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Radial basis function simulation and metamodelling of surface roughness in centreless grinding

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Analysis and modelling

ABSTRACT

Purpose: The purpose of this study was to investigate the efficiency of artificial neural networks and the related metamodels to simulate and identify complex centreless grinding process.

Design/methodology/approach: The modelling is founded on the system approach, which is efficiently dealing with the complexity of the grinding process. The unknown process transfer function is identified via artificial neural network that requires fewer assumptions and less precise information about the process modelled than other conventional modelling techniques. The developed metamodel is a response surface (polynomial fit) of the simulated process that is achieved by the computer model.

Findings: The metamodel quality is strongly related to the prediction accuracy of the underlying simulation model. The generalisation capability of an artificial neural network is sensitive to the training samples (design of experiments). The predictive ability of a metamodel is comparable to the accuracy of the response surface regression model.

Research limitations/implications: Improved simulation model and application of unconventional metamodels (Gaussian process regression) will significantly improve the presented preliminary results.

Originality/value: Metamodelling of computer experiments is an expansion of response surface methodology and the classical designs of experiments and represents a new paradigm in empirical modelling of machining operations.

Keywords: Manufacturing and Mechanical Engineering; Statistic Methods; Artificial Intelligence Methods; Grinding; Modelling

1. Introduction

Centreless grinding is characterised by its complexity, nonlinearity and sensibility to a large number of input factors that influence system stability and output performance [1]. The most important quality constraints for the set-up of centreless grinding system are workpiece roundness and surface roughness. The latter will often reveal unsuitable wheel topography, incorrect grinding gap set-up or wrong kinematical engagements. The set-up of centreless grinding is still largely based on empirical competence of machine-tool operator. The enhancement of the process efficiency and the reduction of the set-up efforts require model based process simulation, which is a powerful tool for evaluating the performance of complex systems.

Within the framework of modelling, experimental data is transferred into an radial basis function artificial neural network (RBFANN) that enable modelling of highly-uncertain, nonlinear data and that can be therefore used to represent the real centreless grinding system [2-3]. The developed simulation model is subsequently approximated by advanced polynomial regression. Approximation of a simulation model is called a metamodel and is a curve fit over a series of simulated data points. The resulting response surface does not exactly reproduce the observations used

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to build the simulation model. Metamodel can reveal the general characteristics of the more complex simulation model or grinding process itself and identify the statistical significance of the input factors [4].

One of the major metamodelling steps in the framework of response surface methodology (RSM) is the selection of design of experiments (DoE), which determine design points for which the data are to be simulated [5]. DoE has a significant role in developing simulation metamodels. D-optimal DoE has been employed to develop second-order polynomial metamodel.

2. Plunge centreless grinding

Plunge centreless grinding has been widely employed in industries that require large batches of precise, rotationally symmetrical components. It is a complex manufacturing process with a great number of influencing factors that are nonlinear, interdependent, and difficult to quantify. A special process characteristic is the simultaneous support of the workpiece on the grinding wheel, control wheel and workrest blade, shown in Figure 1. Surface roughness, has been investigated according to the following controllable centreless grinding system factors:

- Geometrical grinding gap set-up factor: the workpiece centre height, h,
- Grinding wheel dressing factor: the longitudinal dressing feed-rate, f_d,
- Kinematical factor: the regulating wheel speed, n_r,
- Kinematical factor: the in-feed speed, v_{fa}.

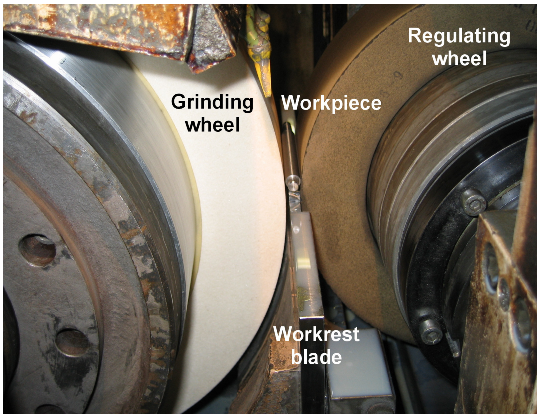

Fig. 1. Plunge centreless grinding gap

3. Grinding process modelling

The input-output approach to grinding process modelling is dealing with the identification of a transfer function denoted by $f(\cdot)$ that represents the relation between the outputs $\boldsymbol{Y}$ and the controllable inputs $\boldsymbol{X}$, considering process fluctuations $\boldsymbol{V}$ causing errors:

$$\boldsymbol{Y} = f(\boldsymbol{\theta}, \boldsymbol{X}) + \boldsymbol{V} \tag{1}$$

Transfer function $f(\cdot)$ with unknown structure and coefficients $\boldsymbol{\theta}$ can be modelled via $g(\cdot)$:

$$\hat{\boldsymbol{Y}} = g(\hat{\boldsymbol{\theta}}, \boldsymbol{X}) \tag{2}$$

where $\hat{\boldsymbol{Y}}$ represents the prediction vector, and $\hat{\boldsymbol{\theta}}$ the estimated model coefficients that minimize a scalar valued loss function $L(\boldsymbol{\theta})$, individually defined for particular modelling approach.

The input-output approach for identification and analysis of complex manufacturing systems originates in the correlation theory for the grinding process [6] and can be transferred to other machining operations [7]. In the context of empirical process modelling, the centreless grinding system is identified in form of ANN, which is able to acquire, store, and utilize experiential knowledge. ANN can effectively explore relationships in the input-output data sets through the iterative presentation of the data and the intrinsic characteristics of neural topologies. Several studies employed ANN for modelling of grinding processes [8]. Let suppose that the individual grinding process output can be modelled by a single-layered RBFANN:

$$\hat{Y}_i = g(\hat{\boldsymbol{\theta}}, \boldsymbol{X}, \boldsymbol{q}_i, \sigma) = \sum_{i=1}^{k} \hat{\theta}_i \exp\left[\frac{-D^2(\boldsymbol{X}, \boldsymbol{q}_i)}{2\sigma^2}\right] \tag{3}$$

where $\hat{Y}_i$ represents the network scalar output, θ_i is the ith weight parameter of RBFANN, $g(\cdot)$ the Gaussian function, which have two adjustable parameters: the centreing vector $\boldsymbol{q}_i$ of each RBF and a constant width parameter σ, analogous to the variance, to adjust the distribution of the Gaussian RBF.

The most widely used method of estimating the centres and widths is to use an unsupervised training technique called the k-nearest neighbour rule. The input space is first clustered. The centres of the clusters give the centres of the RBFs, while the distances between the clusters provide the width of the Gaussians. The determination of the width is nontrivial. Computer algorithms use competitive learning to compute the centres and widths. It sets each width proportional to the distance between the centre and its nearest neighbour [9].

The synaptic weights in turn are obtained through supervised learning. Here the loss function is the normalized sum of mean squared errors:

$$L(\boldsymbol{\theta}) = \frac{1}{2k} \sum_{i=1}^{k} E\left(Y_i - g(\hat{\boldsymbol{\theta}}, \boldsymbol{X}_i)\right)^2 \tag{4}$$

Common method of supervised training for synaptic weights determination is the backpropagation training algorithm. This algorithm which is a stochastic gradient algorithm, that recursively processes one input-output pair $\{X_i, Y_i\}$ at a time or momentum learning, which improves the gradient algorithm in the way that a past weight increment, is used to speed up and stabilize convergence. More detailed characteristics of backpropagation algorithm can be found in [8].

4. Metamodelling and D - Optimality

The fundamental idea of metamodelling relates to the assumption that metamodels can be used to approximate the computer simulation model within experimental region of interest. In this paper, metamodeling deals with the polynomial approximation of the RBFANN simulation. Metamodel is hence a polynomial of the input simulation vector X_n weighted by regression coefficients θ that need to be estimated. By polynomial regression, we mean that for the input simulation vector approximation is performed whose output has the form:

$$\hat{Y}_n = \hat{\theta} X_n \tag{5}$$

The unknown regression coefficients can be estimated by least squares, which loss function is defined as:

$$L(\theta) = \frac{1}{2n} \sum_{j=1}^{n} (Y_j - \theta X_j^{\,T})^2 \tag{6}$$

A solution to the least squares problem of estimating θ is solved by setting the root-finding function $d(\theta) = \partial L(\theta) / \partial(\theta)$ to zero [10]. The solution is straightforward if there are at least as many simulation points as coefficients to be estimated:

$$\hat{\theta} = (X_n^{\,T} X_n)^{-1} X_n^{\,T} Y_n \tag{7}$$

It is further important to introduce the covariance matrix of the least square $\hat{\theta}$ estimator:

$$Cov(\hat{\boldsymbol{\theta}}) = \sigma^2 (\mathbf{X}_n^{\,T} \mathbf{X}_n)^{-1} \tag{8}$$

In DoE $\mathbf{X}_n^{\,T} \mathbf{X}_n$ is called the design matrix. The fundamental problem is to choose n input vectors X_n, such that when RBFANN simulation is run, the corresponding output vector $\hat{Y}_n$ is as informative as possible. Therefore the focus is to choose X_n in some optimal way to enhance the accuracy of the coefficients estimates. In the context of DoE the goal is to select a design ξ such that θ is estimated with as much precision as possible. The precision is quantified by the determinant of the precision matrix, $\det\left[M(\theta,\xi)\right]$, which represents the accuracy of the θ estimate based on the n inputs of X_n. Due to the close connection of the inverse of the covariance matrix to the precision matrix, a goal is to find a ξ^* that minimizes $\det\left[Cov(\hat{\boldsymbol{\theta}})\right]$; a design minimizing this determinant is called D-optimal [10]:

$$\xi^* = \max_{\xi}\left\{\det\left[M(\theta,\xi)\right]\right\} = \min_{\xi}\left\{\det\left[(X_n^{\,T} X_n)^{-1}\right]\right\} \tag{9}$$

The polynomial fitting assessment is based on two standard statistics calculated via analysis of variance (ANOVA). The R^2, coefficient of multiple determination, which estimates the fraction of total variation in the data accounted by the metamodel, and the $R_{adj}^{\,2}$ statistics, adjusted to the number of terms in the metamodel relative to the number of simulation points, which measures the amount of variation about the mean explained by the metamodel. The determination of significant metamodel degree and the determination of significant metamodel factors is based on F-value and P-value, also calculated via ANOVA. P-values smaller than 0.05 imply significance of the metamodel degree and particular, linear, quadratic or interaction term.

5. Experimental details

Grinding experiments were conducted on a Studer Mikrosa, Kronos M, centreless grinding machine-tool. The grinding was conducted under chatter free conditions and to keep the cutting speed (63 m/s), the grinding depth (0.2 mm), the depth of grinding wheel dressing (0.02 mm), the spark out time (0.1 s), and the coolant flow constant.

A vitrified grinding wheel, 22A60L6V63L, with an abrasive blend of monocrystalline and white aluminium oxide was used. Wheel dimensions were 500x88x304.8 mm. Besides, a standard rubber bonded control wheel of 300x103x304.8 mm dimensions was employed.

The workpiece material was 9SMn28, free-cutting unalloyed steel, used for serial production of shafts for electric motors. The test workpieces of 11.15 mm diameter and 116.2 mm length were supported by the specially made workrest blade with the 30° angle.

For the research, the surface roughness was quantified by the most used parameter R_a. It is a measure of arithmetic average of the absolute vertical changes of the roughness profile from the centre line. The measurements were carried out with a stylus type measuring instrument according to an ISO standard, which employs a high pass Gaussian filter, a sampling length of 0.8 mm and evaluation length of 4 mm. Each ground workpiece was measured three times. The surface roughness measurements, summarized in Table 1 and Table 2, represent the average readings of three consecutive measurements.

6. RBFANN model

For RBFANN modelling a Neuro Solutions ANN simulator has been employed. RBFANN has three-layer feed-forward (4-24-1) topography. Here the hidden layer with 24 neurons, cluster centres respectively, performs a fixed nonlinear input-output transformation. The transfer functions of the hidden layer are

Gaussian, which have two adjustable parameters determined by unsupervised learning. The transfer function of the output layer is a hyperbolic tangent. In this research, 29 sets of experiments have been carried out. The region of interest, coded {-1, 1}, is a region determined by factor level setting combinations that are of major interest. This region has been extended to the region of operability, coded {-2, 2}, which is determined by factor level setting combinations that can be operationally achieved with acceptable safety and will output a testable workpiece. Coded factor levels are summarized in Table 1.

Table 1.
Design factor levels

Code	h [mm]	f_d [mm/min]	n_r [rpm]	v_{fa} [μm/s]
-2	10	100	46	10
-1	11.5	200	51	20
-0.5	12.25	250	53.5	25
-0.33	12.5	267	54.3	26.7
0	13	300	56	30
0.33	13.5	333	57.7	33.3
0.5	13.75	350	58.5	35
1	14.5	400	61	40
2	16	500	66	50

The experimental data set has been divided into 24 training sets in Table 2 and 5 test sets in Table 5. The training sets used for process modelling have not been used for testing the generalisat ion capability of trained RBFANN. The training sets include five levels that associate the levels of four considered centreless grinding factors with measured surface roughness.

The number of the training epochs, that is the number of processing runs through the complete training data, is set to 20000 for supervised learning and 100 for unsupervised learning.

The performance of the trained RBFANN has been measured via different criteria of the training sets [9]. The trained RBFANN has yielded a mean square error (MSE) of 0.004, the correlation coefficient of 0.992, Akaike's information criterion (AIC) value of 158.25, and Rissanen's minimum description length (MDL) value of 98.66.

7. D - optimal metamodel

The major two issues in metamodelling include the determination of the degree of polynomial metamodel and the selection of adequate DoE that supports presupposed polynomial fitting. D-optimal design for fitting a quadratic polinomial consists of 35 sets of experiments that distribute the region of interest, coded {-1, 1} on 7 levels, coded {-1, -0.5, -0.33, 0, 0.33, 0.5, 1} and are simulated by trained RBFANN according to the experimental design matrix, shown in Table 3.

Metamodel fitting is computer-aided and uses a special decomposition algorithm on the design matrix, which is used for solving linear algebraic equations and linear least squares. The full metamodel includes some terms that are not statistically significant. Therefore, the next step is the metamodel reduction, which eliminates terms that are not significant in the way in which statistical hierarchy is not violated. A metamodel is hierarchal if the presence of quadratic and interactions terms requires the inclusion of all linear terms contained within those of higher order, even if they do not appear to be significant on their own. The model reduction follows the stepwise regression algorithm, which combines the forward and the backward elimination procedures [11].

Table 2.
RBFANN model training set

Set	h [mm]	f_d [mm/min]	n_r [rpm]	v_{fa} [μm/s]	R_a [μm]
1	13	300	66	30	0.88
2	16	300	56	30	1.12
3	14.5	200	51	40	0.70
4	13	100	56	30	0.35
5	11.5	200	61	40	0.70
6	14.5	400	61	20	1.27
7	11.5	200	51	40	0.69
8	11.5	200	61	20	0.70
9	14.5	200	61	40	0.71
10	11.5	400	51	40	1.32
11	14.5	200	61	20	0.67
12	14.5	400	61	40	1.32
13	13	500	56	30	1.20
14	10	300	56	30	0.60
15	13	300	56	50	1.27
16	14.5	200	51	20	0.73
17	13	300	56	30	1.20
18	11.5	400	61	20	1.26
19	13	300	56	30	1.23
20	13	300	56	10	0.79
21	13	300	46	30	0.84
22	14.5	400	51	40	1.23
23	11.5	400	51	20	1.33
24	13	300	56	30	1.21

The developed D-optimal metamodel has three significant factors, h, f_d, v_{fa}^2 and one hierarchal factor, v_{fa}. The metamodel fitting assessment yields $R^2 = 0.9575$, and the $R_{adj}^2 = 0.9501$. The D-optimal metamodel can be formulated in a form of reduced polynomials in terms of dimensionless coded factors:

$$R_a = 0.9 + 0.028h + 0.3f_d + 0.018v_{fa} + 0.083v_{fa}^2 + 0.025h \cdot v_{fa} \quad (10)$$

Response surface plots give a good overview of the design space, displaying how the surface roughness varies with two selected input factors. Figure 2 and Figure 3 present the three dimensional response surface plots of the surface roughness plotted against the two most influential plunge centreless grinding system factors within the region of interest, while the remaining two off-axis factors were fixed to their central level.

Table 3.
D-optimal DoE

Set	h [mm]	f_d [mm/min]	n_r [rpm]	v_{fa} [μm/s]	R_a [μm]
1	11.5	266.7	61	26.7	0.68
2	11.5	266.7	54.3	20	0.80
3	14.5	200	51	33.3	0.63
4	13.5	200	61	33.3	0.61
5	11.5	333.3	51	33.3	1.02
6	11.5	400	61	40	1.14
7	14.5	333.3	51	20	1.05
8	11.5	400	57.7	26.7	1.19
9	11.5	333.3	54.3	40	1.17
10	14.5	300	51	40	1.01
11	13.5	333.3	61	20	1.05
12	12.5	200	51	40	0.69
13	13.75	250	53.5	25	0.82
14	13	250	58.5	35	0.83
15	14.5	400	61	20	1.26
16	11.5	200	51	20	0.70
17	14.5	200	56	40	0.80
18	14.5	400	61	30	1.28
19	14.5	400	57.7	40	1.32
20	13.5	400	61	40	1.30
21	11.5	400	54.3	33.3	1.21
22	11.5	200	54.3	33.3	0.43
23	11.5	200	61	20	0.69
24	11.5	200	61	40	0.70
25	14.5	200	54.3	20	0.65
26	11.5	400	51	40	1.26
27	14.5	200	61	20	0.67
28	13.5	400	51	40	1.27
29	13.5	400	54.3	20	1.27
30	11.5	400	61	20	1.26
31	13.5	200	51	20	0.67
32	11.5	400	51	20	1.28
33	12.25	350	53.5	25	1.18
34	14.5	400	51	30	1.22
35	14.5	266.7	61	40	1.00

The metamodel assessment is based on ANOVA, summarized in Table 4.

Table 4.
ANOVA for D-optimal metamodel

Source	Sum of Squares	DF	Mean Square	F-value	P-value
Model	2.34	5	0.47	130.58	< 0.0001
h	0.020	1	0.020	5.64	0.0244
f_d	2.27	1	2.27	631.32	< 0.0001
v_{fa}	0.008	1	0.008	2.20	0.1484
v_{fa}^2	0.041	1	0.041	11.44	0.0021
h x v_{fa}	0.011	1	0.011	3.19	0.0845
Residual	0.10	29	0.0035		
Total	2.45	24			

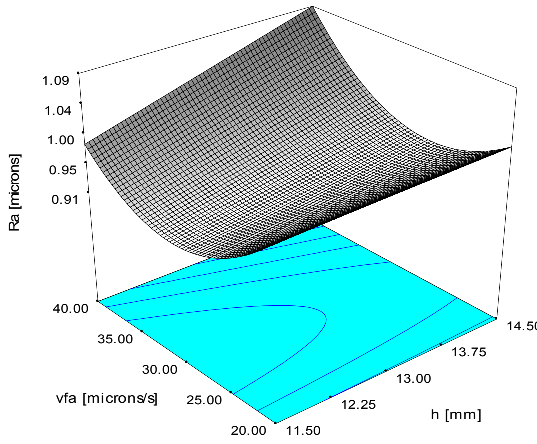

Fig. 2. Metamodel response surface plot h - v_{fa}

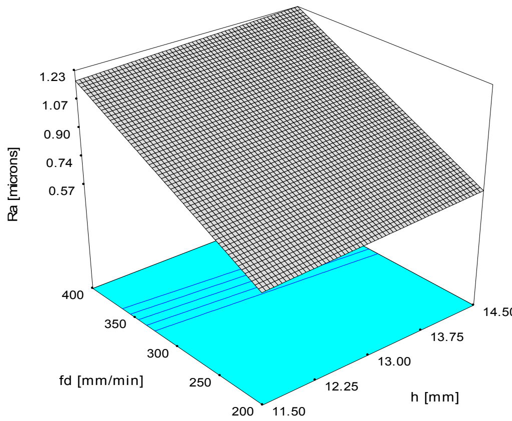

Fig. 3. Metamodel response surface plot h - f_d

In addition to response surface plot it is useful to plot the standard error of design to show how the error in the predicted metamodel response varies over the design space. The plot, shown in Fig. 4, exhibits nonsymmetrical contours, which are characteristic for D-optimal designs.

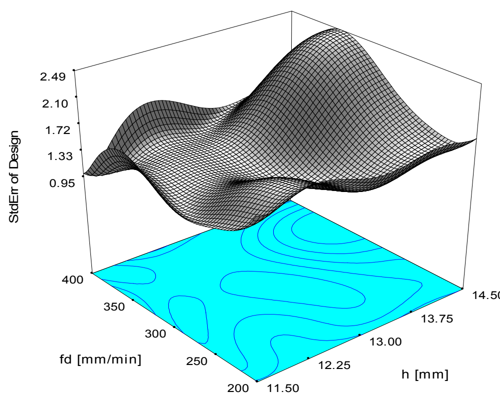

Fig. 4. Standard error of the D-optimal design

8. Modelling and metamodelling performance assessment

The simulation of the RBFANN model and accuracy of D-optimal metamodel are evidented in Table 5, where the simulated values (R_a*) of the RBFANN model and its metamodel (R_a**) are compared to the measurements (R_a).

Table 5.
RBFANN model and D-optimal metamodel testing set

Set	h [mm]	f_d [mm/min]	n_r [rpm]	v_{fa} [µm/s]	R_a [µm]	R_a* [µm]	R_a** [µm]
1	14.5	400	51	20	1.34	1.27	1,24
2	11.5	400	61	40	1.27	1.14	1,10
3	13	300	56	30	1.23	1.21	0,97
4	11.5	200	51	20	0.77	0.70	0,66
5	13	300	56	30	1.22	1.21	0,97

The difference between the measured and simulated surface roughness is illustrated in Figure 5.

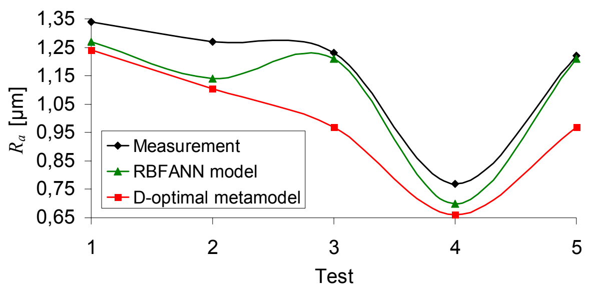

Fig. 5. Modelling and metamodelling efficiency

The relative performance assessment of modelling and metamodelling is quantified with two different criteria related to the testing set in Table 2. The first is the mean squared error of prediction:

$$MSEP = 1/m \sum_{l=1}^{m} (Y_l - \hat{Y}_l)^2 \quad (11)$$

and the second is the mean absolute percentage deviation:

$$MAPD = 1/m \sum_{l=1}^{m} \left| (\hat{Y}_l - Y_l)/Y_l \right| \quad (12)$$

The relative performance assessment of developed model and its metamodel is quoted in Table 6.

Table 6.
Relative performance assessment

Model / metamodel	MSEP	MAPD [%]
RBFANN model	0,00544	5,399
D-optimal metamodel	0,03601	15,297

9. Conclusions

The objectives of this study refer to development of surface roughness computer simulation model and its polynomial metamodel, for the plunge centreless grinding process.

When dealing with complex systems, simulation is a good alternative for process performance evaluation and subsequent optimisation [12]. Usually, RSM is applied to a real process, such as grinding, milling, forming. However, RSM can also be applied to computer simulation model of a real system in which RSM is used to develop a model of the system being modelled by the computer simulation, i.e. metamodel. In this way, computer simulation model represents an abstraction of real centreless grinding system in terms of its components, factors and relationships. To obtain an acceptable understanding of a simulated system, experiments must be performed on their elements through adequate simulation runs. However, as abstractions of the real process, all simulations have limits of credibility. Therefore there is no shortcut to having sufficiently deep understanding of the real system and its relationship to the simulation. With the limitations in mind, the methods in this paper are powerful tools of required process improvement as stressed in the paper introduction.

Because of the nonlinear nature of the grinding processes use of ANN has been attempted. The experimental data, Table 2, have been utilized to train the RBFANN, which proved adequate predictive simulation capability, as shown in Figure 3. The determination of the RBFANN training epochs and rates is largely dependent on modeller competence. Therefore, it is hard to find adequate ANN training parameters and to ensure the quality of the model and overfitting. In practice the fact remains, however, that ANN modelling still requires expertise and know-how. Further it is useful to stress that ANN is only a complement to the classical statistical tools of regression analysis, RSM, and DoE advocated in [13-14], but not a complete replacement for them, because ANN can only give a prediction model and not fundamental insight into the process. Besides RBFANNs, feedforward backpropagation ANNs are also universal function approximators that are widely employed in modelling of machining operations.

The developed metamodel is a polynomial approximation of the input-output transformation that is implied by the simulation RBFANN model. Metamodels can be used for better process understanding, prediction, optimisation or the validation of simulation model. Metamodelling consists of two phases: DoE, in which a set of experiments in the design space is selected, and polynomial fitting, in which the simulated values from the DoE are evaluated and used to build a reasonably accurate approximation for a response surface.

The importance of using optimum design of experiments when selecting the simulation input vector has been highlighted. In this way the D-optimality criterion has been used to improve the estimates of unknown metamodel coefficients and to enhance the metamodel robustness via minimisation of the determinant of the covariance matrix.

All experimental data obtained from previous studies, have been used to compare the models/metamodels based on the relative prediction accuracy and their ability to interpolate and extrapolate. The predictive ability of D-optimal metamodel is comparable to the accuracy of response surface regression model, while RBFANN model surpasses it [14].

On the basis of metamodel ANOVA, it has been found out that the grinding wheel dressing condition most significantly affects the ground surface roughness, which is additionally affected by the geometrical grinding gap set-up factor and the in-feed speed. Factor interaction effects proved to be insignificant.

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