous section, be replaced by their principal component scores using the transformation $P_{c_i} = e_i^T[Z(Y_p)]$. Estimating a quadratic model for the principal component scores, $y(\mathbf{x},\mathbf{z})_i$ may be interpreted as $P_c(\mathbf{x},\mathbf{z})_i$. One can now apply the propagation of error principle to $P_c(\mathbf{x},\mathbf{z})_i$ in order to obtain their respective mean and variance equations. Considering the multivariate optimization of mean and variance, one may set the weight ω and then solve the multiple correlated responses and noise variables as follows:

$$Min\ MMSE(Fi)(\mathbf{x}) = \left\{ \prod_{i=1}^{m} \left[\begin{array}{c} \omega\cdot(E_z[P_c(\mathbf{x},\mathbf{z})_i] - \zeta_{PCz_i})^2 + \\ (1-\omega)\cdot\left[\sigma_z^2\cdot\sum_{j=1}^{r}\left(\frac{\partial P_c(\mathbf{x},\mathbf{z})_i}{\partial z_j}\right)^2 + \sigma^2\right] \end{array} \right]^{\phi_i} \middle| \sum_{i=1}^{m-r}\phi_i \geqslant \xi \right\}^{\left(\frac{\frac{1}{m-r}}{\sum_{i=1}\phi_i}\right)} \tag{13}$$

$$\text{subject to}: \mathbf{x}^T\mathbf{x} \leqslant \rho^2$$

$$\text{with}: \zeta_{PCz_i} = e_{1i}[Z(Y_1|\zeta_{Y_1})] + e_{2i}[Z(Y_2|\zeta_{Y_2})] + \ldots + e_{pi}[Z(Y_p|\zeta_{Y_p})] \tag{14}$$

$$P_c(\mathbf{x},\mathbf{z})_i = b_{0i} + [\nabla f(\mathbf{x})^T]_i + \left\{\frac{1}{2}\mathbf{x}^T[\nabla^2 f(\mathbf{x})]\mathbf{x}\right\} \tag{15}$$

$$i = 1,2,\ldots,p; \quad m \leqslant p$$
$$\mathbf{x} = [x_1, x_2, \ldots, x_k]$$
$$\mathbf{z} = [z_1, z_2, \ldots, z_r]$$

The value of ζ_{Y_p} corresponds to a utopia point obtained as $\zeta_{Y_p} = Min_{\mathbf{x}\in\Omega}[\hat{y}_i(\mathbf{x})]$ and Z represents the standardized value of the ith response considering the target ζ_{Y_p}, such that $Z(Y_p - \zeta_{Yp}) = [(\zeta_{Yp}) - \mu_{Yp}] \times (\sigma_{Yp})^{-1}$. Furthermore, the term ϕ_i is an exponent that stands for the relative importance of each component used to compose the *MMSE (Fi)*($\mathbf{x}$), being obtained by:

$$\phi_i = \frac{\lambda_i}{\left(\sum_{i=1}^{p}\lambda_i\right)} \tag{16}$$

where λ_i is the eigenvalue associated to the ith largest principal component. Gomes et al. (2013) and Paiva et al. (2010) have applied similar approach, using weighted sum though. The conditional parameter ξ represents the acceptable cumulative proportion of explanation associated with the ith largest principal components, fixed as the practitioner so desires. So as to compare with traditional uncorrelated and correlated approaches, this method was labeled "MMSE (Fi)".

Alternatively, the global multiobjective function *MMSE (Fi)*($\mathbf{x}$) from Eq. (13) can be written to suppress the exponential term ϕ_i from the expression and to adopt the geometric mean of Multivariate Mean Square Error functions whose principal components have an explanation higher than 80% (ξ = 0.8). This modification allows one to evaluate the influence of ϕ_i on the optimization results, leading to the following global multiobjective function:

$$MMSE(\mathbf{x}) = \left\{ \prod_{i=1}^{m} \left[\begin{array}{c} \omega\cdot(E_z[P_c(\mathbf{x},\mathbf{z})_i] - \zeta_{PCz_i})^2 + \\ (1-\omega)\cdot\left[\sigma_z^2\cdot\sum_{j=1}^{r}\left(\frac{\partial P_c(\mathbf{x},\mathbf{z})_i}{\partial z_j}\right)^2 + \sigma^2\right] \end{array} \right] \right\}^{\left(\frac{1}{m}\right)} \tag{17}$$

The constraint $\mathbf{x}^T\mathbf{x} \leqslant \rho^2$ remains the same. With this modification, the multivariate approach described above is hereafter referred to as the "MMSE" method. It is also a point of comparison for the other methods discussed in this work.

Once the global multiobjective function is established, its optimum can be generally reached by using several methods available

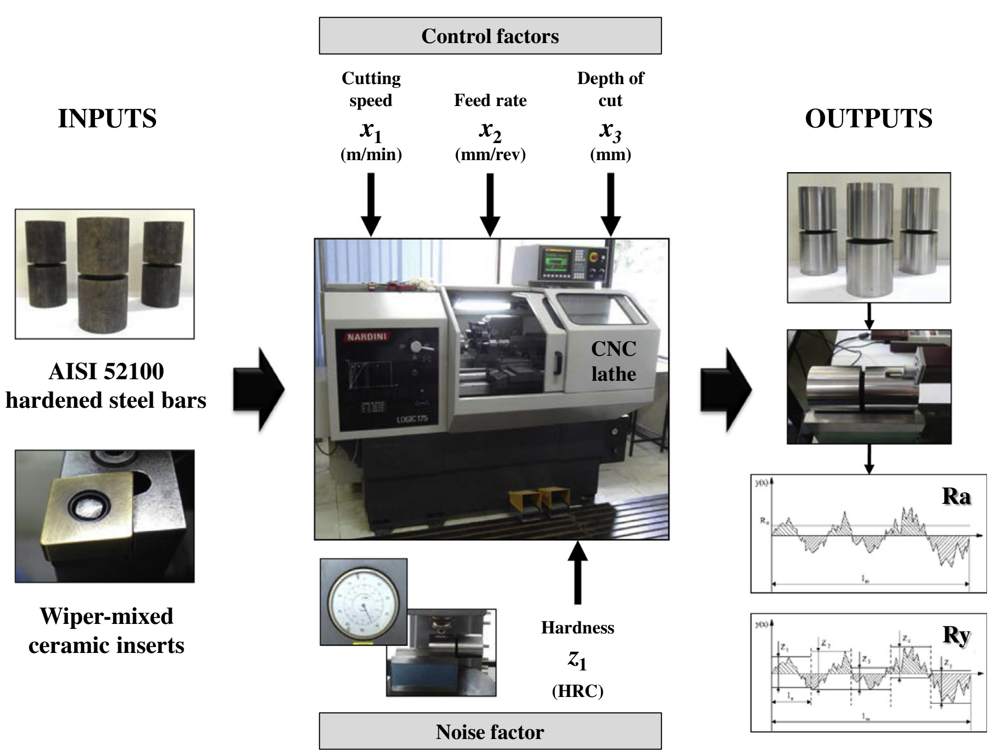

Fig. 1. Turning process of the AISI 52100 hardened steel.

to solve nonlinear programming problems (NLP), such the Generalized Reduced Gradient (GRG) (Haggag, 1981; M'silti & Tolla, 1993; Paiva et al., 2012; Sadagopan & Ravindran, 1986; Tang & Xu, 2002). GRG is considered one of the most robust and efficient gradient algorithms for nonlinear optimization and, as an attractive feature, it exhibits an adequate global convergence, mainly when initiated sufficiently close to the solution (Lasdon, Waren, Jain, & Ratner, 1978). Moreover, one can note that the transformed multiobjective function remains convex, so that a strict minimum should exist. For these reasons, this work used the GRG.

Given the discussion above, the MMSE approach proposed in this section may be summarized as follows:

Procedure:

Step 1: Experimental design
Establish an adequate combined array as an experimental design, including as many control and noise variables as desired. Run the experiments in random order and store the responses.

Step 2: Principal Component Analysis
Conduct the Principal Component Analysis (PCA) using the correlation matrix of original data, storing the PC-scores (whose explained variance is at least 80%) and respective eigenvalues and eigenvectors.

Step 3: Modeling of responses including control and noise variables
Establish equations for $y(\mathbf{x},\mathbf{z})_i$ and $P_c(\mathbf{x}, \mathbf{z})_i$ using experimental data for original responses and PC-scores.

Step 4: Means and variances definition
Establish equations for mean and variance of $y(\mathbf{x},\mathbf{z})_i$ and $P_c(\mathbf{x},\mathbf{z})_i$ using Eqs. (11) and (12).

Step 5: Constrained optimization of Y_p
Establish the response targets (ζ_{Y_p}) using the individual constrained minimization of each response surface, such as $\zeta_{Y_p} = Min_{\mathbf{x}\in\Omega}[\hat{y}_i(\mathbf{x})]$.

Step 6: Choose the PC-score target values
Transform the original targets (ζ_{Y_p}) in PC-targets using $\zeta_{PC_i} = \sum_{i=1}^{p}\sum_{j=1}^{q} e_{ij}[Z(Y_p|\zeta_{Y_p})]$.

Step 7: Choose means and variances weights
Choose a desired value for ω, generally using the range [0; 1] and observe the value of the percentage of explanation for PC_i (ϕ_i). This value is needed only if the practitioner needs more than one principal component.

Step 8: Build the Multivariate Mean Square Error index
With the previous steps, write the global objective function for the problem using Eq. (13) (or Eq. (17) alternatively).

Step 9: Run the multiobjective nonlinear optimization algorithm
Using the Generalized Reduced Gradient (GRG) algorithm, minimize the value of $MMSE\ (Fi)(\mathbf{x})$ obtained in **Step 8**, using as constraints the experimental region, non-negative variances or some other constraint $g_i(\mathbf{x})$ desired by the practitioner.
The next section presents a numerical illustration of our proposal and checks its adequacy.

5. Experiment description

This work, to achieve its aims, carried out dry turning tests of AISI 52100 hardened steel (1.03% C; 0.23% Si; 0.35% Mn; 1.40% Cr; 0.04% Mo; 0.11% Ni; 0.001% S; 0.01% P). AISI 52100 hardened steel is especially recommended for the manufacturing of dies, profiling rollers, ball and bearing cages. It is also employed in the cold work of forming matrices, profiling cylinders, besides wear coating purposes.

Table 1
Experimental design.

Run	Control parameters			Noise	Responses		PC-scores	
	x_1	x_2	x_3	z_1	*Ra*	*Ry*	PC_1	PC_2
1	200	0.20	0.150	40	0.317	2.194	−1.601	−1.018
2	240	0.20	0.150	40	0.327	2.179	−1.407	−0.727
3	200	0.40	0.150	40	0.341	2.212	−0.960	−0.494
4	240	0.40	0.150	40	0.421	2.543	2.061	0.371
5	200	0.20	0.300	40	0.366	2.575	0.830	−1.069
6	240	0.20	0.300	40	0.355	2.311	−0.297	−0.476
7	200	0.40	0.300	40	0.382	2.742	1.762	−1.224
8	240	0.40	0.300	40	0.383	2.718	1.708	−1.122
9	200	0.20	0.150	60	0.385	2.194	0.050	0.633
10	240	0.20	0.150	60	0.379	2.245	0.071	0.322
11	200	0.40	0.150	60	0.392	2.181	0.178	0.846
12	240	0.40	0.150	60	0.456	2.686	3.377	0.756
13	200	0.20	0.300	60	0.393	2.180	0.199	0.873
14	240	0.20	0.300	60	0.367	1.931	−1.243	1.053
15	200	0.40	0.300	60	0.387	2.141	−0.074	0.855
16	240	0.40	0.300	60	0.367	2.258	−0.178	−0.012
17	180	0.30	0.225	50	0.368	2.156	−0.486	0.344
18	260	0.30	0.225	50	0.382	2.181	−0.065	0.603
19	220	0.10	0.225	50	0.361	2.145	−0.692	0.210
20	220	0.50	0.225	50	0.412	2.699	2.351	−0.355
21	220	0.30	0.075	50	0.373	2.143	−0.407	0.508
22	220	0.30	0.375	50	0.352	2.151	−0.891	−0.028
23	220	0.30	0.225	50	0.347	2.175	−0.935	−0.228
24	220	0.30	0.225	50	0.351	2.184	−0.808	−0.160
25	220	0.30	0.225	50	0.349	2.175	−0.886	−0.179
26	220	0.30	0.225	50	0.351	2.179	−0.824	−0.144
27	220	0.30	0.225	50	0.351	2.177	−0.831	−0.137

Table 2
Principal Component Analysis.

Eigenvalue	1.5567	0.4433
Proportion	0.7780	0.2220
Cumulative	0.7780	1.0000
Eigenvectors	PC_1	PC_2
Ra	0.7070	0.7070
Ry	0.7070	−0.7070

Table 3
Response surface models with noise variables.

Coefficient	*Ra*	*Ry*	PC_1	PC_2
b_0	0.3521	2.2081	−0.7034	−0.2125
x_1	0.0050	0.0209	0.1896	0.0533
x_2	0.0143	0.1158	0.7234	−0.0311
x_3	−0.0025	0.0183	−0.0013	−0.1202
z_1	0.0146	−0.1036	0.0178	0.6927
$x_1 \cdot x_1$	0.0072	0.0089	0.2028	0.1447
$x_2 \cdot x_2$	0.0100	0.0723	0.4791	0.0081
$x_3 \cdot x_3$	0.0040	0.0036	0.1094	0.0863
$x_1 \cdot x_2$	0.0099	0.0879	0.5261	−0.0463
$x_1 \cdot x_3$	−0.0128	−0.0808	−0.5727	−0.0467
$x_1 \cdot z_1$	−0.0043	0.0248	−0.0226	−0.1838
$x_2 \cdot x_3$	−0.0103	0.0032	−0.2384	−0.2596
$x_2 \cdot z_1$	−0.0053	−0.0150	−0.1764	−0.0787
$x_3 \cdot z_1$	−0.0111	−0.1259	−0.6802	0.1397
Adj. R^2 (%)	87.76	86.11	86.76	85.89
Residual error	0.000112	0.006650	0.2192	0.0546

The experiments were conducted on a CNC lathe, with the maximum rotational speed and power of 4000 rpm and 5.5 kW. Also employed were Wiper-mixed ceramic (Al_2O_3 + TiC) inserts (ISO code CNGA 120408 S01525WH) coated with a thin layer of titanium nitride (TiN; Sandvik-Coromant GC 6050). The tool holder presented a negative geometry with ISO code DCLNL 1616H12 and an entering angle χ_r = 95°. The workpieces, with dimensions

Table 4
Mean and variance equations.

Coefficient	*Ra*	*Ry*	PC_1	PC_2	*Var Ra*	*Var Ry*	*Var* PC_1	*Var* PC_2
b_0	0.3521	2.2081	−0.7034	−0.2125	0.000214	0.010738	0.000316	0.479890
x_1	0.0050	0.0209	0.1896	0.0533	−0.000124	−0.005129	−0.000804	−0.254710
x_2	0.0143	0.1158	0.7234	−0.0311	−0.000154	0.003109	−0.006269	−0.109004
x_3	−0.0025	0.0183	−0.0013	−0.1202	−0.000325	0.026088	−0.024177	0.193567
$x_1 \cdot x_1$	0.0072	0.0089	0.2028	0.1447	0.000018	0.000613	0.000512	0.033798
$x_2 \cdot x_2$	0.0100	0.0723	0.4791	0.0081	0.000028	0.000225	0.031110	0.006190
$x_3 \cdot x_3$	0.0040	0.0036	0.1094	0.0863	0.000124	0.015845	0.462653	0.019519
$x_1 \cdot x_2$	0.0099	0.0879	0.5261	−0.0463	0.000045	−0.000743	0.007983	0.028928
$x_1 \cdot x_3$	−0.0128	−0.0808	−0.5727	−0.0467	0.000095	−0.006231	0.030787	−0.051369
$x_2 \cdot x_3$	−0.0103	0.0032	−0.2384	−0.2596	0.000117	0.003776	0.239942	−0.021984

Table 5
Payoff matrices.

Payoff matrix for *Ra* and *Ry*		Payoff matrix for MSE_1 and MSE_2	
0.3382	2.0956	0.000278	0.054144
0.3490	1.9920	0.001996	0.009048

of ϕ 49 mm × 50 mm, were machined considering three control variables: cutting speed (x_1, m/min), feed rate (x_2, mm/rev), and depth of cut (x_3, mm). Prior to machining, the workpieces were quenched and tempered to attain three levels of hardness (40, 50, and 60 HRC) up to a depth of 3 mm below the surface. This paper considers these hardness values as noise factor levels (z_1).

The aim of different noise conditions is to simulate the general phenomena that occur during a turning operation, reproducing, in some sense, the decreasing of the workpiece surface hardness during the machining operation. It is expected that the surface roughness values will suffer some kind of variation due to noise conditions. So, the main objective of the Robust Parameter Design is to determine the control parameters capable of achieving a reduced surface roughness with minimal variance. The multiple correlated responses associated with the machining process considered here were the arithmetic average surface roughness (*Ra*) and the maximum surface roughness (*Ry*). Fig. 1 represents the turning process of the AISI 52100 hardened steel used in this experimental study.

Because *Ra* is an average value, it is not strongly correlated with defects on the surface and not suitable for defect detection (Correa, Bielza, & Pamies-Teixeira, 2009). Thus, most practitioners use a second surface roughness metric, like *Ry*. *Ry* is the greatest partial roughness value (Z_i) observed among several sample lengths (l_e). This parameter is used extensively by researchers because it is capable of informing the maximum vertical deterioration of the surface. To measure these responses, both measures of surface roughness were assessed using a Mitutoyo portable roughness tester, model Surftest SJ 201, set to a cut-off length of 0.25 mm.

Following the experimental sequence of a combined array (Montgomery, 2009), a CCD for $k = 4$ variables (x_1, x_2, x_3, and z_1) was used as a response surface design, deleting the axial points referent to the noise variable z_1 (**Step 1** of the proposed procedure).

Table 6
Optimization results for the MMSE (Fi) method.

ω	Coded parameters			Responses				MSE_1	MSE_2
	x_1	x_2	x_3	*Ra*	*Ry*	*Var Ra*	*Var Ry*		
0.05	1.190	−1.098	0.456	0.3496	2.0545	0.0002	0.0199	0.000348	0.023814
0.10	1.294	−1.041	0.270	0.3513	2.0657	0.0002	0.0147	0.000419	0.020183
0.20	1.228	−1.104	0.322	0.3503	2.0616	0.0002	0.0161	0.000395	0.020953
0.30	1.205	−1.115	0.364	0.3500	2.0593	0.0002	0.0172	0.000380	0.021775
0.40	1.195	−1.111	0.408	0.3498	2.0570	0.0002	0.0185	0.000364	0.022694
0.50	1.190	−1.098	0.456	0.3496	2.0545	0.0002	0.0199	0.000348	0.023814
0.60	1.187	−1.077	0.512	0.3494	2.0518	0.0002	0.0217	0.000330	0.025255
0.70	1.182	−1.048	0.578	0.3492	2.0491	0.0002	0.0239	0.000309	0.027177
0.80	1.176	−1.008	0.657	0.3490	2.0467	0.0002	0.0268	0.000287	0.029832
0.90	1.162	−0.953	0.756	0.3487	2.0451	0.0002	0.0309	0.000263	0.033733
0.95	1.149	−0.910	0.826	0.3486	2.0450	0.0001	0.0340	0.000248	0.036861

Table 7
Optimization results for the compared methods.

Weights	MMSE (Fi)		MMSE		WSum		Beta	
	MSE1a	MSE2a	MSE1b	MSE2b	MSE1c	MSE2c	MSE1d	MSE2d
0.05	0.000348	0.023814	0.000930	0.034948	0.001218	0.012885	0.001918	0.013791
0.10	0.000419	0.020183	0.000605	0.023690	0.001221	0.012505	0.001915	0.013798
0.20	0.000395	0.020953	0.000463	0.020508	0.001229	0.012344	0.000756	0.020821
0.30	0.000380	0.021775	0.000419	0.020484	0.001237	0.012265	0.000699	0.021324
0.40	0.000364	0.022694	0.000394	0.021046	0.001245	0.012217	0.000640	0.022165
0.50	0.000348	0.023814	0.000374	0.021884	0.001253	0.012196	0.000579	0.023482
0.60	0.000330	0.025255	0.000354	0.023006	0.001262	0.012201	0.000516	0.025509
0.70	0.000309	0.027177	0.000333	0.024540	0.001270	0.012233	0.000452	0.028655
0.80	0.000287	0.029832	0.000309	0.026820	0.000361	0.022600	0.000390	0.033669
0.90	0.000263	0.033733	0.000273	0.031540	0.000306	0.027190	0.000334	0.042115
0.95	0.000248	0.036861	0.000256	0.035461	0.000278	0.030820	0.000314	0.048679

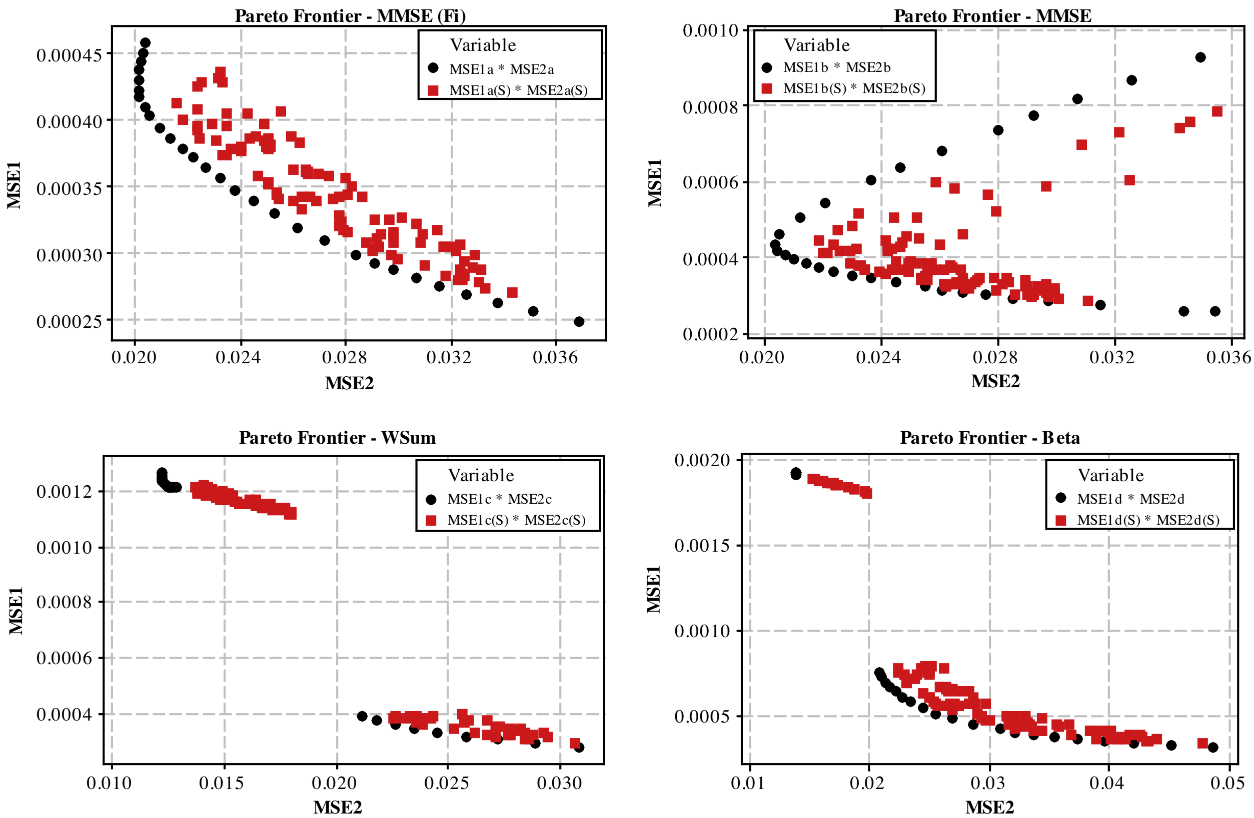

Fig. 2. Comparison among Pareto frontiers obtained through different methods.

It resulted, as shown in Table 1, in 27 experiments. The surface roughness was measured three times at each of the four positions in the middle of the workpiece, the mean of the twelve measurements were computed for sake of adequacy.

6. Results and discussion

6.1. Procedure application

A top issue of this multiobjective optimization approach regards the correlation among the responses. For the results found in Table 1 the Pearson's correlation coefficient is 0.557 (*P-value* = 0.003), representing a moderate level of correlation with statistical significance. Conducting a spectral decomposition on the correlation matrix (**R**), one can obtain the respective eigenvalues and eigenvectors of **R**, as shown in Table 2 (**Step 2**). This table shows that the first principal component explains about 77.80% of variance–covariance structure established between Ra and Ry. This finding allows one to replace the original response variables with their respective principal component scores (PC_1 and PC_2). Once the PC-scores are obtained, the OLS algorithm is applied, yielding the second order models of original data $y(\mathbf{x},\mathbf{z})_i$ and principal components $P_c(\mathbf{x},\mathbf{z})_i$. Table 3 shows the coefficients and model's adequacy measures for Ra, Ry, PC_1 and PC_2 (**Step 3**). All *adj.* R^2 values were higher than 85.00%, which can be considered excellent adjustments. Bearing in mind previous works by Paiva et al. (2009) and Paiva et al. (2012), where surface roughness metrics were also used as responses, one can conclude that the inclusion of the noise variables z_1 into the design naturally decreases the values of Pearson's correlation coefficient and the *adj.* R^2 values.

After the modeling task, mean and variance equations for Ra, Ry, PC_1, and PC_2 were established with the help of the POE principle (**Step 4**). The full quadratic models of these characteristics are shown in Table 4. The surface roughness targets (ζ_{Y_p}) were then calculated using the individual constrained minimization of each response (**Step 5**). For the present data, $\zeta_{Ra} = 0.3382$ μm and $\zeta_{Ry} = 1.992$ μm. These values were used in order to compose each $MSE(\mathbf{x})$. After individual optimization, one can obtain the values of $MSE_i^{\max}(\mathbf{x})$ and $MSE_i^I(\mathbf{x})$. For both cases, the utopia points lead to the Payoff matrix of Table 5. To apply the MMSE (Fi) and MMSE methods, the original targets must be transformed into PC-targets (ζ_{PC_i}) (**Step 6**). Thus, it was found -1.744 for PC_1 and 0.154 for PC_2. Table 6 shows different chosen values for the weight ω (**Step 7**). For the MMSE (Fi) method, the multivariate coefficients for the first and second principal components were $\phi_1 = 0.778$ and $\phi_2 = 0.222$, respectively. To conclude this setup, the nonlinear constraint $\mathbf{x}^{\mathrm{T}}\mathbf{x} \leqslant 2.829$ was considered since the axial distance (ρ) for a CCD with $k = 3$ control factors is 1.682. With this information, the four models discussed earlier could be tested (**Step 8** and **Step 9**).

6.2. Methods' comparisons

Mean square error models typically contain fourth-order terms which in turn may generate non-convex and supported efficient solutions when weighted sums are used as a global optimization criterion. Therefore, weighted sums may generate discontinuous Pareto frontiers. On the other hand, the compromise solutions, generated by geometric and weighted geometric means, avoid such drawback. Table 7 summarizes the optimization results for each multiobjective method. Moreover, Fig. 2 compares the Pareto frontiers obtained using the four optimization approaches discussed in this paper.

Note that multivariate approaches using a multiplicative operator to agglutinate the objective functions present convex and continuous Pareto frontiers. However, this is not the case with "Beta" and "Weighted Sum" approaches, both of which generated an extremely large gap between two consecutive weights.

```
Chi-Square = 21.60    DF = 3    P = 0.000

                                         Individual 95.0% CIs
Method  N<=  N>   Median    Q3-Q1   --+---------+---------+---------+----
MSE1a    24   6  0.00035  0.00012   (*)
MSE1b    18  12  0.00039  0.00030   (-*-)
MSE1c     9  21  0.00122  0.00087                          *)
MSE1d     9  21  0.00062  0.00151     (----*------------------------)
                                    --+---------+---------+---------+----
                                    0.00040   0.00080   0.00120   0.00160

(a)     Overall median = 0.00042

Chi-Square = 13.87    DF = 3    P = 0.003

                                        Individual 95.0% CIs
Method*  N<=  N>  Median   Q3-Q1   -----+---------+---------+---------+-
MSE2a     13  17  0.0235  0.0089                   (----*------)
MSE2b      9  21  0.0251  0.0076                      (----*-----)
MSE2c     23   7  0.0126  0.0098   *)
MSE2d     15  15  0.0225  0.0188         (-------------*-----------)
                                   -----+---------+---------+---------+-
                                      0.0150    0.0200    0.0250    0.0300

(b)     Overall median = 0.0223

Chi-Square = 5.60    DF = 3    P = 0.133

                                        Individual 95.0% CIs
Method**  N<=  N>  Median   Q3-Q1   -+---------+---------+---------+-----
Bias a     20  10  0.0746  0.0193    (-----*-----)
Bias b     15  15  0.0817  0.0593        (--------*----------------------)
Bias c     11  19  0.0829  0.0087                (-*-)
Bias d     14  16  0.0821  0.0149      (----------*
                                    -+---------+---------+---------+-----
                                    0.070     0.080     0.090     0.100

(c)     Overall median = 0.0817

Chi-Square = 8.27    DF = 3    P = 0.041

                                         Individual 95.0% CIs
Method***  N<=  N>  Median   Q3-Q1   ----+---------+---------+---------+--
Var a       10  20  0.0198  0.0111                  (------*-------)
Var b       14  16  0.0167  0.0110            (-----*--------)
Var c       21   9  0.0079  0.0101   *
Var d       15  15  0.0159  0.0201     (-------------*--------------)
                                     ----+---------+---------+---------+--
                                       0.0100    0.0150    0.0200    0.0250

(d)     Overall median = 0.0164
```

Fig. 3. Mood's median test for optimization models properties: (a) MSE_1, (b) MSE_2, (c) Bias, and (d) Variance.

In addition to the mentioned analyses, Figs. 3 and 4 respectively compare accuracy and precision of evaluated methods. Fig. 3 shows the results from Mood's median test comparing MSE_1, MSE_2, Bias, and Variance for each model. Mood's median test is a robust statistical procedure against outliers, to test the equality of medians from two or more populations. It is mainly used when the data does not follow a normal distribution. Hence, this test provides a nonparametric alternative to the one-way Analysis of Variance (Montgomery, 2009). Examining Fig. 3a for the property MSE_1 (mean square error for *Ra*), one can note significant differences among the four approaches discussed in this paper (*P-value* < 0.05). Furthermore, observing the confidence intervals for individual medians, it is immediately clear that the MMSE (Fi) method presents the lowest value for MSE_1 and that WSum exhibits the largest. This method presents the narrowest 95% C.I. for the medians, implying that it provides the lowest variance among the optimization results obtained through different weights. The first graphic in Fig. 4, where the Levene's nonparametric test was used, also shows this result. Thus, low levels of variance among optimization results are a reflection of the smoothness and continuity of the Pareto frontier. Indeed, these results are somewhat expected, since *Ra* is a "mean-type" measure and the variance of a mean tend to be less than the variance of a difference (or range).

On the other hand, for MSE_2 (mean square error for *Ry*), the difference is also statistically significant, but the WSum method exhibited the lowest median (Fig. 3b). This is understandable since *Ry* is a "range-type" metric. Besides, it can be noted that no difference was found among the three methods considering the correlation between *Ra* and *Ry*, as there was an overlap of their 95% confidence intervals. Once the variance of the optimization results obtained with these three multivariate methods are less than the weighted sum, the smallest values of MSE_2 were achieved by the WSum because this method ignores the correlation term (see Fig. 4 and compare Eqs. (2) and (5)). Splitting the MSE term into "Bias" and "Variance", no significant differences were found among

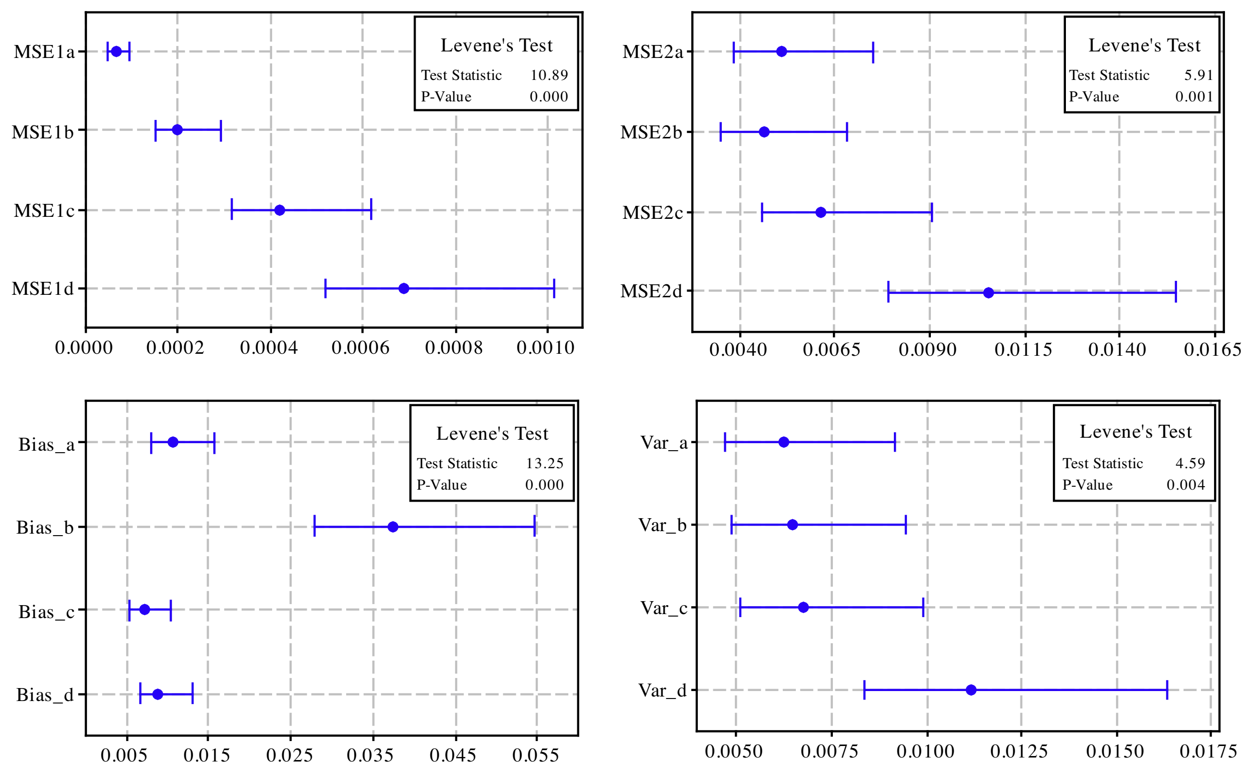

Fig. 4. Levene's test for optimization models properties MSE_1, MSE_2, Bias, and Variance.

bias of the compared methods (Fig. 3c). Finally, *P-value* presented in Fig. 3d identified significant difference among methods for "Variance" component, in which WSum method has determined the lowest median.

It is essential to highlight that the variance of optimization results, obtained with different weights, comes mainly from the discontinuity of the Pareto frontier. Thus, methods that use weighted sums as agglutination operations exhibited discontinuous frontiers, providing a drastic and abrupt change in the values of the MSE_1 and MSE_2. This, in turns, increases substantially the amount of variance in the data. Looking for such evidence, Levene's test was employed to evaluate the differences among confidence intervals for the standard deviation of each method. Similarly to the Mood's median test, Levene's test is a nonparametric statistical procedure adequate to evaluate the homoscedasticity when the data come from continuous, but not necessarily normal distributions. As can be seen in Fig. 4, methods' variances are different (all *P-values* < 5%). For MSE_1, the PCA-based approaches (MMSE (Fi) and MMSE) are statistically different from the weighted sums (WSum and Beta), with the PCA-approaches presenting substantially smaller standard deviations (and, in consequence, variances). Note the absence of a statistical difference between WSum and Beta confidence intervals. For MSE_2, the differences were less than MSE_1, but the variance values obtained with PCA-based methods are still less than the traditional weighted sums methods. For the "Bias" property, MMSE (Fi) presents results that were similar to those exhibited by weighted sums and significantly smaller than MMSE. For "Variance" component, the test has shown significant difference, mainly, due to the standard deviation provided by Beta method.

Based on the previous conclusions, more detailed analyses among multivariate approaches were performed. In Fig. 5, the Pareto frontiers of the MMSE (Fi) and MMSE methods were plotted and compared. Note that the solution region, for both methods, is convex and the frontier is continuous. Although they seem the same, the reference anchorage points are considerably different.

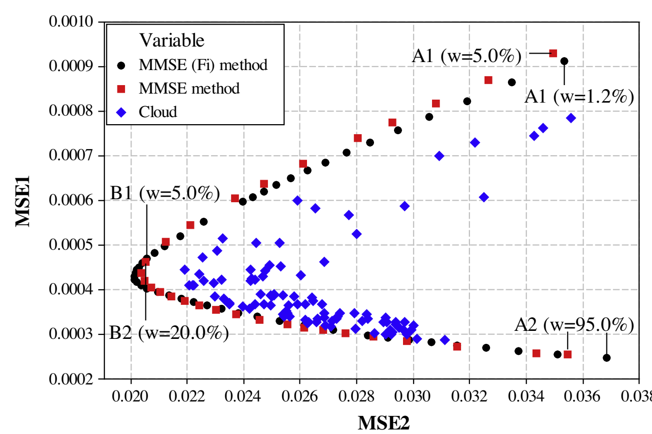

Fig. 5. Comparison between MMSE (Fi) and MMSE Pareto frontiers.

For low weights, for example, the same MSE_1 and MSE_2 are reached in the MMSE (Fi) with a lower weight ($\omega = 1.2\%$) than that in the MMSE method ($\omega = 5.0\%$). Around the inflection point, however, this difference is greater: $\omega = 5.0\%$ for MMSE (Fi) corresponding to a $\omega = 20.0\%$ for MMSE for the same values of the pair $MSE_1 \times MSE_2$. This discrepancy clearly highlights the influence of the coefficients ϕ_i used in the MMSE (Fi) model. Indeed, when compared to further components – in this case, the second one – these coefficients emphasize the importance of the first principal component. As PC_1 contains much more information regarding variation than PC_2, its objective function should be prioritized.

Analyzing the Pareto frontiers in Fig. 5, it can be seen that some points of the proposed method are apparently dominated by MMSE method. Nevertheless, besides the previous explanation, it is important to evidence that there is variation associated to those estimates. Taking into consideration that the objective functions

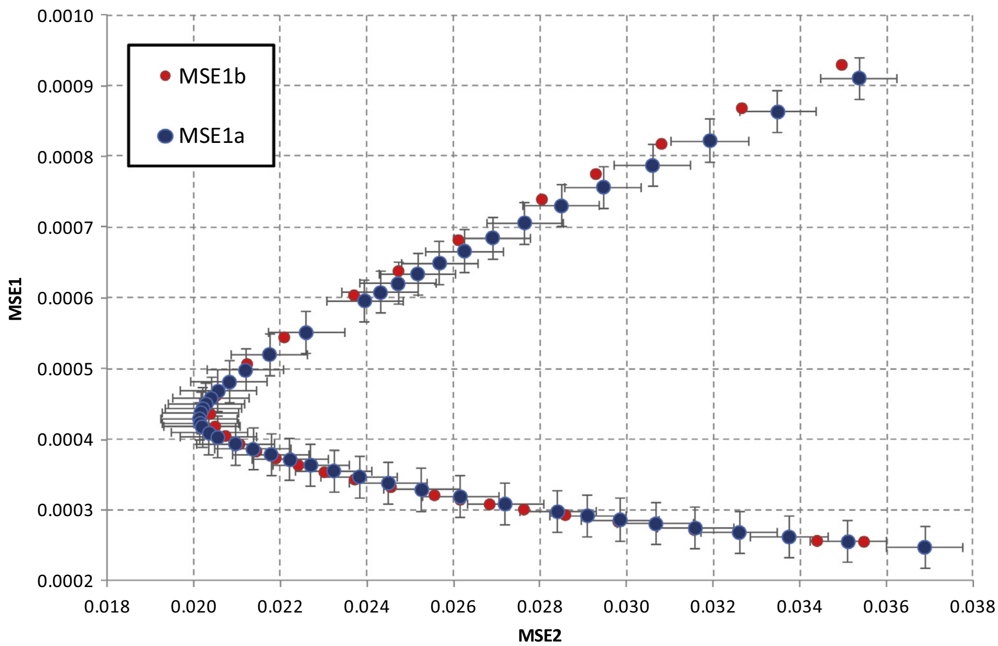

Fig. 6. Pareto frontier with combined confidence intervals from simulated results.

Table 8
Manova hypothesis test for MMSE (Fi) (w = 1.2%) and MMSE (w = 5.0%) methods.

MANOVA: Optimization Method versus MSE1 and MSE2 (s = 1; m = 0; n = 13.5)					
Criterion	Test	F	DF Num	DF Denom	*P-value*
Wilks'	0.98488	0.223	2	29	0.802
Lawley–Hotelling	0.01535	0.223	2	29	0.802
Pillai's	0.01512	0.223	2	29	0.802
Roy's	0.01535				
Pearson Correlation MSE1 × MSE2:			0.732	*P-value*:	0.000

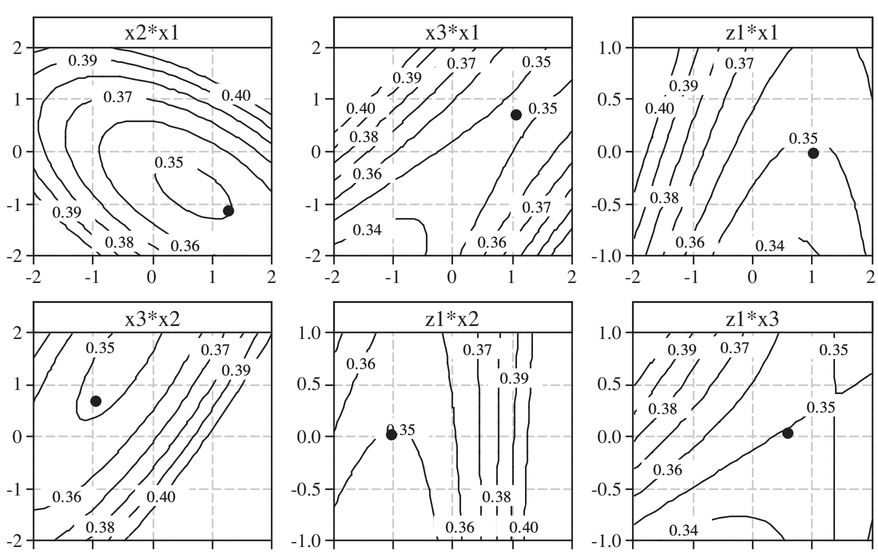

Fig. 7. Optimum obtained by the MMSE (Fi) with ω = 0.70 (projection in the plane of *Ra*).

are response surface obtained from experimental data, there are standard errors associated to expected values of the regression coefficients. Based on this particularity, it is reasonable to admit that there is a population of objective functions. Hence, a confidence interval was supposed to be assigned to each frontier point. Therefore, if there is an overlapping between MMSE and MMSE (Fi) confidence intervals, it is not reasonable to affirm that there is dominance of a particular frontier over another one.

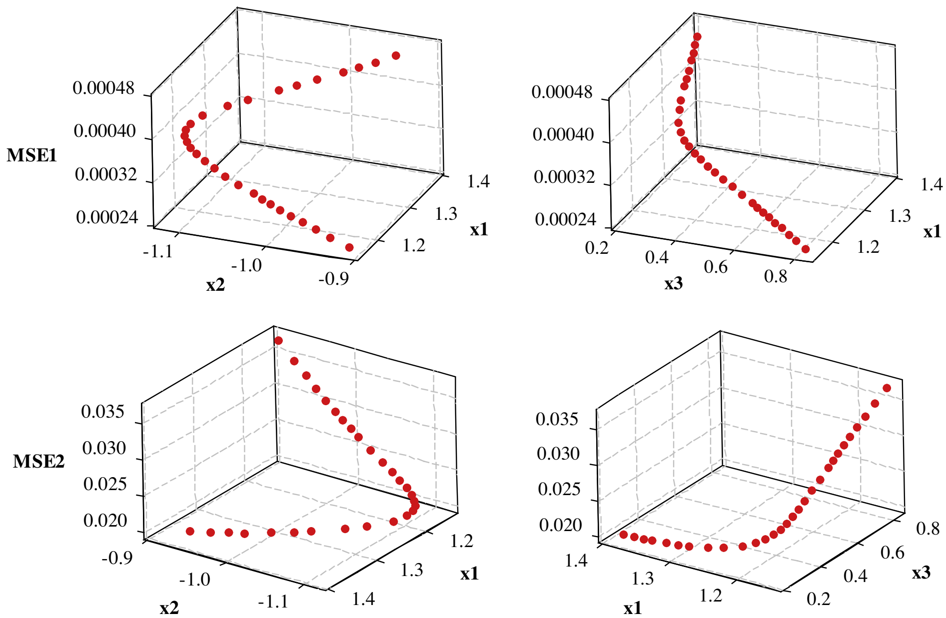

Fig. 8. Pareto frontiers for MSE_1 and MSE_2 in the space of ρ^2.

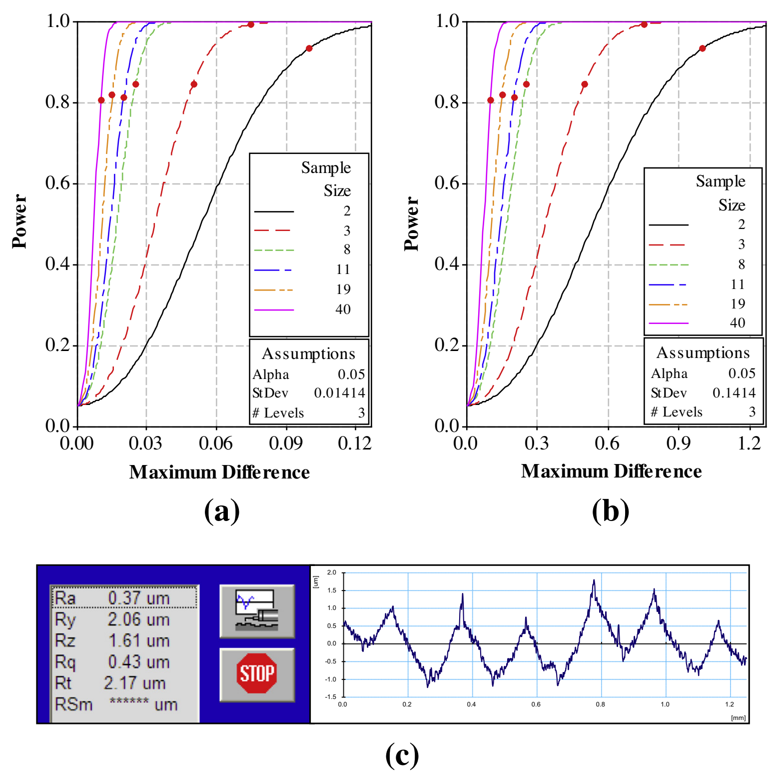

Fig. 9. (a) Power curve for Ra, (b) power curve for Ry, and (c) measurement of the workpiece: *Hardness* = 50HRC, *i* = 3 and *j* = 3 in Table 9.

For sake of comparison, a simulation study was performed in order to compare MMSE (Fi) and MMSE Pareto frontiers. Fig. 6 shows the combined confidence interval for MSE_1 and MSE_2 estimated by the multivariate approaches. To illustrate how similar two estimates are, the points A1 (MMSE: $w = 5.0\%$) and A1 (MMSE (Fi): $w = 1.2\%$) highlighted in Fig. 5 were compared by using a multivariate analysis of variance. As can be seen from Table 8, the hypothesis tests have emphasized that there were no statistical difference of MSE_1 and MSE_2 estimated from the multivariate approaches.

The comparison study has evidenced that MMSE (Fi) provided better properties in relation to the other methods. Hence, another analysis was conducted to project MMSE (Fi) results into the space of original variables. As emphasized earlier, the multiplicative operator used in MMSE approaches avoided the lack of continuity in the frontier. Fig. 7, for instance, represents an optimum obtained

Table 9
Confirmation test's measurements.

Hardness	i	Ra				Ra mean	Ry				Ry mean
		j = 1	j = 2	j = 3	j = 4		j = 1	j = 2	j = 3	j = 4	
60	1	0.35	0.34	0.35	0.35	0.348	2.04	2.00	2.09	2.04	2.043
	2	0.36	0.34	0.36	0.35	0.353	2.05	2.03	2.06	2.06	2.050
	3	0.35	0.35	0.34	0.34	0.345	2.05	2.07	2.00	2.02	2.035
	4	0.36	0.34	0.34	0.35	0.348	2.07	2.06	2.07	2.06	2.065
	5	0.35	0.34	0.34	0.34	0.343	2.08	2.04	2.05	2.05	2.055
50	1	0.35	0.35	0.35	0.34	0.348	2.08	2.05	2.07	1.98	2.045
	2	0.36	0.34	0.36	0.33	0.348	2.08	2.09	2.08	2.00	2.063
	3	0.36	0.33	0.37	0.36	0.355	2.12	1.99	2.06	2.07	2.060
	4	0.35	0.34	0.35	0.36	0.350	2.07	2.04	1.98	2.11	2.050
	5	0.36	0.35	0.36	0.34	0.353	2.07	2.08	2.07	2.05	2.068
40	1	0.34	0.37	0.35	0.36	0.355	2.03	2.08	2.10	2.07	2.070
	2	0.34	0.36	0.35	0.34	0.348	2.07	2.13	2.04	2.03	2.068
	3	0.34	0.33	0.36	0.37	0.350	2.05	1.99	2.06	2.05	2.038
	4	0.35	0.33	0.35	0.36	0.348	2.11	1.99	2.04	2.10	2.060
	5	0.36	0.35	0.35	0.35	0.353	2.07	2.08	2.07	2.10	2.080
LCB						0.3473					2.0493
UCB						0.3513					2.0637
MMSE (Fi)						0.3496					2.0545

by the MMSE (Fi) with $\omega = 0.70$, projected in the plane of average surface roughness (*Ra*). It is easy to see that the MMSE (Fi) optimum is quite close to the stationary point of *Ra* surface. According to Shin et al. (2011), a bi-objective optimization problem is convex if the feasible set $\mathbf{x}$ is convex and both objective functions are convex. In this case, the Pareto set can be viewed as a convex curve in the space of ρ^2. Furthermore, the constraint $\mathbf{x}^T\mathbf{x} - \rho^2 \leqslant 0$ is convex since it represents a hypersphere of radius ρ. The graphics presented in Fig. 8 show convex curves of MSE_1 and MSE_2, written in terms of x_1, x_2, and x_3 obtained by the MMSE (Fi) method. These three variables belong to the space of solution ρ^2.

Taking into account not only the methods' comparative study for accuracy and precision, but also the detailed analyses among multivariate methods, it can be concluded that the MMSE (Fi) approach has presented lower variance values than did the other methods. Therefore, confirmation experiments were performed to investigate the adequacy of the proposed multiobjective optimization method.

6.3. Confirmation runs

Before designing and running confirmation experiments, power and sample size capabilities were evaluated to ensure enough certainty detecting differences of magnitude 0.01 for Ra and 0.1 for Ry. Fig. 9a and b respectively present power curves for *Ra* and *Ry*, based on the variances with $w = 0.5$ in Table 6. Examining the power curves, 19 samples are able to detect differences of magnitude 0.015 for Ra and 0.15 for Ry, with power = 0.82%. As a result, 20 samples were measured for each hardness level. Fig. 9c illustrates a measurement result obtained by the roughness tester.

In order to validate the effectiveness of the proposed MMSE (Fi) method, a set of confirmation experiments was then carefully carried out, machining $i = 5$ workpieces, measuring $j = 4$ repetitions on the middle of the bars, for each noise condition (hardness 40, 50 and 60 HRC). Table 9 shows roughness measurements of *Ra* and *Ry*, according to the uncoded experimental condition $x_1 = 244$, $x_2 = 0.19$, and $x_3 = 0.26$, using $w = 0.50$ in Table 6.

To verify whether *Ra* and *Ry* means are at their targets and the variability around those targets are as small as possible, accuracy and precision studies were conducted. Based on a multivariate analysis of variance for *Ra* and *Ry* means, the optimal experimental condition has proved to be insensible, at 5% significance, to the distinct hardness levels of workpieces. Moreover, 95% confidence intervals for *Ra*and *Ry* means were estimated and their results are shown in Table 9. As expected, the optimum provided by MMSE (Fi) method was estimated inside the confidence bounds, LCB (lower confidence bound) and UCB (upper confidence bound).

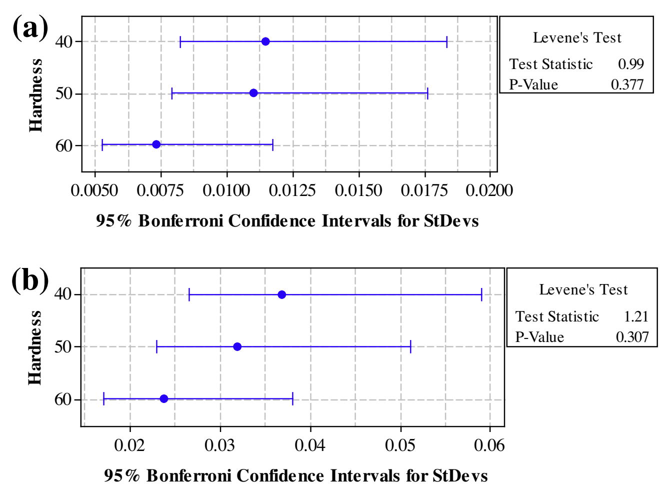

Fig. 10. Levene's tests for (a) *Ra* and (b) *Ry*.

Finally, variability around the optimum result was evaluated with Levene's tests. As shown in Fig. 10, no significant differences of roughness parameters *Ra* (*P-value* = 0.377) and *Ry* (*P-value* = 0.307) were found among hardness levels. In summary, the proposed multivariate optimization approach with combined array design has revealed to be an effective strategy for determining robustness to this dry turning process of AISI 52100 hardened steel.

7. Conclusions

This paper presented a new approach for robust multiobjective optimization of experiments considering Principal Component Analysis and the propagation of error principle. For this sake, PCA was employed in the modeling of multi-response experiments, and, in optimization procedure, POE was used to account for noise variables.

The POE principle allows for inference interactions among control and noise variables, such that optimization results may differ according to varying noise scenarios. PCA was used to avoid correlation issues in multi-response analysis.

The approach proposed in this paper, labeled MMSE (Fi), was then compared to other methods for multiobjective optimization, such as MMSE, WSum and Beta, by means of a turning experiment of AISI 52100 hardened steel.

The results showed the MMSE (Fi) method for multiobjective optimization to be a useful and reliable approach. It presented convex solution regions, continuous and smooth Pareto frontiers, non-dominated solutions, few variances and a lack of frontier peaks or disruptions. For the AISI 52100 hardened steel turning case, the surface roughness mean and variance values were quite small (for any weight used), being compatible with products meeting the highest levels of quality.

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