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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

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