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A multivariate surface roughness modeling and optimization under conditions of uncertainty

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ABSTRACT

Correlated responses can be written in terms of principal component scores, but the uncertainty in the original responses will be transferred and will influence the behavior of the regression function. This paper presents a model building strategy that consider the multivariate uncertainty as weighting matrix for the principal components. The main objective is to increase the value of R^2 predicted to improve model's explanation and optimization results. A case study of AISI 52100 hardened steel turning with Wiper tools was performed in a Central Composite Design with three-factors (cutting speed, feed rate and depth of cut) for a set of five correlated metrics (R_a, R_y, R_z, R_q and R_t). Results indicate that different modeling methods conduct approximately to the same predicted responses, nevertheless the response surface to Weighted Principal Component – case b – (WPC1^b) presented the highest predictability.

1. Introduction

The uncertainty's measurement is a problem that affects the result's accuracy. Pérez [1] affirms that the uncertainties' measurement can both affect the response variable (**y**) and the predictor variables (**x**). Ignoring these uncertainties makes inefficient the results obtained through any design of experiments.

Correlated response may be written in terms of principal component scores. The uncertainty contained in the original responses will contaminate the principal components through the transfer function. The presence of correlation greatly influences the model building tasks causing its instability and provoking errors in the regression coefficients. In other words, the regression equations are not adequate to represent the objective functions without considering the variance–covariance (or correlation) structure [2,3]. The later aspect of the multi objective optimization is the influence of the correlation among the responses over the global solution. As pointed out by some researchers [4–6] the individual analyses of each response may lead to a conflicting optimum, since the factor levels that improve one response can, otherwise, degrade another.

Wang [7] confirms that median or high correlations existing among multiple responses significantly affect the product quality and these correlations must be considered when resolving the optimizing problem of multiple responses. Chiang and Hsieh [8] considered the correlation between quality characteristics and applied the principal component analysis to eliminate the multiple colinearity. McFarland and Mahadevan [9] affirmed that large correlation suggest that the parameters can be characterized using a reduced set of variables and the standard method for finding such a reduced set is PCA.

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Tong et al. [10] used PCA to simplify the optimization process and multi-response problems and concluded that the procedure is valid with some modifications. Wentzel and Lohanes [11] applied a procedure based on the method of Maximum Likelihood Principal Component Analysis (MLPCA) to include measurement error covariance in multivariate decomposition. The method is similar to conventional PCA, but it considers the uncertainty's measurement in the process placing less emphasis on measurements with large variance. Bratchell [12] employed a second-order response surface based on PCA to adequately represent the original set of responses in a small number of latent variables. The Bratchell's approach do not present alternatives for the cases where the largest principal component is not able to explain the most part of variance as well as do not indicate how the specification limits and targets of each response could be transformed to the plane of principal components. In spite of these gaps, the use of PCA's to overcome the correlation influence is very extensive in the machining literature, mainly associated with Taguchi designs [13,14].

PCA has become an indispensable tool for multivariate analysis in areas such as exploratory data analysis, modeling, mixture analysis and calibration, but the major weakness of this approach, however, is that it makes implicit assumptions about measurement errors which are often incorrect. This corrupts the quality of information provided and may lead to erroneous results [15].

In this context, this study proposes a model building approach to estimate the total uncertainties' measurement that affects all response variables ($Y = f(x_1, x_2, \ldots, x_k)$), using the inverse of multivariate uncertainty as weighting matrix for principal components scores used to replace the set of correlated variables in a set of uncorrelated ones. The main objective of this proposal is to achieve a satisfactory variance explanation, making the prediction R^2 as higher as possible, once it is useful in assessing the prediction ability of models [16]. After the uncertainty correction, a multi-objective optimization method – based on the concept of Multivariate Mean Square Error (MMSE) – was used to improve the multiple correlated characteristics combining PCA and RSM.

To illustrate the proposal, Wiper CNGA120408 S01525WH inserts were used in a AISI 52100 hardened steel turning operation.

2. Development of the method

Correlated variables can always be replaced by principal components scores without significative loss of information. Additionally, the rotation of axes which PC's representation can also be used to improve the variance–covariance explanation.

Then, to develop a WPCR (Weighted Principal Component Regression) method using the uncertainties' measurement or the experimental variance and evaluate how the weighting and rotation can influence the determination of the regression coefficients, this approach combines PCA, Factor Analysis (FA) and Weighted Least Square (WLS) in the model building task.

The principal component analysis is one of the most widely applied tools used to summarize common patterns of variation among variables. Supposed that $f_1(\mathbf{x})$, $f_2(\mathbf{x}), \ldots, f_p(\mathbf{x})$ are correlated with values written in terms of a random vector $Y^T = [Y_1, Y_2, \ldots, Y_p]$. Assuming that Σ is the variance–covariance matrix associated to 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 uncorrelated linear combination may be stated as $PC_i = e_i^T Y = e_{1i}Y_1 + e_{2i}Y_2 + \cdots + e_{pi}Y_p$ with $i = 1, 2, \ldots, p$. The ith principal component can be obtained as maximization of this linear combination [17]. According Antony [18] the principal components are created in order of decreasing variance, so that the first principal component accounts for most variance in the data, the second principal component less, and so on. Thus this is able to retain meaningful information in the early PCA axes. The geometric interpretation of these axes is shown in Fig. 1.

Generally, as the parameters Σ e ρ are unknown the sample correlation matrix R_{ij} and the sample variance–covariance matrix S_{ij} may be used [17]. If the variables studied are taken in the same system of units or if they are previously standardized, S_{ij} is a more appropriate choice. Otherwise, R_{ij} must be employed in the factorization. The sample variance–covariance matrix can be written as follows:

$$S_{ij} = \begin{bmatrix} s_{11} & s_{12} & \cdots & s_{1p} \\ s_{21} & s_{22} & \cdots & s_{21} \\ \vdots & \vdots & \ddots & \vdots \\ s_{p1} & s_{p2} & \cdots & s_{pp} \end{bmatrix}, \quad \text{with} \quad s_{ii} = \frac{1}{n}\sum_{j=1}^{n}(y_i - \bar{y}_i)^2$$

$$s_{ij} = \frac{1}{n}\sum_{j=1}^{n}(y_i - \bar{y}_i)(y_j - \bar{y}_j) \tag{1}$$

Then, the elements of sample correlation matrix R_{ij} can be obtained as:

$$r_{(y_i,y_j)} = \frac{\mathrm{Cov}(y_i, y_j)}{\sqrt{\mathrm{Var}(y_i) \times \mathrm{Var}(y_j)}} = \frac{\hat{e}_{ij}\sqrt{\hat{\lambda}_i}}{\sqrt{s_{ii}}} = \frac{s_{ij}}{\sqrt{s_{ii} \times s_{jj}}} \times i, j = 1, 2, \ldots, p \tag{2}$$

In practical terms, PC is an uncorrelated linear combination expressed in terms of a score matrix, defined by Johnson and Wichern [17] as

$$PC_k = \mathbf{Z}^\mathbf{T}\mathbf{E} = \begin{bmatrix} \left(\frac{x_{11}-\bar{x}_1}{\sqrt{s_{11}}}\right) & \left(\frac{x_{21}-\bar{x}_2}{\sqrt{s_{22}}}\right) & \cdots & \left(\frac{x_{p1}-\bar{x}_p}{\sqrt{s_{pp}}}\right) \\ \left(\frac{x_{12}-\bar{x}_1}{\sqrt{s_{11}}}\right) & \left(\frac{x_{22}-\bar{x}_2}{\sqrt{s_{22}}}\right) & \cdots & \left(\frac{x_{p2}-\bar{x}_p}{\sqrt{s_{pp}}}\right) \\ \vdots & \vdots & \ddots & \vdots \\ \left(\frac{x_{1n}-\bar{x}_1}{\sqrt{s_{11}}}\right) & \left(\frac{x_{2n}-\bar{x}_2}{\sqrt{s_{22}}}\right) & \cdots & \left(\frac{x_{pn}-\bar{x}_p}{\sqrt{s_{pp}}}\right) \end{bmatrix}^\mathbf{T} \times \begin{bmatrix} e_{11} & e_{12} & \cdots & e_{1p} \\ e_{21} & e_{22} & \cdots & e_{2p} \\ \vdots & \vdots & \ddots & \vdots \\ e_{1p} & e_{2p} & \ldots & e_{pp} \end{bmatrix} \tag{3}$$

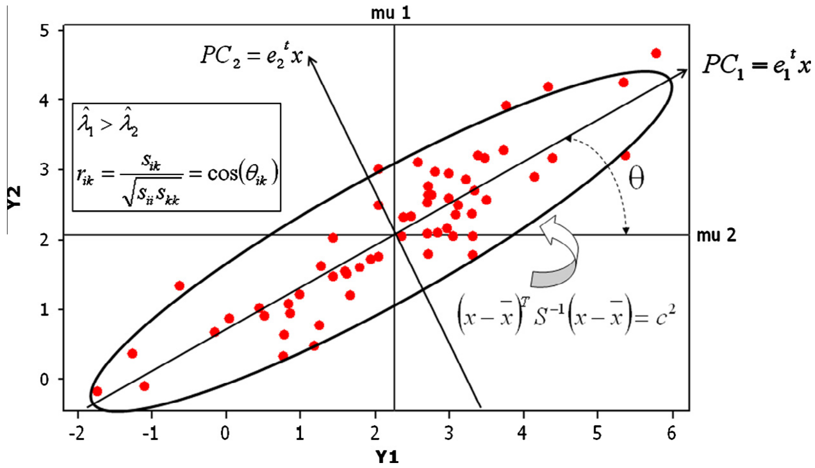

Fig. 1. Geometric interpretation of principal components.

Factor analysis is a multivariate statistical technique very useful and powerful tool for effectively extracting information from large databases and makes sense of large collections of interrelated data [6].

According Johnson and Wichern [17] the observable random vector **x**, with p components, has mean μ and covariance matrix Σ. The factor model postulates that **x** is linearly dependent upon a few unobservable random variables $F_1, F_2, \ldots, F_m$, called common factors, and p additional sources of variation $\varepsilon_1, \varepsilon_2, \ldots, \varepsilon_p$, called errors or, sometimes, specific factors. In particular, the factor analysis model is,

$$\begin{aligned} X_1 - \mu_1 &= \ell_{11}F_1 + \ell_{12}F_2 + \cdots + \ell_{1m}F_m + \varepsilon_1 \\ X_2 - \mu_2 &= \ell_{21}F_1 + \ell_{22}F_2 + \cdots + \ell_{2m}F_m + \varepsilon_2 \\ \vdots & \qquad\qquad \vdots \\ X_p - \mu_p &= \ell_{p1}F_1 + \ell_{p2}F_2 + \cdots + \ell_{pm}F_m + \varepsilon_p \end{aligned} \tag{4}$$

or in matrix notation,

$$\underset{(p\times1)}{X} = \mu + \underset{(p\times m)}{L}\ \underset{(m\times1)}{F} + \underset{(p\times1)}{\varepsilon} \tag{5}$$

The coefficient ℓ_{ij} is called the *loading* of the ith variable on the jth factor, so the matrix L is the *matrix of factor loadings*. Note that the ith specific factor ε_i is associated only with the ith response X_i. The p deviations $X_1 - \mu_1$, $X_2 - \mu_2, \ldots, X_p - \mu_p$, are expressed in terms of $p + m$ random variables $F_1, F_2, \ldots, F_m, \varepsilon_1, \varepsilon_2, \ldots, \varepsilon_p$ which are unobservable. This distinguishes the factor model of Eq. (5) from the multivariate regression model in Eq. (6), in which the independent variables whose position is occupied by **F** in Eq. (5) can be observed.

The multivariate linear regression model is,

$$\underset{(n\times m)}{Y} = \underset{(n\times(r+1))}{Z}\ \underset{((r+1)\times m)}{\beta} + \underset{(n\times m)}{\varepsilon}$$

With

$$E(\varepsilon_i) = 0 \text{ and } \mathrm{Cov}(\varepsilon_{(i)}, \varepsilon_{(k)}) = \sigma_{ik}\mathbf{I} \quad i,k = 1,2,\ldots,m \tag{6}$$

The m observations on the jth trial have covariance matrix $\Sigma = \{\sigma_{ik}\}$, but observation from different trials are uncorrelated. Here β and σ_{ik} are unknown parameters; the design matrix **Z** has jth row $[Z_{j0}, Z_{j1}, \ldots, Z_{jr}]$.

With so many unobservable quantities, a direct verification of the factor model from observations on $X_1, X_2, \ldots X_p$ is hopeless. However, with some additional assumptions about the random vectors **F** and ε, the model in Eq. (5) implies certain covariance relationships, which can be checked.

We assume that

$$E(F) = \underset{(m\times1)}{0},\ \mathrm{Cov}(F) = E[FF'] = \underset{(m\times m)}{\mathrm{I}} \tag{7}$$

$$E(\varepsilon) = \underset{(p\times1)}{0},\ \mathrm{Cov}(\varepsilon) = E[\varepsilon\varepsilon'] = \underset{(p\times p)}{\Psi} = \begin{bmatrix} \psi_1 & 0 & \ldots & 0 \\ 0 & \psi_2 & \ldots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \ldots & \psi_p \end{bmatrix} \tag{8}$$

and that **F** and ε are independent, so $\mathrm{Cov}(\varepsilon, F) = E(\varepsilon, F') = \underset{(p\times m)}{0}$.

These assumptions and the relation in Eq. (5) constitute the orthogonal factor model, where,

μ_i = mean of variable i
ε_i = ith specific factor
F_j = jth common factor
L_{ij} = loading of the ith variable on the jth factor
The unobservable random vectors F and ε satisfy the following conditions:
F and ε are independent
$E(F) = 0$, Cov $(F) = \mathrm{I}$
$E(\varepsilon) = 0$, Cov $(\varepsilon) = \Psi$, where Ψ is a diagonal matrix

2.1. Multivariate uncertainty for PC score regression

To develop an appropriate equation for the multivariate uncertainty for correlated quantities the basic model can be written as

$$u_m^2(y) = \sum_{i=1}^{n} \left[\frac{\partial f}{\partial x_i}\right]^2 u_c^2(x_i) + 2\sum_{i}^{n-1}\sum_{j=i+1}^{n} \left(\frac{\partial f}{\partial x_i}\right) \times \left(\frac{\partial f}{\partial x_j}\right) \times u(x_i) \times u(x_j) \times r(x_i, x_j) \tag{9}$$

Considering that in the PCA, the multiple responses can be combined in the form of principal component scores, such as $PC_k = \mathbf{Z^TE}$, where Z can be established as:

$$Z_P = \frac{(x_{ip} - \mu_p)}{\sigma_p} \tag{10}$$

Then, applying Eq. (9) to the case of Principal Component Analysis (PCA), we have:

$$y = f(x) = PC_{score} = \sum_{i=1}^{p}(e_i \times Z_i) = \sum_{i=1}^{p}\left[e_i \times \left(\frac{x_i - \mu}{\sigma}\right)\right] \tag{11}$$

where

$$\frac{\partial f}{\partial x_i} = \frac{e_i}{\sigma} \tag{12}$$

Finally, the combination of Eqs. (9) and (11) can be written as:

$$u_m^2(PC) = \left(\frac{e_1}{\sigma_{x_1}}\right)^2 u^2(x_i) + \left(\frac{e_2}{\sigma_{x_2}}\right)^2 u^2(x_j) + 2 \times \left(\frac{e_1}{\sigma_{x_i}}\right) \times \left(\frac{e_2}{\sigma_{x_j}}\right) \times u(x_i) \times u(x_j) \times r(x_i, x_j) \tag{13}$$

where e_i is eigenvector of the correlation matrix used in the extraction of principal components; σ_{x_i} is the standard deviation of the response data (column) I; σ_{x_j} is the standard deviation of the response data (column) j; $u^2(x_i)$ is the uncertainty (or variance) of each observation response I; $u^2(x_j)$ is the uncertainty of each observation of the response j and $r(x_i, x_j)$ is the coefficient of correlation between x_i and x_j responses.

2.2. Multivariate uncertainty for PC score obtained by factor analysis

The optimization by PCA cannot always produce satisfactory results. Bratchell [12] points out that some difficulties can be resolved or avoided by using other techniques. Using the principal component analysis to model and optimize multivariate response was observed that in some situation the rotation of the principal components provides an easy and accessible means of analyzing and optimizing a multivariate response which simplifies interpretation of the overall response and retains the flexibility associated with linear or non-linear modeling. Factor analysis is one of techniques that can improve the adjustments. It is a mathematical tool for examining a wide range of data sets, with applications especially important to the design of experiments (DOEs).

Following Bratchell's recommendation, the component scores were obtained by factor analysis, thus the weighted matrix will be the inverse of multivariate uncertainty calculated using the equation below,

$$u_m^2(FA_{rotated}) = \left(\frac{k_1}{\sigma_{x_1}}\right)^2 u^2(x_i) + \left(\frac{k_2}{\sigma_{x_2}}\right)^2 u^2(x_j) + 2 \times \left(\frac{k_1}{\sigma_{x_i}}\right) \times \left(\frac{k_2}{\sigma_{x_j}}\right) \times u(x_i) \times u(x_j) \times r(x_i, x_j) \tag{14}$$

where k_1 and k_2 are the coefficients of the factors obtained by varimax rotation. Rotation is applied to simplify the data structure and according Johnson and Wichern [17] varimax rotation is the most common choice.

2.3. Weighted least squares

When the errors ε are uncorrelated but have unequal variances so that the covariance matrix of ε is

$$\sigma^2\mathbf{V} = \sigma^2\begin{bmatrix} \frac{1}{w_1} & & 0 & \\ & \frac{1}{w_1} & & \\ & & \ddots & \\ 0 & & & \frac{1}{w_n} \end{bmatrix} \tag{15}$$

say, the estimation procedure is usually called weighted least squares. Let $\mathbf{W} = \mathbf{V^{-1}}$. Since $\mathbf{V}$ is a diagonal matrix, $\mathbf{W}$ is also diagonal with diagonal elements or weights w_1, $w_2, \ldots, w_n$. The weighted least squares normal equations is

$$\hat{\boldsymbol{\beta}} = (\mathbf{X^TWX})^{-1}\mathbf{X^TWY} \tag{16}$$

which is the weighted least squares estimator. The observation with large variances will have smaller weights than observations with small variances [19].

To use weighted least squares in a practical sense, we must know the weights $w_1, w_2, \ldots, w_n$. Sometimes prior knowledge or experience or information based on underlying theoretical considerations can be used to determine the weights. In order situations we may find empirically that the variability in the response is a function of one or more regressors, and so a model may be fit to predict the variance of each observation and hence determine the weights. In some cases we may have to estimate the weights, perform the analysis, re-estimate a new set of weights based on these results, and then perform the analysis again [19].

Cho and Park [20] recommend the use of weighted least squares method to balance the data with weights that are inversely proportional to the variance at each level of the explanatory variables when the variance is not constant. Through this method, Pérez [1] weighted the regressors of surface roughness for R_a and R_q using the inverse of the uncertainty's measurement as weighting matrix, which is determined in the following equation,

$$\mathbf{W_y} = \frac{1}{u_y^2} \tag{17}$$

where $\mathbf{W_y}$ is a diagonal array with its main diagonal elements and u^2 is the total uncertainty of the process for each of the response values.

Applying the mathematical method developed in Eqs. (13) and (14) is possible to establish the W matrix to apply the WLS (Weighted Least Square) method on principal component scores, such as:

$$\mathbf{W_{PC}} = \frac{1}{\boldsymbol{u}_M^2 PC} \tag{18}$$

where W matrix is adopted as variance inverse of PC or PC rotated and U_m is the total uncertainty of the process.

To explain the method application Fig. 2 shows the fundamental steps in the proposed approach using PCA.

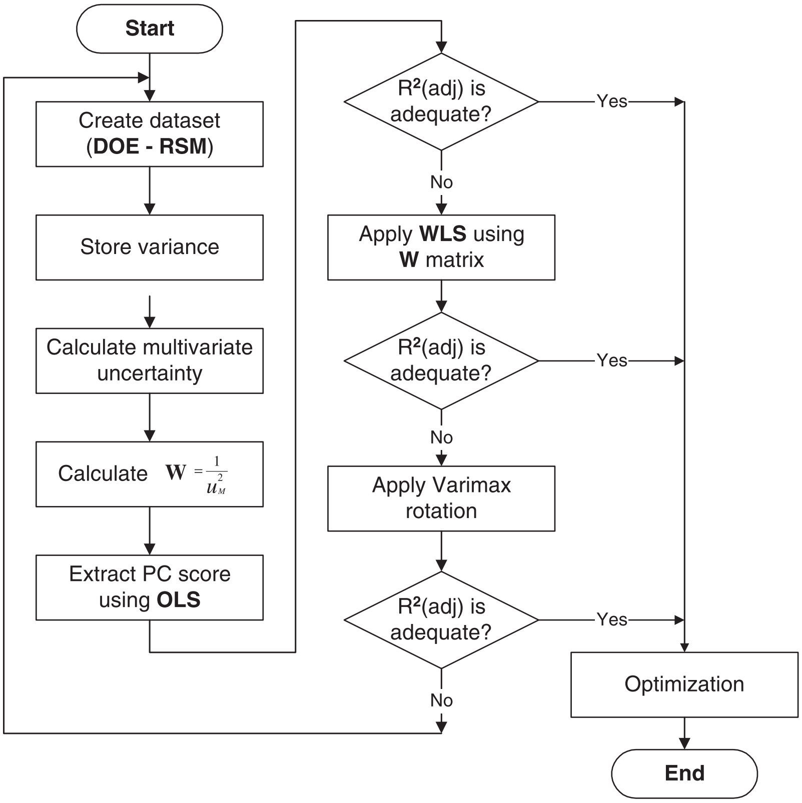

Fig. 2. Flow of searching for WLS models.

3. Optimization

This section discusses the application of multivariate optimization based in MMSE. Under various circumstances the multiple responses considered in a process present conflict of objectives, with individually optimization leading to different solution sets. This fact characterizes a multiobjective optimization problem and, also considering inequality constraints, can be stated as the following equation:

$$\begin{aligned}&\text{Minimize } f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_p(\mathbf{x})\\&\text{Subject to}: \ g_j(\mathbf{x}) \leqslant 0, \quad j = 1, 2, \ldots, m\end{aligned} \tag{19}$$

Supposed that $f_1(\mathbf{x}), f_2(\mathbf{x}), \ldots, f_p(\mathbf{x})$ are correlated with values written in terms of a random vector $Y^T = [Y_1, Y_2, \ldots, Y_p]$. Assuming that Σ is the variance–covariance matrix associated to this vector then Σ can be factorized in pairs of eigenvalues–eigenvectors $(\lambda_i, e_i), \ldots \geqslant (\lambda_p, e_p)$, where $\lambda_1 \geqslant \lambda_2 \geqslant \cdots \geqslant \lambda_p \geqslant 0$, such as the i^{th} uncorrelated linear combination may be stated as $PC_i = e_i^T Y = e_{1i}Y_1 + e_{2i}Y_2 + \cdots + e_{pi}Y_p$ with $i = 1, 2, \ldots, p$.

Multivariate Mean Square Error (MMSE) is a multivariate dual response surface criteria developed to replace the estimated mean $\hat{y}$ by an estimated principal component score regression (PC_i) and the variance $\hat{\sigma}^2$ by the respective eigenvalue λ_i [21]. Taking ζ_{PC_i} as the target for the ith principal component, a multivariate mean square error formulation can be defined as:

$$\text{MMSE}_i = (PC_i - \zeta_{PC_i})^2 + \lambda_i \tag{20}$$

In Eq. (20) PC_i is the fitted second-order polynomial and 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. This relationship may be established using Eq. (21) such as:

$$\begin{aligned}&\zeta_{PC_i} = e_i^T[Z(Y_p|\zeta_{Y_p})] = \sum_{i=1}^{p}\sum_{j=1}^{q} e_{ij}[Z(Y_p|\zeta_{Y_p})]\\&i = 1, 2, \ldots p; \quad j = 1, 2, \ldots, q\end{aligned} \tag{21}$$

In Eq. (21) e_i are the eigenvectors associated to the ith principal component and ζ_{Y_p} represents the target for each of the p original responses. With this transformation, it can be established a coherent value for the target of the ith principal component, that is compatible with the targets of the original problem.

If more than one principal component is needed, then the MMSE functions whose eigenvalues are equal or greater than the unity, may be written in following form:

$$\begin{aligned}\text{Minimize MMSE}_T &= \left[\prod_{i=1}^{k}(\text{MMSE}_i|\lambda_i \geqslant 1)\right]^{\left(\frac{1}{k}\right)}\\&= \left\{\prod_{i=1}^{k}[(PC_i - \zeta_{PC_i})^2 + \lambda_i|\lambda_i \geqslant 1]\right\}^{\left(\frac{1}{k}\right)}\\&\times i = 1, 2, \ldots, k; \ k \leqslant p\end{aligned} \tag{22}$$

$$\text{Subject to}: \mathbf{x}^T\mathbf{x} \leqslant \rho^2 \tag{23}$$

$$\hat{g}_i(\mathbf{x}) \leqslant 0 \tag{24}$$

$$\text{With}: \zeta_{PC_i} = e_{1i}[Z(Y_1|\zeta_{Y_1})] + e_{2i}[Z(Y_2|\zeta_{Y_2})] + \cdots + e_{pi}[Z(Y_p|\zeta_{Y_p})] \tag{25}$$

$$PC_i = b_{0i} + [\nabla f(\mathbf{x})^T]_i + \left\{\frac{1}{2}\mathbf{x}^T[\nabla^2 f(\mathbf{x})]\mathbf{x}\right\}_i \quad i = 1, 2, \ldots, p. \tag{26}$$

where Z represents the standardized value of the ith response considering its target value ζ_{Yi}, such that $Z(Y_i|\zeta_{Yi}) = [(\zeta_{Yi}) - \mu_{Yi}]\cdot(\sigma_{Yi})^{-1}$. k is the number of factors and ε is the error term; $\mathbf{x}$ is the vector of parameters, b_0 is the regression constant term, $\nabla f(\mathbf{x})^T$ is the gradient of the objective function corresponding to the first-order regression coefficients and $\nabla^2 f(\mathbf{x})^T$ is the Hessian matrix, formed by the quadratic and interaction terms of the estimated model of Y.

4. Experimental procedure

To accomplish with the goals of this paper, dry turning tests were conducted on a CNC lathe with maximum rotational speed of 4000 rpm and power of 5.5 kW. The workpieces used in the turning process were made with dimensions of Ø49 mm × 50 mm. All of them were quenched and tempered. After this heat treatment, their hardness was between 49 and 52 HRC (Rockwell Hardness), up to a depth of 3 mm below the surface. The workpiece material was AISI 52100 steel, with the following chemical composition: 1.03% C; 0.23% Si; 0.35% Mn; 1.40% Cr; 0.04% Mo; 0.11% Ni; 0.001% S; 0.01%. The Wiper mixed ceramic (Al_2O_3 + TiC) inserts (CNGA 120408 S01525WH) coated with a very thin layer of titanium nitride (TiN) were used in the experiment. The WIPER inserts represent a new technology on turning operations, manly by their new type of nose configuration. Depending on the machining parameters, this insert is capable of generating a better surface finish at a much higher feed. Therefore, the use of Wiper inserts increase the productivity, keeping the surface roughness as lower as possible. This particular characteristic can be used to eliminate grinding operations, which represents a great advantage to the manufacturers. Correia and Davim [22] and Asiltürk and Neseli [23] reported similar results obtained using the wiper insert. Fig. 3 represents the turning process of AISI 52100 hardened steel with Wiper inserts used in this experimental study.

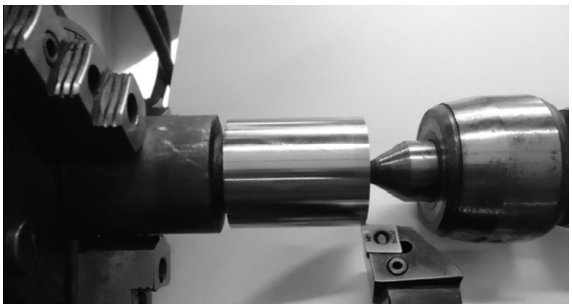

Fig. 3. Hard Turning process with Wiper geometry tool.

Table 1
Assignment of the variables levels.

Parameters	Levels				
Coded units	−1.682	−1	0	1	1.682
Cutting speed (m/min)	186.4	200	220	240	253.6
Feed rate (mm/rev)	0.132	0.20	0.30	0.40	0.468
Depth of cut (mm)	0.099	0.15	0.225	0.30	0.351

Adopting this experimental condition, the workpieces were machined using the range of parameters reported in Table 1.

A sequential set of experimental runs was established using a CCD built according to the design shown in Table 2. The following surface roughness parameters were obtained by means of a Mitutoyo Surftest 201 roughness meter set to a cut-off length of 0.25 mm: arithmetic average surface roughness (R_a), maximum surface roughness (R_Y), root mean square roughness (R_q), ten point height (R_z) and maximum peak to valley (R_t). After turning each part, the surface roughness was measured at four positions at the center of the workpiece. An average of three measurements was taken for each position by rotating the part 90° after measuring its roughness. The mean values of these measurements are represented in Table 2. In the same table, PC1^A correspond to the scores of the first principal component for R_aR_q and PC1^B represent the scores of the first principal component for $R_aR_yR_zR_qR_t$, both extracted from the correlation matrix of the respective dataset. The detailed procedure of the principal component analysis is shown in Table 4.

Table 3 represents the experimental variance obtained with the four measurements of each metric of surface roughness.

5. Results and discussion

Applying Eq. (3), the scores of the first principal component (PC1) were obtained as can be seen in Table 2. Using the Principal Component Analysis (PCA) to decompose the correlation structure, it can be verified that the first principal component (PC1^A) for R_aR_q explains 97.3% of the total variation observed in the two surface roughness responses, with an eigenvalue equals to 1.946 and respective eigenvectors. Working with a set of data for five surface roughness responses (R_a; R_y; R_z; R_q; R_t), PC1^B explains 96.4% of the total variation with the largest eigenvalue equals to 4.821 and respective eigenvectors listed in Table 4. This multivariate analysis was done with Minitab 15.0 but it is also available in many statistical packages.

Table 2
Parameters and responses measured.

Machining parameters			Responses					PCA scores		FA scores	
Vc	Fn	d	R_a	R_y	R_z	R_q	R_t	$PC1^A$	$PC1^B$	$FPC1^A$	$FPC1^B$
−1	−1	−1	0.15	0.97	0.85	0.19	0.99	−2.09	−3.29	−1.11	−0.97
+1	−1	−1	0.22	1.13	1.07	0.26	1.16	−1.31	−2.38	−1.02	−1.05
−1	+1	−1	0.39	2.65	2.11	0.53	2.67	1.06	2.04	0.67	1.08
+1	+1	−1	0.38	2.34	1.87	0.50	2.42	0.90	1.35	0.33	0.46
−1	−1	+1	0.18	1.15	0.99	0.23	1.17	−1.73	−2.70	−0.82	−0.79
+1	−1	+1	0.17	1.09	1.00	0.22	1.13	−1.81	−2.80	−0.95	−0.81
−1	+1	+1	0.36	2.22	1.75	0.46	2.39	0.57	0.93	0.16	0.52
+1	+1	+1	0.41	2.65	2.09	0.53	2.73	1.25	2.18	0.39	1.08
−1.68	0	0	0.37	2.04	1.84	0.47	2.07	0.71	0.78	0.05	−0.19
1.68	0	0	0.36	2.20	1.95	0.48	2.23	0.64	1.05	0.34	0.26
0	−1.68	0	0.10	0.74	0.63	0.12	0.79	−2.79	−4.20	−1.30	−1.03
0	1.68	0	0.53	3.46	2.48	0.68	3.52	2.76	4.53	0.88	2.05
0	0	−1.68	0.35	1.93	1.71	0.42	1.98	0.31	0.29	−0.43	−0.05
0	0	1.68	0.42	2.36	2.12	0.52	2.43	1.23	1.81	0.14	0.42
0	0	0	0.30	2.02	1.82	0.40	2.05	−0.10	0.22	0.12	0.36
0	0	0	0.29	2.15	1.73	0.39	2.19	−0.21	0.26	−0.11	0.85
0	0	0	0.31	1.77	1.61	0.60	1.70	0.88	0.25	3.22	−2.32
0	0	0	0.29	1.86	1.60	0.36	1.92	−0.36	−0.33	−0.47	0.26
0	0	0	0.32	1.88	1.60	0.42	1.98	0.10	0.02	−0.09	−0.12
	Mean	μ	0.310	1.925	1.622	0.409	1.975	0.000	0.000		
	SD	σ	0.108	0.678	0.494	0.149	0.692				
	Target	(ζ_{Yi})	0.090	0.710	0.620	0.120	0.690	−2.815	−4.323		
	Z	$Z(Y_i\|\zeta_{Yi})$	−2.042	−1.793	−2.027	−1.940	−1.856				

Table 3
Experimental variances and multivariate weights.

Var R_a	Var R_y	Var R_z	Var R_q	Var R_t	W ($PC1^A$)	W ($PC1^B$)	$WPC1^BF$	$WPC1^AF$
0.0002	0.0232	0.0107	0.0004	0.0186	31.8272	6.5503	58.12865	12.40494
0.0010	0.0076	0.0097	0.0009	0.0065	8.6627	5.9594	35.36257	81.42054
0.0003	0.0533	0.0058	0.0001	0.0455	33.6697	4.6105	56.99478	3.517637
0.0004	0.0247	0.0217	0.0012	0.0287	11.9647	3.6576	12.34147	15.13378
0.0003	0.0059	0.0815	0.0004	0.0045	24.6972	4.4011	74.51362	31.48883
0.0004	0.0052	0.0060	0.0006	0.0063	17.2311	9.9061	40.86533	104.4103
0.0006	0.0119	0.0274	0.0009	0.0227	10.9044	3.9134	34.58623	21.58304
0.0006	0.0391	0.0150	0.0010	0.0302	10.6690	3.4098	25.28757	10.20686
0.0009	0.0191	0.0075	0.0012	0.0165	7.8056	4.4605	28.45866	34.05698
0.0004	0.0577	0.0197	0.0013	0.0503	11.4857	2.6853	10.77569	5.872338
0.0000	0.0015	0.0008	0.0000	0.0040	236.2661	57.1103	580.9875	97.51999
0.0016	0.0278	0.0584	0.0020	0.0176	4.5319	2.0128	15.9641	21.82228
0.0009	0.0102	0.0162	0.0007	0.0039	9.7889	5.6581	38.95572	83.56822
0.0010	0.0568	0.0480	0.0020	0.0485	5.9276	1.7805	10.29008	6.847434
0.0012	0.0413	0.0293	0.0018	0.0393	5.6953	2.1960	15.92233	10.33892
0.0010	0.0567	0.0010	0.0008	0.0467	8.7744	3.5038	35.40306	6.400632
0.0003	0.0034	0.0013	0.2239	0.1719	0.1820	0.3218	0.016693	0.071986
0.0005	0.0249	0.0056	0.0007	0.0098	14.0235	6.2319	42.29087	30.1927
0.0003	0.0074	0.0222	0.0006	0.0349	19.1635	4.8936	42.00797	14.27545

5.1. Analysis and results for $PC1^A$

Table 5 shows the results for $\mathbf{PC1^A}$ (R_aR_q) obtained from the Analyze Response Surface Design and Regression Analysis. The value of R-Sq(adj) in the unweighted matrix is below of 75%. The model needs to be increased to explain its relationship with one or more predictor variables. Thus to determinate the multivariate uncertainty involved in the experiment, Eq. (13) was applied to calculate the total uncertainty for $\mathbf{PC1^A}$. The regressors were weighted using the weight matrix ($WPC1^A$), as shown in Eq. (18). Pérez [1] used a similar model to modeling the response values for R_a and R_q.

The equation for $\mathbf{PC1^A}$ unweighted is

$$\mathbf{PC1^A} = 0.096 + 0.080Vc + 1.467Fn + 0.092d + 0.025Vc^2 - 0.217Fn^2 + 0.059d^2 - 0.022Vc \times Fn - 0.001Vc \times d + 0.001Fn \times d \quad (27)$$

The result in Table 5 ($WPC1^A$) shows that the mathematical model through the use of a weighted matrix can filter the uncertainty and thereby raise the value of

Table 4
Principal component analysis for $PC1^A$ and $PC1^B$.

Eigenanalysis of the correlation matrix							
PC	$PC1^A$ (R_a, R_q)		$PC1^B$ (R_a, R_y, R_z, R_q, R_t)				
Eigenvalue	1.946	0.054	4.821	0.123	0.031	0.024	0.001
Proportion	0.973	0.027	0.964	0.025	0.006	0.005	0.000
Cumulative	0.973	1.000	0.964	0.989	0.995	1.000	1.000
Variable	PC1	PC2	PC1	PC2	PC3	PC4	PC5
R_a	0.707	0.707	0.451	−0.075	−0.525	−0.711	0.101
R_y			0.451	0.360	0.388	0.062	0.716
R_z			0.451	0.050	−0.564	0.687	−0.063
R_q	0.707	−0.707	0.436	−0.811	0.375	0.075	−0.076
R_t			0.449	0.451	0.340	−0.111	−0.684

Table 5
Response surface regression and regression analysis: $PC1^A \times Vc$, Fn and d.

Unweighted estimated regression coefficients for $PC1^A$					Weighted analysis using weights in $WPC1^A$			
Term	Coef	SE Coef	T	P	Coef	SE Coef	T	P
Constant	0.096	0.320	0.301	0.771	−0.074	0.291	−0.250	0.806
Vc	0.080	0.194	0.413	0.689	0.135	0.148	0.910	0.386
Fn	1.467	0.194	7.561	0.000	1.386	0.148	9.370	0.000
d	0.092	0.194	0.473	0.647	0.039	0.157	0.250	0.808
Vc^2	0.025	0.194	0.127	0.901	0.046	0.169	0.270	0.790
Fn^2	−0.217	0.194	−1.120	0.292	−0.145	0.139	−1.050	0.323
d^2	0.059	0.194	0.303	0.769	0.019	0.178	0.110	0.917
$Vc \times Fn$	−0.022	0.254	−0.087	0.933	−0.067	0.181	−0.370	0.720
$Vc \times d$	−0.001	0.254	0.000	1.000	−0.068	0.180	−0.380	0.714
$Fn \times d$	0.001	0.254	0.003	0.998	−0.002	0.176	−0.010	0.994
S = 0.72	R-Sq(pred) = 14.81%		R-Sq(adj) = 73.57%		S = 2.01	R-Sq(pred) = 96.49%	R-Sq(adj) = 93.70**%**	

R-Sq(adj). Now it's possible to explain 93.70% of the variability in $\mathbf{PC1^A}$. It means an improvement of 20.13%. The regression equation for $\mathbf{PC1^A}$ weighted is

$$\mathbf{WPC1^A} = -0.074 + 0.135Vc + 1.386Fn + 0.039d + 0.046Vc^2 - 0.145Fn^2 + 0.019d^2 - 0.067Vc \times Fn - 0.068Vc \times d - 0.002Fn \times d \quad (28)$$

As can be seen in both equations, feed (Fn) is the only one significant effect on the surface roughness set of data. Asiltürk and Neseli [23], Davim [24] and Aouici et al. [25] agree that feed rate (Fn) have statistical influence on the surface roughness in piece.

Bratchell [12] affirms that in some situations rotation of the principal components may provide factors which can be interpreted physically. In order to investigate the rotation effect over the model, a multivariate factor analysis was carried out. The method of extraction is principal components and type of rotation is varimax. The attained results are demonstrated in Table 6, where $PC1^{\mathbf{A}}F$ means factor analysis of principal component with varimax rotation.

Throughout factor analysis with varimax rotation the result of R-Sq(adj) was not improved as expected. The results of this analysis are exposed in the following equation:

$$\mathbf{PC1^A}F = 0.541 + 0.025Vc + 0.669Fn + 0.065d - 0.163Vc^2 - 0.306Fn^2 - 0.283d^2 - 0.007Vc \times Fn + 0.045Vc \times d - 0.101Fn \times d \quad (29)$$

Thus, to obtain a better explanation of the model, the regressors were pondering with a weighted matrix ($WPC1^AF$) as exposed in Table 6.

Now the model is capable to explain 94.0% of the variability in $PC1^AF$ and the Lack of Fit, as can be seen in Table 7 is over than 0.05.

Then using the actual variables the regression equation can be written as:

$$\mathbf{WPC1^A}F = -0.181 + 0.007Vc + 0.672Fn - 0.002d + 0.054Vc^2 - 0.002Fn^2 - 0.093d^2 - 0.003Vc \times Fn + 0.021Vc \times d - 0.128Fn \times d \quad (30)$$

5.2. Analysis and results for $\mathbf{PC1^B}$ (R_a; R_y; R_z; R_q; R_t)

$PC1^B$ represents a set of data for five surface roughness responses. Eq. (13) was developed to works with a pair of response (R_aR_q), but to identify the total multivariate uncertainty for (R_a; R_y; R_z; R_q; R_t) another equation must be developed. So the total multivariate uncertainty for $PC1^B$ is then calculated using the following equation:When

$$
\begin{aligned}
u_m^2(\mathrm{PC1}_{RaRyRzRqRt}) = {} & \left(\frac{e_1}{\sigma_{x_1}}\right)^2 u^2(x_1) + \left(\frac{e_2}{\sigma_{x_2}}\right)^2 u^2(x_2)\left(\frac{e_3}{\sigma_{x_3}}\right)^2 u^2(x_3) + \left(\frac{e_4}{\sigma_{x_4}}\right)^2 u^2(x_4) + \left(\frac{e_5}{\sigma_{x_5}}\right)^2 u^2(x_5) \\
& + 2 \times \left(\frac{e_1}{\sigma_{x_1}}\right) \times \left(\frac{e_2}{\sigma_{x_2}}\right) u(x_1) \times u(x_2) \times r(x_1, x_2) \\
& + 2 \times \left(\frac{e_1}{\sigma_{x_1}}\right) \times \left(\frac{e_3}{\sigma_{x_3}}\right) u(x_1) \times u(x_3) \times r(x_1, x_3) \\
& + 2 \times \left(\frac{e_1}{\sigma_{x_1}}\right) \times \left(\frac{e_4}{\sigma_{x4}}\right) u(x_1) \times u(x_4) \times r(x_1, x_4) \\
& + 2 \times \left(\frac{e_1}{\sigma_{x_1}}\right) \times \left(\frac{e_5}{\sigma_{x5}}\right) u(x_1) \times u(x_5) \times r(x_1, x_5) \\
& + 2 \times \left(\frac{e_2}{\sigma_{x_2}}\right) \times \left(\frac{e_3}{\sigma_{x_3}}\right) u(x_2) \times u(x_3) \times r(x_2, x_3) \\
& + 2 \times \left(\frac{e_2}{\sigma_{x_2}}\right) \times \left(\frac{e_4}{\sigma_{x_4}}\right) u(x_2) \times u(x_4) \times r(x_2, x_4) \\
& + 2 \times \left(\frac{e_2}{\sigma_{x_2}}\right) \times \left(\frac{e_5}{\sigma_{x_5}}\right) u(x_2) \times u(x_5) \times r(x_2, x_5) \\
& + 2 \times \left(\frac{e_3}{\sigma_{x_3}}\right) \times \left(\frac{e_4}{\sigma_{x_4}}\right) u(x_3) \times u(x_4) \times r(x_3, x_4) \\
& + 2 \times \left(\frac{e_3}{\sigma_{x_3}}\right) \times \left(\frac{e_5}{\sigma_{x_5}}\right) u(x_3) \times u(x_5) \times r(x_3, x_5) \\
& + 2 \times \left(\frac{e_4}{\sigma_{x_4}}\right) \times \left(\frac{e_5}{\sigma_{x_5}}\right) u(x_4) \times u(x_5) \times r(x_4, x_5)
\end{aligned}
\tag{31}
$$

Eq. (31) is used to calculate the total multivariate uncertainty for the scores obtained with rotation in factor analysis ($\mathrm{PC1}^B F$), $\boldsymbol{e}_i$ is substituted by $\boldsymbol{k}_i$. Where $\boldsymbol{k}_i$ is the coefficient of the factor obtained by varimax rotation.

Table 8 provides the comparative data between $\mathrm{PC1}^B$ unweighted and $\mathrm{PC1}^B$ weighted.

Unweighted Estimated Regression Coefficients for $\mathrm{PC1}^B$ shows an average for R-Sq(adj) of 81.02% and the equation is

$$
\begin{aligned}
\mathbf{PC1^B} = {} & 0.134 + 0.132\mathrm{V}c + 2.370\mathrm{F}n + 0.179d + 0.010\mathrm{V}c^2 \\
& - 0.255\mathrm{F}n^2 + 0.058d^2 - 0.032\mathrm{V}c \times \mathrm{F}n + 0.116\mathrm{V}c \\
& \times d - 0.056\mathrm{F}n \times d
\end{aligned}
\tag{32}
$$

To determine the multivariate uncertainty involved in the experiment, Eq. (31) was applied to calculate the total uncertainty for $\mathrm{PC1}^B$. The regressors were weighted using the weight matrix ($\mathrm{WPC1}^B$) as shown in Eq. (18). The results observed in Table 8 show that R-Sq(adj) improved from 81.02% to 92.4%.

The regression equation with actual variables can be written as:

$$
\begin{aligned}
\mathbf{WPC1^B} = {} & 0.030 + 0.077\mathrm{V}c + 2.281\mathrm{F}n + 0.001d \\
& + 0.017\mathrm{V}c^2 - 0.164\mathrm{F}n^2 - 0.063d^2 - 0.005\mathrm{V}c \\
& \times \mathrm{F}n - 0.028\mathrm{V}c \times d - 0.036\mathrm{F}n \times d
\end{aligned}
\tag{33}
$$

In order to better understand the rotation effect over the model, as suggested by Bratchell, the multivariate factor analysis was carried out. The additional **F** to $\mathrm{PC1}^B$ means the first principal component with factor analysis and varimax rotation. The results shown in Table 9 (Unweighted Estimated Regression Coefficients for $\mathrm{PC1}^B F$)

Table 6
Response surface regression and regression analysis: $\mathrm{PC1}^A\mathrm{F} \times \mathrm{V}c$, $\mathrm{F}n$ and d.

	Unweighted estimated regression coefficients for $\mathrm{PC1}^A F$				Weighted analysis using weights in $\mathrm{WPC1}^A F$			
Term	Coef	SE Coef	T	P	Coef	SE Coef	T	P
Constant	0.541	0.459	1.176	0.270	−0.181	0.112	−1.620	0.140
Vc	0.025	0.279	0.091	0.929	0.007	0.069	0.110	0.917
Fn	0.669	0.279	2.402	0.040	0.672	0.061	11.000	0.000
d	0.065	0.279	0.231	0.822	−0.002	0.067	−0.030	0.979
$\mathrm{V}c^2$	−0.163	0.279	−0.584	0.573	0.054	0.074	0.740	0.479
$\mathrm{F}n^2$	−0.306	0.279	−1.098	0.301	−0.002	0.055	−0.030	0.975
d^2	−0.283	0.279	−1.017	0.336	−0.093	0.069	−1.350	0.210
Vc × Fn	−0.007	0.364	−0.020	0.984	−0.003	0.077	−0.040	0.966
Vc × d	0.045	0.364	0.125	0.903	0.021	0.075	0.280	0.783
Fn × d	−0.101	0.364	−0.279	0.787	−0.128	0.074	−1.730	0.118
S = 1.03	R-Sq(pred) = 4.52%		R-Sq(adj) = 0.00%		S = 1.30	R-Sq(pred) = 96.90%	R-Sq(adj) = 94.0%	

Table 7
Analysis of variance.

Source	DF	SS	MS	*F*	*P*
Regression	9	497.576	55.286	32.530	0.000
Residual error	9	15.297	1.700		
Lack of Fit	5	9.492	1.898	1.310	0.409
Pure error	4	5.804	1.451		
Total	18	512.872			

are worse than the results extracted without factor analysis with varimax rotation. But when the regressors were weighted by a weight matrix, the results were improved. It can be seen in Table 9 where the results for *R*-Sq(adj) raised from 25.00% to 92.4%.

The equation for $\mathbf{PC1^BF}$ unweighted is given below in:

$$\mathbf{PC1^B}F = -0.182 + 0.043\mathrm{V}c + 0.874\mathrm{F}n + 0.093d + 0.010\mathrm{V}c^2 + 0.179\mathrm{F}n^2 + 0.063d^2 + 0.005\mathrm{V}c \times \mathrm{F}n + 0.156\mathrm{V}c \times d - 0.042\mathrm{F}n \times d \quad (34)$$

Once weighted the regression equation with actual variables can be written as:

$$\mathbf{WPC1^B}F = 0.263 - 0.012\mathrm{V}c + 0.865\mathrm{F}n + 0.029d - 0.188\mathrm{V}c^2 + 0.054\mathrm{F}n^2 - 0.104d^2 + 0.068\mathrm{V}c \times \mathrm{F}n + 0.115\mathrm{V}c \times d - 0.001\mathrm{F}n \times d \quad (35)$$

The Lack of Fit, as can be seen in Table 10 is over than 0.05.

In statistics, the coefficient of determination is used in cases of statistical models, whose main purpose is the prediction of future outcomes on the basis of other related information [26]. To assess and compare the efficiency of each model (normal, weighted or rotated) we will use the predicted $\mathbf{R^2}$ coefficient ($\mathbf{R^2}$ **pred**). This coefficient provides a measure of how well future outcomes are likely to be predicted by the model. It takes values between zero and the unit ($0 \leqslant R^2 \leqslant 1$). The closer the value is to the unit, the better and more accurate is the prediction. The predicted $\mathbf{R^2}$ can be calculated as:

$$R^2(\text{pred.}) = \frac{\sum_{i=1}^{n}\left(\frac{e_i}{1-h_i}\right)^2}{1 - \sum_{i=1}^{n}(y_i - \bar{y})^2} \quad (36)$$

where y_i is the *i*th observed response value, $\bar{y}$ is the mean response, *n* is the number of experiments or observations, e_i is the ith residual and h_i is the *i*th diagonal element of $\mathbf{X}(\mathbf{X^TX})^{-1}\mathbf{X^T}$. *X* is the matrix of predictors.

For summarize and compare the results obtained in the two case studies, we will use a full factorial design, as can be seen in Table 11. With this approach we can analyze the influence of the presence or absence of the weights or rotation over the explanation property of the models. Considering the cases "A" and "B" as two replicates of 2^2 full factorial design, we obtain the following results.

The interaction analysis in Fig. 4 clearly shows that the multivariate weighting strategy is more important for R^2

Table 8
Response surface regression and regression analysis: $\mathrm{PC1^B} \times Vc$, F*n* and *d*.

	Unweighted estimated regression coefficients for $\mathrm{PC1^B}$				Weighted analysis using weights in $\mathrm{WPC1^B}$			
Term	Coef	SE Coef	*T*	*P*	Coef	SE Coef	*T*	*P*
Constant	0.134	0.427	0.313	0.761	0.030	0.436	0.070	0.947
V*c*	0.132	0.259	0.511	0.622	0.077	0.238	0.320	0.754
F*n*	2.370	0.2589	9.155	0.000	2.281	0.229	9.960	0.000
d	0.179	0.2589	0.690	0.508	0.001	0.243	0.010	0.996
Vc^2	0.010	0.2589	0.040	0.969	0.017	0.252	0.070	0.948
Fn^2	−0.255	0.2589	−0.984	0.351	−0.164	0.213	−0.770	0.461
d^2	0.058	0.2589	0.224	0.828	−0.063	0.255	−0.250	0.810
V*c* × F*n*	−0.032	0.338	−0.094	0.927	−0.005	0.290	−0.020	0.987
V*c* × *d*	0.116	0.338	0.344	0.739	−0.028	0.284	−0.100	0.923
F*n* × *d*	−0.056	0.338	−0.166	0.872	−0.036	0.291	−0.120	0.905
S = 0.96	*R*-Sq(pred) = 28.03%		*R*-Sq(adj) = 81.02%		*S* = 1.81	*R*-Sq(pred) = 94.64%	*R*-Sq(adj) = 92.40%	

Table 9
Response surface regression and regression analysis: $\mathrm{PC1^B}F \times Vc$, *f* and *d*.

	Unweighted estimated regression coefficients for $\mathrm{PC1^B}F$				Weighted analysis using weights in $\mathrm{WPC1^B}F$			
Term	Coef	SE Coef	*T*	*P*	Coef	SE Coef	*T*	*P*
Constant	−0.182	0.387	−0.469	0.650	0.263	0.152	1.730	0.118
V*c*	0.043	0.234	0.184	0.858	−0.012	0.077	−0.150	0.884
F*n*	0.874	0.234	3.730	0.005	0.865	0.065	13.400	0.000
d	0.093	0.234	0.395	0.702	0.029	0.076	0.390	0.705
Vc^2	0.010	0.234	0.042	0.967	−0.188	0.079	−2.380	0.041
Fn^2	0.179	0.234	0.765	0.464	0.054	0.070	0.770	0.462
d^2	0.063	0.234	0.271	0.793	−0.104	0.074	−1.410	0.193
V*c* × F*n*	0.005	0.306	0.016	0.987	0.068	0.099	0.680	0.512
V*c* × *d*	0.156	0.306	0.509	0.623	0.115	0.087	1.330	0.218
F*n* × *d*	−0.042	0.306	−0.138	0.893	−0.001	0.098	−0.010	0.989
S = 0.87	*R*-Sq(pred) = 19.48%		*R*-Sq(adj) = 25.00%		*S* = 1.19	*R*-Sq(pred) = 95.98%	*R*-Sq(adj) = 92.40%	

Table 10
Analysis of variance.

Source	DF	SS	MS	F	P
Regression	9	326.011	36.223	25.390	0.000
Residual error	9	12.841	1.427		
Lack of Fit	5	8.055	1.611	1.350	0.398
Pure error	4	4.786	1.196		
Total	18	338.852			

Table 11
Summary of results.

Method	Weight	Rotation	R^2 adj (%)	R^2 pred (%)
PC1[a]	Without	Without	73.57	14.81
WPC1[a]	With	Without	93.70	96.49
PC1F[a]	Without	With	0.00	4.52
WPC1F[a]	With	With	94.00	96.90
PC1[b]	Without	Without	81.02	28.03
WPC1[b]	With	Without	92.40	94.64
PC1F[b]	Without	With	25.00	19.48
WPC1F[b]	With	With	93.20	96.01

adjusted and R^2 predicted than varimax rotation. It is observed that the rotation is only significant when there is interaction with the weighting. Although this conclusion cannot be extrapolated or generalized to other models, in this specific case we will follow with the optimization phase using only the principal component response normal and weighted to assess the efficiency of MMSE optimization approach.

5.3. Optimization

The process optimization is an important task due to accurate means of shaping the parts into final product with required surface finish and high dimensional accuracy. Problems are formulated to attend a specific target. In this work the objective is to minimize a certain response.

The optimization based on the concept of multivariate mean square error is capable of finding out the best combination to attend all the established targets for a correlated set of responses. Eq. (37) was applied to optimize the variables responses for R_a; R_y; R_z; R_q and R_t.

$$\begin{aligned} &\text{Minimize } MMSE_i = (PC_i - \zeta_{PC_i})^2 + \lambda_i \\ &\text{Subject to}: \ \mathbf{x}^T\mathbf{x} \leqslant \rho^2 \end{aligned} \tag{37}$$

According to Table 2, the targets for the surface roughness (ζ_{Yi}) are, respectively, 0.090, 0.710, 0.620, 0.120, and 0.690. Standardizing these values and using the respective eigenvectors (Table 4), it is possible to calculate the targets for the principal components (ζ_{PC_i}). So, for case A, $\zeta_{PC_1^A} = -2.815$ and for case B, $\zeta_{PC_1^B} = -4.323$. Table 12 shows the MMSE optimization's results taking into consideration the principal component regression for normal and weighted responses.

The results indicate that different modeling methods conduct approximately to the same predicted responses at optimum, without significant difference between results obtained with MMSE. But nevertheless, the multivariate weighted response surfaces (WPC1[a]; WPC1[b]) presented

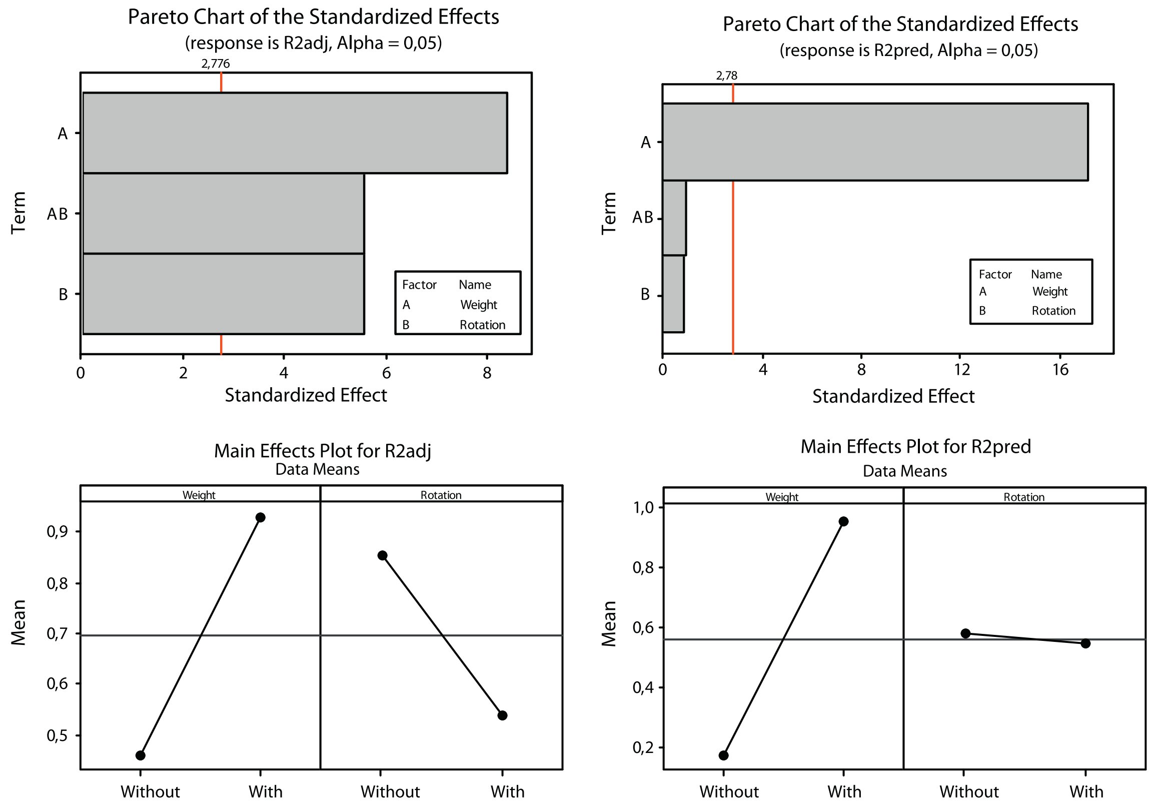

Fig. 4. Statistical analysis of the influence of weights and rotation on R^2 adj and R^2 pred.

Table 12
Optimization results.

Method	R^2 Pred (%)	Optimum parameters			Predicted RESPONSES at optimum				
		Vc	Fn	d	R_a	R_y	R_z	R_q	R_t
					0.090[A]	0.710	0.620	0.120	0.690
PC1[a]	14.81	−0.087	−1.595	−0.101	0.093	0.712	0.568	0.116	0.736
		218.3[B]	0.141	0.217	3.6%[C]	0.3%	−8.3%	−3.7%	6.6%
WPC1[a]	96.49	0.005	−1.681	−0.052	0.081	0.650	0.502	0.096	0.676
		220.1	0.132	0.221	−10.1%	−8.4%	−18.9%	−20.1%	−2.1%
PC1[b]	28.03	−0.089	1.590	−0.120	0.094	0.714	0.571	0.117	0.738
		218.2	0.141	0.216	4.5%	0.6%	−7.9%	−2.9%	7.0%
WPC1[b]	94.64	−0.050	−1.681	−0.040	0.081	0.650	0.500	0.096	0.675
		219.0	0.132	0.222	−10.5%	−8.4%	−19.3%	−20.4%	−2.2%

[A] Targets.
[B] Uncoded units.
[C] Percentual error of optimization method.

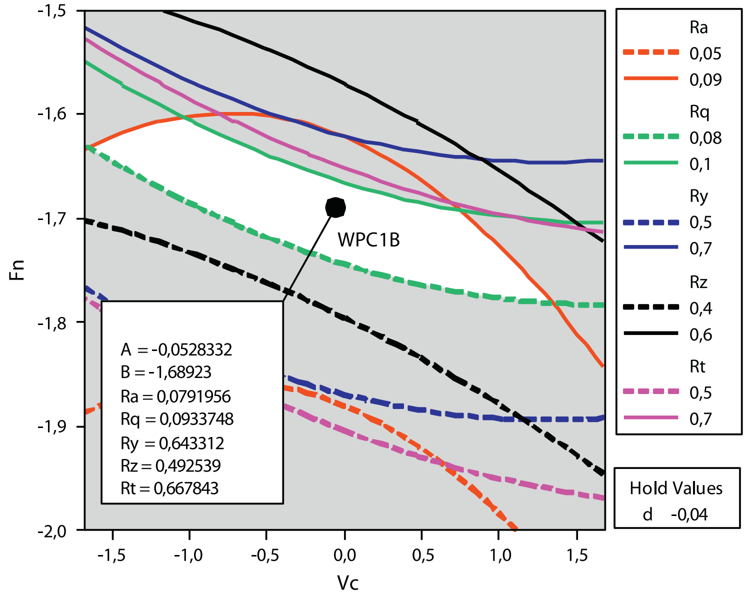

Fig. 5. Overlaid contour plot showing the MMSE optimum obtained with WPC1[B] case.

higher predicted $\mathbf{R^2}$. Then, it is possible to conclude that the solutions obtained with the weighted principal component regression equations achieve the proposed targets through multivariate mean square error approach while keeps the highest predictability. These solutions (cases *a* and *b*) are better because they are consistent and ensure that the optimization results will be reproduced in the industrial practical situations. Fig. 5 shows the overlaid of the five correlated surface roughness equations with their respective upper and lower bounds. The figure also present the solution obtained with the application of MMSE optimization routine to the objective function of WPC1[b].

5.4. Confirmation runs

The confirmation runs were conducted to check whether the responses at optimum highlighted by the optimization method employed are really attainable. To this purpose, ten confirmation experiments for case A were performed to analyze the surface roughness for R_a; R_y; R_z; R_q and R_t. The parameters adopted for these experiments were: Vc = 220.00 Fn = 0.13 and d = 0.22. The targets are presented in Table 12.

Table 13
Responses measured.

Runs	Responses				
	R_a	R_y	R_z	R_q	R_t
1	0.12	0.81	0.74	0.15	0.84
2	0.12	0.77	0.68	0.14	0.79
3	0.11	0.76	0.68	0.14	0.79
4	0.10	0.76	0.69	0.13	0.78
5	0.10	0.76	0.70	0.13	0.82
6	0.12	0.75	0.67	0.15	0.79
7	0.13	0.78	0.71	0.15	0.80
8	0.10	0.61	0.58	0.12	0.66
9	0.10	0.73	0.64	0.13	0.74
10	0.11	0.73	0.66	0.13	0.79
Mean	0.11	0.75	0.68	0.14	0.78

Table 14
95% CI lower bound/upper bound.

Forecast model		Results			Fit (predicted values)	
Target		Experiment mean	Lower bound	Upper bound	Perez	Proposed model
R_a	0.090	0.110	0.059	0.111	0.090	0.081
R_y	0.710	0.746	0.584	0.927	0.757	0.650
R_z	0.620	0.675	0.488	0.762	0.627	0.502
R_q	0.120	0.137	0.076	0.141	0.114	0.096
R_t	0.690	0.780	0.542	0.991	0.763	0.676

After turning each workpiece, the surface roughness was measured at four positions at the center of the piece. An average of three measurements was taken for each position. These values are presented in Table 13.

The means obtained from confirmation runs indicate that all responses were positioned within the confidence interval. The 95% prediction interval is the range in which we can expect any individual value to fall into 95% of the time [27]. The results can be observed in Table 14.

All response variables were positioned within the confidence interval. However the method has proved more efficient for R_y, R_z and R_t, which are more sensitive to dispersion because they are based on the amplitude.

The Paired *T*-Test was applied to compare Perez's Model vs. the Proposed Model. The value of $p = 0.054$ indicates that both methods lead to equal results. However the proposed model has an advantage. While Pérez [1] works with individual responses, the proposed model works with the principal components.

6. Conclusions

This paper presented a model building strategy to estimate the total uncertainty that affects all response variables, using the inverse of multivariate uncertainty as weighting matrix for principal components scores used to replace the original correlated dataset. The main objective of this proposal is to achieve a satisfactory variance explanation, making R^2 (adj) and R^2 (pred) as higher as possible and consequently, reducing the predictive error of the model. According to the results some conclusions can be drawn from the previous sections:

a. The weight matrix represents strong influence over the model and raise the result of *R*-Sq(adj) to satisfactory level, over 80%. On the other hand, the weight matrix does not reduce the prediction error (S) such as expected, but conducted to a better predictability, mainly evidenced from the larger values of the obtained predicted $\mathbf{R^2}$.
b. Following Bratchell's recommendation a Factorial Analysis with varimax rotation was applied to the data. In both case to $PC1^AF$ and $PC1^BF$ the results of R^2 (adj) and R^2 (pred) were low. The Factorial Analysis showed itself to be not capable of improve these particular results such as expected. But when $PC1^AF$ and $PC1^BF$ were weighting with weight matrix, the results of *R*-Sq(adj) achieved 94% and 92.4% respectively. Besides, the factorial analysis with varimax rotation keeps the *p*-value of the lack-of-fit upper 5%.
c. Considering the optimization results it was possible to observe that the MMSE approach applied to hard turning of steel 52100 produced very close solutions to all the targets. The best point for case A is achieved with $Vc = 220$ m/min, $Fn = 0.13$ mm/rev and $d = 0.22$ mm and for case B, $Vc = 219$ m/min, $Fn = 0.13$ mm/rev and $d = 0.22$ mm. The results indicate that different modeling methods conduct approximately to the same predicted responses at optimum, without significant difference between results obtained with MMSE. However, the multivariate weighted response surfaces ($WPC1^a$, $WPC1^b$) presented higher predicted R^2, suggesting that the weighted principal component regression equations achieve the proposed targets through multivariate mean square error approach while keeps the highest predictability. These solutions are preferable because they are consistent, ensuring that the optimization results will be reproduced in the industrial context.
d. The confirmation runs showed that this method provides relative accurately the behavior of response variables, since all the results of the variables analyzed were within the confidence interval. The method was able to indicate an optimal point that provides a solution for the response variables. All response variables were positioned within the confidence interval. However the method was more efficient for R_y, R_z and R_t, which are more sensitive to the dispersion since they are based on the amplitude.

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