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ORIGINAL ARTICLE

A multivariate mean square error optimization of AISI 52100 hardened steel turning

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Abstract Hardened steel turning has received special attention in recent years due to its many applications in modern industries. The characteristics that define its machinability—expressed in terms of multiple response problems—are usually represented by experimental model building strategies like response surface methodology (RSM). Such strategies, however, have a particular drawback when multiple correlated regression functions are present. The optimization of multiple process characteristics without considering the variance–covariance structure among the responses may lead to an inadequate optimum. To deal with this constraint, this paper presents a novel multiobjective optimization method; it correctly focuses the multiple correlated characteristics of the AISI 52100 hardened steel, based on the concept of multivariate mean square error. This novel approach combines principal component analysis with RSM focusing a multidimensional nominal-the-best problem. In this kind of optimization, all the characteristics (tool life, cutting time, cost, material removal rate, and surface roughness) have a specific target while maintaining a strong correlation structure. Transforming the original responses and respective targets to the plane of a multivariate principal component scores, an optimization routine is capable of finding out a compromise solution that attends all the established targets. The following AISI 52100 turning process variables were considered in this study: cutting speed, feed rate, and depth of cut. Theoretical and experimental results were convergent and confirmed in a case study.

Keywords Hard turning · Multivariate mean square error (MMSE) · Response surface methodology (RSM) · Principal component analysis (PCA)

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1 Introduction

In recent years, considerable attention has been focused on the understanding of hardened steel machinability [1–10]. The hard turning is a machining process that offers a number of potential benefits over traditional grinding in some applications and has, nonetheless, several unique characteristics, as segmented chip formation and micro-structural alterations at the machined surfaces, fundamentally different from conventional turning [1]. According to Tamizharasan et al. [2], hard turning is a profitable alternative to finish grinding. Considering that the ultimate aim of hard turning is to remove work piece material in a single cut rather than a lengthy grinding operation, a great deal of improvements can be obtained, since this machining process may to reduce processing time, the production cost, and setup time, besides an adequate surface roughness. Furthermore, many of its properties are predictable as tool wear, tool life, quality of surface turned, and amount of material removed [2]. Trying to achieve the best hard turning process comprehension, several works have been done recently [1–20]. Singh and Rao [3] and Ozel et al. [4] studied the effect of cutting conditions, workpiece hardness, and tool geometry on surface roughness and cutting forces. Many researchers developed studies considering the effects of cutting fluids on the hard turning performance [5–7]. Concerns about the wear and tribochemical wear mechanisms are found in the work of Hwang et al. [1]. In the same way, the monitoring of the flank tool wear and its influence to the geometric error, accuracy, and thermal damage were contemplated by Zhou et al. [8] and Quiza et al. [9]. The influence of solid lubricants [10] and the surface integrity (surface roughness, residual stress and thermal damage layer) [11] are also extensively studied. To overcome the limitations of cutting fluids in machining, more attention is also being paid to the internal cooling of cutting tools. The elevated cutting zone temperature in hard turning causes the instant boiling of coolant in the cutting zone, which pulls down the tool life and surface finish, by making thermal distortions and, hence, in most of the hard turning operations [12].

As cited in Tamizharasan [2], the most of hard turning performance characteristics are predictable and, therefore, can be modeled. These models, obtained in different ways, may be used as objective functions in optimization, simulation, control, and prediction algorithms. In a first approach, these characteristics can be separated in two sets of responses: one that prioritizes the product quality and other that is concerned with the cutting productivity. These two sets of characteristics are generally conflicting in nature [11] and in a competitive manufacturing environment; the simultaneous optimization is required and desirable for the manufactures. Nonetheless, the attainment of a high quality machining process that takes into account the particularities of each measurable aspect of a product is not an easy task.

The multiresponse optimization requires, sometimes, the employment of several mathematical techniques involving the models building and optimization. The model building is the first aspect of the machining optimization. Whereas the behavior of the cutting parameters as well as their relationship with the process performance indexes is generally unknown, it is necessary to establish reliable equations to be used as objective or constraint functions. Sometimes, the large number of experiments necessary to establish this relationship between the observed responses and the cutting parameters makes the experimentation cost-prohibitive. To accomplish with the model building task, many researchers have been using response surface methodology (RSM) [7, 14–21] In this methodology, the effects of the cutting parameters on the machining outputs are obtained using experiments capable of generating appropriate data for efficient statistical analysis which, in turn, produces valid and objective conclusions and models [23].

Many examples of RSM in the study of hardened steel machining are found in the literature. Benga and Abrão [19] studied the tool life and the surface finish in the turning of the hardened 100Cr6 bearing steel using RSM. Singh and Rao [3] conducted an experimental investigation of the effects of cutting conditions and tool geometry on the surface roughness in the finish hard turning of the bearing steel (AISI 52100). Mixed ceramic inserts were made up of aluminum oxide and titanium carbonitride (SNGA), having different nose radius and different effective rake angles. The mathematical models for the surface roughness were developed by using the response surface methodology. In the same direction, the researchers investigated the influence of the *high temperatures developed in hard turning process*, *where the surface quality deteriorates due to the tool wear. The use of solid lubricants during hard turning has been explored using a RSM.* A four-factor two-level factorial design was used by Ozel et al. [4] to determine the effects of the cutting edge geometry, workpiece hardness, feed rate, and cutting speed on surface roughness and resultant tangential and axial forces in the finish hard turning of AISI H13 steel. Although the researches have applied analysis of variance (ANOVA) approach, no multi-objective optimization routine was employed in this case.

Sahin and Motorcu [15] used RSM to model surface roughness (Ra, Rz, and Rmax) in the turning of AISI 1050. Al-Ahmari [17] built empirical models for tool life, surface roughness, and cutting force in a hard turning operation for the austenitic AISI 302.

Whereas the machining output models are established, the second step is the choice of an optimization strategy. Concerned with the aspect of machining improvement, some researchers have investigated the use of multiobjective optimization methods in the hardened steel machining. Karpat and Ozel [24] proposed a methodology based on neural networks and particle swarm to respectively model and optimize three multiresponse hardened steel turning operations: (1) the simultaneous minimization of surface roughness and machining time of an AISI H13 steel; (2) the maximization of tool life and material removal rate of a 100Cr6; and (3) the minimization of tensile residual stress and surface roughness of a AISI 52100 hardened steel. Iqbal et al. [2] used the desirability approach to simultaneously maximize the tool life (y_1) and to minimize the average surface roughness measured along (y_2) and across (y_3) the feed direction in the milling of AISI D2 and in the X210 Cr12 steels. To model the effects of cutting parameters applied to the finish hard-milling process with minimum quantity of lubricant, the researchers have used a D-optimal response surface design. Kwak et al. [4] employed RSM to analyze the grinding power, surface roughness, and material removal rate in external cylindrical grinding o fhardened SCM440 steel. Zhang et al. [11] used the Taguchi method to investigate the surface integrity (surface roughness, residual stress—radial and circumferencial—and thermal damage layer) of hardened bearing steel in hard dry turning. The proposed optimization method was applied individually on each response. However, a common optimal combination was not achieved for the hard turning parameters.

A third aspect of the multiobjective optimization is related to the degree of importance of each objective function (or target functions) and the algorithm of resolution. According to Karpat and Ozel [24] and Busacca et al. [25], two different approaches have been considered when handling such optimization problems: (1) weighted aggregation of all the targets into a single objective function or (2) optimization of the most important target keeping the other target functions as constraints.

Focusing on the weighted aggregation approach, Lin and Tu [26] and Köksoy [27] proposed the mean square error (MSE) concept where the distance among all the responses and their respective targets and variances must be minimized. Consonantly, Ch'ng et al. [28] argue for the use of a capability index (MC_{pm}^{*}) which allows the agglutination of the mean and variance equations in the same objective function while keeping the probability of quality in conformity. Based on the multiplicative criterion, Derringer and Suich [29] presented the desirability function concept. Using a set of transformations considering responses' bounds, a geometric mean is used to compound a single objective function. Likewise, Plante [30] proposed the use of the multiple capability index MCpk to combine the mean and variance of each response of interest.

The later aspect of the multiobjective optimization is the influence of the correlation among the responses over the global solution. As pointed out by many researchers [22, 31–33], the individual analyses of each response may lead to a conflicting optimum, since the factor levels that improve one response can, otherwise, degrade another. The presence of correlation can also cause the model's instability, the overfitting, and the inaccuracy on the regression coefficients. In this case, the regression equations are not adequate to represent an objective function without considering the variance–covariance structure among the multiple responses [22, 32, 33]. Some optimization approaches concerned with the correlation among the multiple responses were recently established to focus on this particular drawback. Chiao and Hamada [31], for example, recognizing the limitations of the desirability in terms of correlation influence over the optimization, have proposed a method based on the multivariate normal probability. In the same direction, Duffy et al. [34] and Liu et al. [35] have presented proposals which take into consideration the maximization of multivariate process yield (the joint likelihood that performance measures' are within the specifications). Khuri and Conlon [36] proposed the minimization of the generalized distance between the responses and respective targets written in terms of estimated variance–covariance matrix $\hat{\Sigma}$. Bratchell [37] employed a second-order response surface based on principal component analysis (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 PCAs to overcome the correlation influence is very extensive in the machining literature, mainly associated with Taguchi designs [38–44].

As the most part of machining processes, hard turning also presents a large set of correlated responses [43]. Regarding this particularity, this paper presents a multiobjective optimization method—based on the concept of multivariate MSE (MMSE)—to improve the multiple correlated characteristics of the AISI 52100 hardened steel. This concept is developed combining PCA and RSM to focuses on a multidimensional nominal-the-best (NTB) problem.

2 Multivariate mean square error approach

Considering the nature of the most part of the manufacturing processes, two objectives must be achieved when attempting to improve their yields: the distance from the target (θ) and its respective variance (σ^2). To achieve both objectives, a dual response surface (DRS) is generally considered to attain the proposed goals in each quality characteristic. This is obtained by building a response surface to the mean (ω_μ) and to the variance or standard deviation (ω_σ). This is the straightforward expression of NTB case. The mean and variance functions can be usually written as a second-order model through ordinary least squares (OLS) algorithm. To accomplish with the objective of the NTB optimization, Vining and Myers [45] and Lin and Tu [26] proposed the minimization of the MSE as an optimization criterion in DRS, where the mean and variance estimated equations can be joined as:

$$\mathrm{MSE} = \left(\widehat{\omega}_\mu - \theta\right)^2 + \widehat{\omega}_\sigma^2 \tag{1}$$

Köksoy [27] and Köksoy and Yalcinoz [46], extending the MSE criterion as a way to optimize multiple responses, have proposed the agglutination of the mean square error equations of each response using a weighted sum or the choice of the MSE of the most important response as objective function while the remaining are kept as constraints.

The aforementioned well-succeeded proposals can be used as a start point to the development of a novel multivariate multiresponse optimization approach. Considering that the most part of the multiobjective optimization methods ignores the correlation among responses [47], the estimated mean and variance described in Eq. 1 can be replaced by the principal component scores regression and its eigenvalues respectively. This new approach are capable of aggregating the several responses into a unique index while keeps its variance–covariance structure and the individual deviation from each target. This proposal promotes the independence from numerical and iterative computation of multivariate integration functions like those need in the Gaussian quadrature or Monte Carlo simulation [31, 35] while employs RSM in the estimation task of multivariate regression equations with experimental data from the process. The original set of responses can be transformed into a set of uncorrelated variables, using a multivariate factorization called PCA. By fitting a second-order model to each uncorrelated variable, the objective functions may be aggregated using a geometric mean. Generally, 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. The targets of the initial dataset can be also transformed into factorized variables. Therefore, a geometrical mean with the larger principal components will generate a multiobjective function that keeps the relationship with the original responses. By associating some constraints, the nonlinear optimization system is completed and can be initialized.

Mathematically, MMSE can be established as a multivariate dual response surface, such as:

$$\mathrm{MMSE}_i = \left(\mathrm{PC}_i - \zeta_{\mathrm{PC}_i}\right)^2 + \lambda_i \tag{2}$$

When a response surface design is used, PC_i is defined as 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 dataset. To establish this relationship, it is possible to use Eq. 3. This transformation was firstly used by Wang and Du [53] to obtain an alternative multivariate capability index. So, the general form of ζ_{PC_i} can be written as:

$$\zeta_{\mathrm{PC}_i} = e_i^T\left[Z\left(Y_p\middle|\zeta_{Y_p}\right)\right] = \sum_{i=1}^{p}\sum_{j=1}^{q} e_{ij}\left[Z\left(Y_p\middle|\zeta_{Y_p}\right)\right] \qquad i = 1,2,\ldots,p; \quad j = 1,2,\ldots,q \tag{3}$$

where 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. 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.

As described before, in the most part of manufacturing processes, one or two principal component equations are enough to represent the original system of p objective functions, since the responses have some degree of correlation. Therefore, considering the optimization routine formed by the MMSE functions whose eigenvalues are equal or greater than the unity, it is possible to write:

$$\text{Minimize} \quad \mathrm{MMSE}_T = \left[\prod_{i=1}^{k}\left(\mathrm{MMSE}_i|\lambda_i \geq 1\right)\right]^{\left(\frac{1}{k}\right)} = \left\{\prod_{i=1}^{k}\left[\left(\mathrm{PC}_i - \zeta_{\mathrm{PC}_i}\right)^2 + \lambda_i|\lambda_i \geq 1\right]\right\}^{\left(\frac{1}{k}\right)} \qquad i = 1,2,\ldots,k; k \leq p \tag{4}$$

$$\textit{Subject to}: \mathbf{x}^T\mathbf{x} \leq \rho^2 \tag{5}$$

where k is the number of MMSE functions according to the significant principal components.

The spectral decomposition represented by PC_i in the Eq. 2 is obtained through the PCA—one of the most widely applied tools used to summarize common patterns of variation among variables. This statistical technique is also able to retain meaningful information in the early PCA axes. Assuming that Σ is the covariance matrix associated to the random vector $Y^T = \left[Y_1, Y_2, \ldots, Y_p\right]$ and that this matrix has pairs of eigenvalues–eigenvectors $(\lambda_i, e_i), \ldots \geq (\lambda_p, e_p)$, where $\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_p \geq 0$, then the ith principal component is given by a uncorrelated linear combination $\mathrm{PC}_i = e_i^T Y = e_{1i}Y_1 + e_{2i}Y_2 + \ldots + e_{pi}Y_p$ with $i = 1,2,\ldots,p$. The ith principal component can be obtained as maximization of this linear combination. The most of statistical software packages has this algorithm implemented. Considering $[Z]$ the standardized data matrix and $[E]$ the eigenvectors matrix of the multivariate set, each principal component score can then be obtained as [51]:

$$\mathrm{PC}_{\mathrm{score}} = [Z].[\mathrm{E}] \tag{6}$$

Since the multivariate score are obtained, a second-order polynomial can be established applying the OLS to set of the independent process parameters (x_i) and the related principal component scores (PC_i), as follows:

$$Y=\beta_0+\sum_{i=1}^{k}\beta_i x_i+\sum_{i=1}^{k}\beta_{ii}x_i^2+\sum\sum_{i<j}^{k}\beta_{ii}x_i x_j+\varepsilon_\mu=b_0+\left[\nabla f(\mathbf{x})^T\right]+\left\{\frac{1}{2}\mathbf{x}^T\left[\nabla^2 f(\mathbf{x})\right]\mathbf{x}\right\} \tag{7}$$

where β is the polynomial coefficient, 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*.

The number of equations used in the geometric mean will be dependent on the number of significant principal components. There is a variety of stopping rules to estimate the adequate number of nontrivial PCA axes (the *PC* scores) that must be adopted to represent the dataset. The most popular rules are those based on the Kaiser's criteria, where only those principal components whose eigenvalues are greater than 1 should be kept to represent the original dataset [49–51]. Moreover, the explained cumulative variance should be greater than 80%. To evaluate whether the eigenvalue of the first principal component is significantly different from the remaining ones, the Bartlett's modified sphericity test can be used [50, 51]. Its formulation is assumed as:

$$\chi^2=-\left[n-\frac{1}{6}(2p+11)\right]\ell n|R| \tag{8}$$

Where $|R|$ is the determinant of the correlation matrix, n is the sample size and p is the number of variables.

In this paper, where PCA is used to replace the original set of AISI 52100 quality characteristics, n is the number of experiments in the chosen central composite design and p is the number of correlated responses. The statistic of test is approximately χ^2distributed, with $p(p-1)/2$ *df*. The null hypothesis is that all variables are uncorrelated.

To test if the eigenvalue of the second principal component is significantly different from the remaining ones, Lawley [51] developed a specific test where the null hypothesis assumption claims that at least two variables are correlated if the second eigenvalue is not significantly different from the remaining ones. By rejecting the null hypothesis, it is assumed that the second eigenvalue (and consequently, the second principal component) is also significant and must be kept to help in the explanation of the variance–covariance structure of the original dataset. The statistic of test is also approximated as a χ^2distribution with $(p+1)(p-2)/2$ *df* and can be expressed as:

$$\chi^2=\frac{n-1}{1-r}\sum_{j\neq i=1}^{p}\sum_{i\neq j=1}^{p}\left(r_{ij}-\bar{r}\right)^2-\psi\sum_{k=1}^{p}\left(\bar{r}_k-\bar{r}\right)^2 \tag{9}$$

where n is the number of experiments and p is the number of response variables. r_{ij} is the Pearson's correlation coefficient between variables i and j. $\bar{r},\psi,\bar{r}_k$ are obtained as follows:

$$\bar{r}=\frac{2}{p(p-1)}\sum_{i=k+1}^{p}\sum_{j=1}^{p}r_{ij},\quad \psi=\frac{(p-1)^2\left[1-(1-\bar{r})^2\right]}{p-(p-2)(1-\bar{r})^2},\quad \bar{r}_k=\frac{1}{(p-1)}\sum_{\substack{i=1\\ i\neq j}}^{p}r_{ik} \tag{10}$$

The null hypothesis is rejected when the statistic of test is less than a critical value (or p value$<\alpha$). In this work, it was assumed that α=0.05. A Matlab 7.0 ® routine was developed to perform the multivariate statistical tests described in Eqs. 8–10.

Although k may be mathematically equal to p, this equality rarely occurs whereas the use of PCA generally reduces the problem dimension according to the strength of variance–covariance structure among the responses. Eventually, it is possible to consider principal component equations with $\lambda<1$, since the Lawley's multivariate hypothesis test reveals its adequacy.

Since the models are established, the multiobjective optimum can be generally found by locating the stationary point of the Eq. 4 only subjected to the constraint that forces the optimum to lie within the experimental region, described in the form of Eq. 5. Other constraints may be added to the system according to the needs of the experimenter. Among the several methods available to solve the nonlinear programming problem (NLP), the generalized reduced gradient (GRG) is considered one of the most robust and efficient [53], and as attractive feature, it exhibits an adequate global convergence, mainly when initiated sufficiently close to the solution [54]. For this reason, the GRG will be used in this article. A general form for a NLP can be written as [44]:

$$\begin{array}{ll} \text{Minimize} & f(\mathbf{x}) \\ \text{Subject to :} & g_i(\mathbf{x}) = 0, \quad i = 1, ..., m \\ & l_j \leq x_j \leq u_j, \quad j = 1, ..., n \end{array} \tag{11}$$

where $\mathbf{x}$ is a vector of n process variables, f is the objective function, and g_i are constraints functions. The l_j and u_j represent respectively the lower and upper bound on the process variables. Some formulations also include inequality constraints although in the GRG method they are converted to equality constraints.

The framework of the GRG method is based on the conversion of a constrained problem into an unconstrained one by using direct substitution [54]. In this way, the vector of process variables x can be partitioned into two subsets $\mathbf{x}=(\mathbf{x^B}, \mathbf{x^N})^\mathbf{T}$, where $\mathbf{x}^\mathrm{B}$ is the m vector of basic variables and $\mathbf{x}^\mathrm{N}$ is the n-m vector of nonbasic variables. Rewriting the NLP problem, the reduced way may be described as [44]:

$$\begin{array}{ll} \text{Minimize} & \mathrm{F}(\mathbf{x}) = f(\mathbf{x^B}(\mathbf{x^N}), \mathbf{x^N}) \\ \text{Subject to :} & \boldsymbol{l}_\mathrm{N} \leq \boldsymbol{x}^N \leq \boldsymbol{u}_N \end{array} \tag{12}$$

where l_N and u_N are the vectors of bounds for $\mathbf{x}^\mathrm{N}$.

Starting with a feasible point $\mathbf{x}^k$, the GRG algorithm tries to find a direction of movement that will optimize the objective function. The direction of steepest descent for a minimization problem is given by the negative of the reduced gradient that can be written as follows:

$$r^k(\mathbf{x}_N) = \left[\frac{\partial f^k}{\partial \mathbf{x}_\mathrm{N}^k}\right] - \left[\frac{\partial f^k}{\partial \mathbf{x}_\mathrm{B}^k}\right]^T \left[\frac{\partial g^k}{\partial \mathbf{x}_\mathrm{B}^k}\right]^{-1} \left[\frac{\partial g^k}{\partial \mathbf{x}_\mathrm{N}^k}\right] \tag{13}$$

The algorithm stops when the magnitude of the reduced gradient at the current point is as small as desired [54, 55]. Otherwise, a line search procedure is performed to find a new point in the direction of the reduced gradient. This operation is repeatedly performed.

Although the MMSE approach presents a good theoretical basis, some limitations can be expected in its usage. As example, the costs inherent to the deviation from the specified targets are not considered. Also, it is not possible to fix weights or an importance degree for the original responses (only to the principal components). It is not possible also to elect a priority response. Some initial simulated cases, however, have shown its efficacy and robustness in NTB problems.

3 Experimental procedure

To comply with the objectives of this research, workpieces of AISI 52100 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) with dimensions of φ49×50 mm were used in the turning process. The workpieces were quenched and tempered before machining and presented after heat treatment, hardness values between 53 and 55 HRC up to a depth of 3 mm below the surface. The machine tool used was a CNC lathe with a 5.5 KW spindle motor with conventional roller bearings.

The mixed ceramic (AL_2O_3+TiC) inserts, ISO code CNGA 120408 S01525, were coated with a very thin layer of titanium nitride presenting a chamfer on the edges, and were manufactured by Sandvik Coromant (Sandvik class CC6050). The tool holder presented a negative geometry with ISO code DCLNL 1616H12 and entering angle χ_r= 95°. Tool flank wear measurements (VB_{max}) were taken through an optical microscope. To evaluate machining conditions, the end of life criteria was adopted as the breaking of the tool point.

Adopting this experimental condition, the work pieces were machined using the range of parameters defined in Table 1. In the set of recorded responses, tool life (T), surface roughness (Ra), and cutting time (C_t) were observed. The total cost (K_p), the total turning cycle time (T_t), and the Material removal rate (MRR) were calculated using Eqs. 14–16. The C_t, also called machining time, is the time that the tool actually spends in the feed mode or cutting and removing chips. Mathematically, this variable can be described in cylindrical turning as [56]:

$$C_t = \frac{l_f \pi D_m}{1000 f V_c} \tag{14}$$

Table 1 CCD factor levels

Parameter	Symbol	Unit	Levels (coded)				
			−1.633	−1	0	+1	+1.633
Cutting speed	V	m min^{-1}	187.34	200	220	240	252.66
Feed	f	mm rev^{-1}	0.0342	0.050	0.075	0.100	0.1158
Depth of cut	d	mm	0.1025	0.150	0.225	0.300	0.3475

Table 2 Parameters symbols and values adopted in the study

Parameters	Symbol	Value
Batch size (units)	Z	1.000
Secondary time (min)	t_s	0.5
Tool approximation and retreat time (min)	t_a	0.1
Set-up time (min)	t_p	60
Insert changing time (min)	t_{ft}	1
Machine and Labor costs ($)	(S_m+S_h)	80
Tool holder price ($)	V_{si}	200
Average tool holder life (Number of edges)	N_{fp}	1.000
Insert price ($)	K_{pi}	50
Number of cutting edges on the insert	N_s	4
Section Length	l_f	50
Initial diameter (mm)	D	49
Final diameter (mm)	d	46
Average diameter (mm)	D_m	47.5

where l_f is the length of part, D_m is the work piece average diameter, f is the feed rate, and V_c is the adopted cutting speed. The T_t in minutes [56] is determined as follows:

$$T_t = \left(1 + \frac{t_{ft}}{T}\right)\left(\frac{l_f \cdot \pi \cdot d}{1000 \cdot f \cdot V_c}\right) + \left(t_s + t_a + \frac{t_p}{Z} - \frac{1}{Z} \cdot t_{ft}\right) \quad (15)$$

As defined in [56], the total cost of the turning process (K_p), considering interchangeable inserts, can be described as:

$$K_p = \left(\frac{T_t}{60} - \frac{1}{Z}\right).(S_h + S_m) + \frac{C_t}{60}(S_h + S_m) + \frac{C_t}{T}\left[\left(\frac{V_{si}}{N_{fp}} + \frac{K_{pi}}{N_s}\right) + t_{ft}(S_h + S_m)\right] \quad (16)$$

The symbols used in Eqs. 14–16 and respective values adopted in this study are shown in Table 2. A sequential set of experimental runs was established using a blocked CCD built according to the design shown in Table 3.

4 Results and discussion

Using a CCD with four center points, two blocks and the axial distance for this design, ρ=1.633, the data of the six machining characteristics was collected and their dependency structure was assessed according to Eqs. 11–13. Through the use of the Minitab software, at a 5% significance level, the critical value for the modified Bartlett's test was $\chi^2_{\text{critical}} = 24,99$ and the statistic of test was χ^2=398.95 which was much larger than the critical

Table 3 Experimental Data for the AISI 52100 hardened steel turning

Number	B	V	f	d	T	C_t	T_t	K_p	MRR	Ra	PC_1	PC_2
1	1	200	0.05	0.15	16.75	7.70	8.82	17.59	1.50	0.33	4.27	−0.59
2	1	240	0.05	0.15	11.50	6.41	7.63	17.26	1.80	0.28	3.01	0.24
3	1	200	0.1	0.15	9.85	3.85	4.90	11.49	3.00	0.70	−0.22	−1.79
4	1	240	0.1	0.15	8.50	3.21	4.24	10.45	3.60	0.57	−0.74	−0.73
5	1	200	0.05	0.3	11.50	3.85	4.84	10.71	3.00	0.25	0.70	1.10
6	1	240	0.05	0.3	7.45	3.21	4.30	11.20	3.60	0.42	−0.50	0.25
7	1	200	0.1	0.3	8.20	1.92	2.82	6.74	6.00	0.57	−2.50	−0.41
8	1	240	0.1	0.3	6.25	1.60	2.52	6.62	7.20	0.61	−3.31	−0.55
9	1	220	0.075	0.225	8.60	3.11	4.13	10.10	3.71	0.36	−0.48	0.63
10	1	220	0.075	0.225	6.80	3.10	4.23	11.44	3.71	0.42	−0.63	0.29
11	2	187.34	0.075	0.225	10.10	3.65	4.67	10.82	3.16	0.34	0.23	0.58
12	2	252.66	0.075	0.225	7.60	2.71	3.72	9.49	4.26	0.45	−1.18	0.18
13	2	220	0.0342	0.225	17.50	6.82	7.87	15.45	1.69	0.32	3.64	−0.36
14	2	220	0.1158	0.225	7.20	2.01	2.95	7.49	5.73	0.72	−2.70	−1.41
15	2	220	0.075	0.1025	12.00	6.82	8.05	17.96	1.69	0.36	3.24	−0.40
16	2	220	0.075	0.3475	6.70	2.01	2.97	7.78	5.73	0.31	−1.97	1.30
17	2	220	0.075	0.225	7.20	3.09	4.20	11.09	3.71	0.37	−0.54	0.61
18	2	220	0.075	0.225	9.10	3.11	4.11	9.82	3.71	0.29	−0.33	1.07
Mean:					9.600	3.788	4.832	11.306	3.711	0.425	0.000	0.000
S.D.:					3.244	1.861	1.931	3.553	1.607	0.145	2.213	0.848
Target ζ_{Yi}:					6.500	1.600	2.600	7.300	6.300	0.400	**−2.560**	**0.786**
$Z(Y_i\|\zeta_{Yi})$:					−0.956	−1.175	−1.156	−1.127	1.611	−0.172	–	–

The bold values were obtained applying the Eq. 15

value. In this way, there is strong evidence against the null hypothesis and, therefore, AISI 52100 data supports the multivariate factorization (Table 4).

Hence, after determining the principal components scores using Eq. 10, PC_1 and PC_2 were also fitted using OLS algorithm. Figures 1 and 2 represent their fitted surfaces in terms of the cutting parameters. Table 5 presents the full quadratic models of each response and respective significance. Tables 6 and 7 present the ANOVA analysis for the full quadratic models of PC_1 and PC_2. Full quadratic models were used for all responses because no lack of fit was detected in the models. The analysis was done using coded units to eliminate any spurious statistical results due to different measurement scales for the factors. Uncoded units often lead to collinearity among the terms in the model which inflates the variability in the coefficients estimation, which makes them difficult to interpret.

Table 4 shows that the first principal component represents 81.6% of the variation in the responses which is a sufficient variance–covariance explanation. This implies that the fitted response surface of PC_1 is an excellent option of representation of a multiobjective function. Moreover, the eigenvectors show that there is a highly positive correlation between PC_1 and the T, C_t, T_t, and K_p, while a negative correlation can be observed between PC_1 and the responses MRR and Ra. This kind of relationship indicates that the minimization of $MMSE_1$ (built only with PC_1) leads to a global normalization, i.e., all the responses are capable to achieve their respective targets.

Although there is a notably explanation in the first principal component, there is a poor correlation among PC_1 and surface roughness, and a strong and negative correlation between PC_2 and Ra, which suggest that PC_2 should also be taken into account. Considering the Lawley's test, according to the Eqs. 14 and 15, and comparing the results

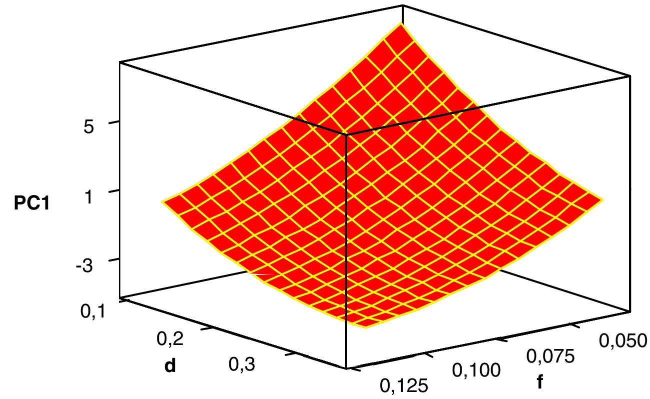

Fig. 1 Response surface plot for PC_1

of the Eq. 14 (χ^2=160.2) with the 5% critical value $\left(\chi^2_{\text{critical}} = 23.7\right)$, it is possible to conclude that the first principal component is extremely significant and the second eigenvalue is considerably different from the smallest ones $(\lambda_3, \ldots, \lambda_6)$. In this way, the choice of the two first principal components to compose the total multivariate mean square error index can be responsible for the explanation of 93.6% of the variation structure of the six turning responses (Table 4). In this case (k=2 principal components), the geometric mean used in MMSE will become a square root.

For the NTB case of the AISI 52100, the distances among the fitted turning responses and their respective targets must be minimized, while the influence of the variance–covariance structure must be considered in the calculation. Adopting these aspects and the minimization criteria, a nonlinear optimization system may be written in terms of the multivariate mean square error using, additionally, a spherical constraint to the factor levels. This constraint ρ^2=2.667 will force the solution to fall within the

Table 4 Principal component analysis of the original turning responses

Eigenvectors matrix (e_{ij})						
Variable	PC_1	PC_2	PC_3	PC_4	PC_5	PC_6
Eigenvalue	4.897	0.720	0.267	0.116	0.001	0.000
Proportion	0.816	0.120	0.044	0.019	0.000	0.000
Cumulative	0.816	0.936	0.981	1.000	1.000	1.000
T	0.403	−0.180	−0.806	0.233	0.317	−0.015
C_t	0.445	−0.160	−0.028	−0.284	−0.548	−0.627
T_t	0.446	−0.154	0.032	−0.296	−0.319	0.767
K_p	0.436	−0.107	0.419	−0.344	0.697	−0.135
MRR	−0.424	−0.018	−0.4	−0.805	0.105	−0.007
Ra	−0.265	−0.952	0.112	0.105	0.003	0.000

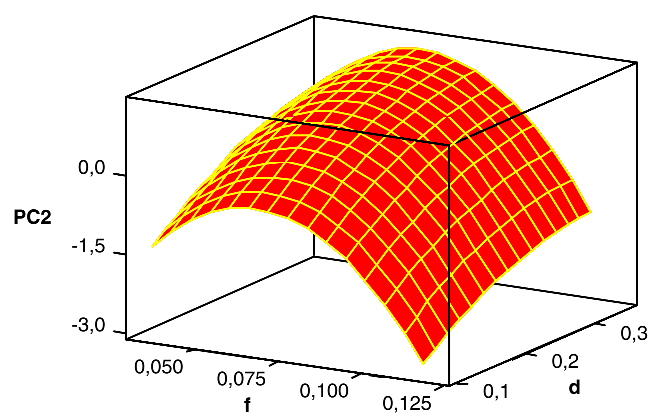

Fig. 2 Response surface plot for PC_2

Table 5 Full quadratic models for each response

Term	PC_1	PC_2	T	C_t	T_t	K_p	MRR	Ra
B_0	**−0.4758**	**0.672**	**7.9680**	**3.1160**	**4.1800**	**10.6220**	**3.7130**	**0.3560**
V	**−0.4569**	0.019	**−1.2510**	**−0.3320**	**−0.3180**	−0.2380	**0.3380**	0.0160
f	**−1.8452**	**−0.465**	**−2.3410**	**−1.3830**	**−1.4360**	**−2.5840**	**1.2380**	**0.1360**
D	**−1.5328**	**0.454**	**−1.6390**	**−1.3830**	**−1.4550**	**−2.8610**	**1.2380**	−0.0080
V^2	−0.0430	−0.154	0.2340	−0.0060	−0.0230	−0.1960	0.0000	0.0230
f^2	**0.3113**	**−0.626**	**1.5470**	**0.4570**	**0.4330**	0.2970	0.0000	**0.0700**
d^2	**0.3732**	−0.127	0.4220	0.4570	**0.4700**	**0.8220**	0.0000	0.0000
Vf	0.1413	0.116	0.7500	0.1210	0.0960	−0.1650	**0.1130**	−0.0260
Vd	−0.0288	**−0.361**	**0.0750**	0.1210	0.1260	0.2180	**0.1130**	**0.0500**
fd	**0.2788**	−0.016	0.6750	**0.4390**	**0.4390**	**0.5450**	**0.4130**	−0.0180
R^2 adj. (%)	99.20	85.00	85.00	99.10	99.30	97.20	99.90	89.10

The bold values represent the individually significant terms ($P<5\%$)

experimental region. Gathering the previous information in comprehensive optimization systems, it is possible to write the following expressions:

Minimize

$$\mathrm{MMSE}_T = \sqrt{\left[\left(\mathrm{PC}_1 - \zeta_{\mathrm{PC}_1}\right)^2 + \lambda_1\right] \cdot \left[\left(\mathrm{PC}_2 - \zeta_{\mathrm{PC}_2}\right)^2 + \lambda_2\right]} \quad (17)$$

$$\text{Subject to :} \qquad \mathbf{x}^T\mathbf{x} \le \rho^2 = V^2 + f^2 + d^2 \quad (18)$$

$$\text{With} \quad \zeta_{\mathrm{PC}_i} = e_{1i}[Z(T|\zeta_T)] + e_{2i}[Z(Ct|\zeta_{Ct})] + e_{3i}[Z(Tt|\zeta_{Tt})] + e_{4i}\left[Z\left(Kp|\zeta_{Kp}\right)\right] + e_{5i}[Z(\mathrm{MRR}|\zeta_{\mathrm{MRR}})] + e_{6i}[Z(Ra|\zeta_{Ra})] \quad (19)$$

$$\mathrm{PC}_i = b_{0i} + \left[\nabla f(\mathbf{x})^T\right]_i + \left\{\tfrac{1}{2}\mathbf{x}^T\left[\nabla^2 f(\mathbf{x})\right]\mathbf{x}\right\}_i \quad i = 1, 2, ..., p. \quad (20)$$

where: $\mathbf{x}=[V, f, d]$. The term Z represents the standardized value of the ith response considering its target value ζ_{Yi}, such that $Z(Y_i|\zeta_{Yi}) = [(\zeta_{Yi}) - \mu_{Yi}].(\sigma_{Yi})^{-1}$. The numerical values of the standardized targets $Z(Y_i|\zeta_{Yi})$ in the present case were cited in the last line of Table 3. In the Eq. 3, e_{ij} represent the eigenvectors associated with the respective principal components, and its numerical values are described in eigenanalysis of Table 4. Using the relationship established by Eq. 3, the principal component targets were calculated as $\zeta_{\mathrm{PC}_1} = -2.56$ and $\zeta_{\mathrm{PC}_2} = 0.786$. From Table 4, the two eigenvalues were $\lambda_1=4.897$ and $\lambda_2=0.720$. The minimization of the distance between each principal component and its respective target can lead to a compromise solution that attends the targets of all the six correlated responses.

To solve the nonlinear optimization system described in the Eqs. 17 to 20, a MS Excel ® spreadsheet was developed and the Solver® routine to the GRG implementation was used. After setting up the problem, the Solver® optimization parameters were chosen considering a precision of 10^{-6}; 100 iterations, a quadratic estimative, forwards derivatives and the Newton's method as a line search option.

Table 8 shows the results using the MMSE approach and the desirability method. The solution with MMSE method, after 12 iterations in the GRG-Solver® software was V=217.7 m/min, f=0.086 mm/rev, and d=0.3424 mm which is compatible to the established targets (Table 8).

Table 6 ANOVA for first principal component PC_1

Source	df	SS	MS	F_0	p_f
Regression	9	82.912	9.212	234.62	0.000
Linear	3	79.511	26.503	674.97	0.000
Square	3	2.614	0.871	22.19	0.000
Interaction	3	0.788	0.263	6.69	0.014
Residual error	8	0.3141	0.039		
Lack-of-fit	5	0.266	0.0533	3.35	0.174
Pure error	3	0.0477	0.0159		
Total	17	83.226			

Table 7 ANOVA for first principal component PC_2

Source	df	SS	MS	F_0	p_f
Regression	9	11.356	1.262	11.9	0.001
Linear	3	5.615	1.872	17.33	0.001
Square	3	4.592	1.530	14.17	0.001
Interaction	3	1.149	0.383	3.55	0.067
Residual error	8	0.864	0.108		
Lack-of-fit	5	0.556	0.111	1.08	0.506
Pure error	3	0.308	0.103		
Total	17	12.220			

Table 8 Comparative results between MMSE and desirability methods

	T min	C_t min	T_t min	K_p \$/piece	MRR cm^3/s	Ra µm	V m/min	f mm/rev	D mm	D[a] –
MMSE	6.270	1.860	2.810	7.430	6.430	0.400	217.736	0.0863	0.3424	0.601
Desirability	6.961	1.866	2.789	7.031	6.403	0.392	203.250	0.0910	0.3440	0.242
Upper bound	7.000	2.000	3.000	8.000	7.000	0.410	252.660	0.1158	0.3475	–
Target	6.500	1.600	2.600	7.300	6.300	0.400	220.000	0.0750	0.2250	–
Lower bound	6.000	1.500	2.500	7.000	6.000	0.390	187.340	0.0342	0.1025	–

[a] Overall desirability index of Eq. 4

As a validation test of the turning process with the aforementioned conditions, four confirmation runs were performed using the available cutting edges values. As can be seen in Table 9, the errors between actual and predicted values for the six responses are considerably small. Using the global desirability as matter of comparison the MMSE outperforms the desirability method. Although the two solutions are not quite different in practical terms, the MMSE approach produces a solution which is closer to all targets. This improvement in the performance may be attributed to the considerable influence of correlation among the responses which is not recognized by the desirability method.

Since the results are compatible with the expected values and the hard turning theory, the multivariate mean square error method may be considered suitable for improving the machining process, mainly when a large set of correlated responses are employed in the NTB context. Although the first principal component was enough to represent an adequate optimization set, the inclusion of the second principal component allowed an adequate representation of the surface roughness.

5 Turning parameters sensitivity analysis

To assess the sensitivity of the turning parameters in an optimal condition, two strategies were used: (1) the change of the right side value of the used constraint and (2) the change of the optimum value $x_* = (V_*, f_*, d_*)$. The adequate approach to develop the strategy (1) is to use the concept of Lagrange multipliers. The Lagrange multipliers—also called *shadow prices* in optimization packages—express the gradient at the optimum as a linear combination of the rows of the constraint matrix and can indicate the sensitivity of the optimal objective value to changes in the data [55]. Assuming that the objective function is twice continuously differentiable, and considering small perturbations (δ) in the right side of the constraints, it is possible to use Taylor series to obtain the approximation [55]:

$$f(\bar{x}) = f(x_*) + \sum_{i=1}^{m} \delta_i \lambda_{*_i} \tag{21}$$

where $\mathbf{x}_*$ represents a local minimum. In particular, Eq. 21 is valid if $\bar{x}$ minimizes the perturbed problem. If the right-hand side of the ith constraint changes by δ_1 then the optimal objective value changes by approximately $\delta_i \lambda_{*_i}$. Hence, λ_{*_i} represents the change in the optimal value per unit increasing (or decreasing) in the ith right-hand side. These constants are found solving a nonlinear constrained optimization problem in terms of a Lagragian function using s_j slack variables (if necessary), such that:

$$L(x_i, \lambda_j, s_j) = f(x_i) - \sum_{j=1}^{n} \lambda_j \left\{ \sum_{i=1}^{p} a_{ji} x_i - b_j \right\} - \sum_{j=n+1}^{m} \lambda_j \left\{ \sum_{i=1}^{p} a_{ji} x_i - b_j - s_j^2 \right\} \tag{22}$$

Table 9 Confirmation runs

Response	Cutting edge				Mean	MMSE (predicted value)	Error %
	First	Second	Third	Forth			
T	6.300	6.400	6.160	5.800	6.165	6.270	1.7
C_t	1.756	1.756	1.756	1.756	1.756	1.860	5.6
T_t	2.693	2.689	2.700	2.718	2.700	2.810	3.9
K_p	7.131	7.070	7.220	7.468	7.222	7.430	2.8
MRR	6.374	6.374	6.374	6.374	6.374	6.430	0.9
Ra	0.435	0.430	0.430	0.420	0.429	0.400	−7.2

Table 10 Sensitivity analysis of the cutting parameters (uncoded units)

	MMSE	T	C_t	T_t	K_p	MRR	Ra	V	f	d
Optimal	1.8787	6.270	1.860	2.810	7.430	6.430	0.400	217.736	0.0863	0.3424
+δ	1.8776	6.438	1.942	2.880	7.344	6.856	0.393	214.594	0.0882	0.3615
−δ	1.8885	6.217	1.845	2.817	7.653	5.920	0.402	220.451	0.0846	0.3174
+2%	1.928	6.101	1.842	2.792	7.357	6.761	0.426	222.360	0.0880	0.3470
−2%	1.916	6.486	1.890	2.850	7.554	6.006	0.373	213.640	0.0840	0.3330

The Lagrange multipliers are determined applying the Karush–Kuhn–Tucker conditions [55] to the Eq. 22. This routine is also available in the Solver® in a spreadsheet called "Sensitivity Report". Whereas only one constraint was used, there is also only one Lagrange multiplier to the problem, whose value is λ_1=−0.0029. Substituting λ_1 in Eq. 21, it follows that:

$$\mathrm{MMSE}_T\left(\bar{x}\right) = \mathrm{MMSE}_T(x_*) + \sum_{i=1}^{n} \delta_i \lambda_{*_i} \tag{23}$$

$$= 1.878 - 0.0029.\delta_{(x^T x)}$$

Adopting $\delta_{(x^T x)} = \pm 1.0$ and newly running the optimization routine, it is observed that the new constraints did not change the optimum value and the MMSE_T or the associated objective functions. Otherwise, introducing an arbitrary change of 2% over the factor levels achieved in the optimization, almost the same results (Table 10) are obtained. This sensitivity analysis shows how robust is the solution found with MMSE method.

Figure 3 shows an overlaid contour plot for the original set of turning quality characteristics. On this graph, all the six response surfaces were plotted taking into account their respective limits. The non hachured area indicates the feasible region. It can be observed that the optimum obtained with MMSE method falls inside of this region.

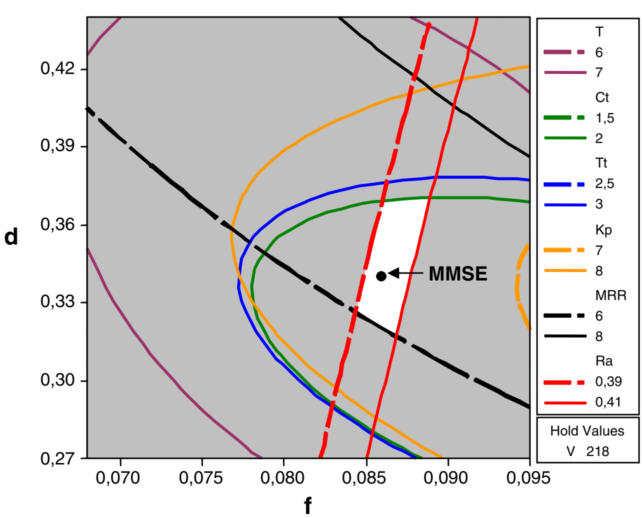

Fig. 3 Overlaid contour plot for the original set of responses and the MMSE solution

6 Conclusions

On the basis of the results presented, the following conclusions can be drawn:

1. The process optimization based on the MMSE approach in situations where the multiple responses exhibited a moderate to high degree of correlation with characteristics of NTB type, showed a consistent adequacy applied to the hard turning of AISI 52100.
2. The results and confirmation runs show that the MMSE approach outperforms the desirability method applied in the optimization of the 52100 hard turning. Although the two solutions are not very different in practical terms, the MMSE approach produces a solution which is closer to all targets. This improvement in the performance may be attributed to the considerable influence of correlation among the responses which is not recognized by the desirability method.
3. In the AISI 52100 case, the first principal component was responsible for most of the variance–covariance present in the original data associated with the tool life, cutting time, total machining cost, total turning cycle time, and material removal rate. The second principal component was used as an alternative to improve the explanation of the surface roughness behavior of the machined parts.
4. Simultaneous normalization (NTB) of the six responses of 52100 hard turning were achieved with V=218 m/min, f=0.086 mm/rot and d=0.34 mm. A variation of ±2% in these values, expressed in the sensitivity analysis, did not significantly modify the multiresponse optimum.
5. Confirmation runs revealed that actual and predicted values obtained with the MMSE method for the six responses presented small differences, which is acceptable since the real experiments can suffer from nuisance factors—not analyzed in this work—like dynamic tool wear, variations in material hardness, among others.

6. The results indicate that RSM combined with PCA is a very useful technique to model and to create equations for forecasting and optimizing, using the fewest experiments possible. Even considering the quality of results of the results of the present approach, these conclusions cannot be extrapolated to different materials, tools or machine tools and they are valid only in the adopted range levels. The approach can, nonetheless, be recommended for optimizing any manufacturing process.

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