Optimization by Estimation of Distribution Algorithms in the Machining of Titanium (Ti 6Al 4V) Alloy using Predicting Surface Roughness using Neural Network Modeling

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1 Introduction

Though the initial applications of titanium alloys have been in aerospace industries such as aero-engine and airframe manufacturing, there is a growing trend in their application in the industrial sector, including petroleum refining, chemical and food processing, surgical implantation, nuclear waste storage, and other automotive and marine applications. One of the more popular titanium alloys for these applications is Ti–6Al–4V, which comprises about 45–60% of the total titanium products in practical use [Mantle et al., 1998; Ezugwu et al., 1997]. Despite the increased usage and production of titanium and its alloys, these materials fall under the category of materials those are the most difficult to machine materials. In the machining of parts, surface quality is one of the most specified customer requirements. A major indication of surface quality on machined parts is surface roughness. Surface roughness is the result of process parameters such as tool geometry and cutting conditions (feed rate, cutting speed, depth of cut, and others). The quality and the integrity of the finish-machined surfaces are affected by the workpiece material hardness and other properties. In quantifying surface roughness, the average surface roughness definition, which is often represented by the Ra symbol, is commonly used. Theoretically, Ra is the arithmetic average value of the departure of the profile from the mean line throughout the sampling length [Sander, 1991]. Ra is also an important factor in controlling machining performance.

Neural networks have been used in many engineering problems as a data analysis tool to map non-linear relationships between process inputs and outputs. Dimla et al. [1997] reported that neural networks could be employed in machining process modeling by using experimental data. Ö zel et al. [2005] used advanced neural network designing techniques to predict the tool life. This technology has become an important computing tool for solving engineering problems [Pawadea et al., 2007; Russell et al., 2003]. It has also led to increased research on a wide variety of industrial applications, such as product manufacturability control, process planning, and others. New research and developments are appearing in the state of the art use of intelligent systems to control and optimize machining, giving support to predictions of and improvements on the surface roughness of different materials [He et al., 2001].

1.1 Literature Review

Ocktem et al. [2006] developed a model for determining the best parameters for optimum roughness in the milling of the faces of a mold to produce a piece by means of biomechanical application (Ortez) using neural networks and genetic algorithms. As an example Che-Haron et al. [2005] worked on an investigation that determined the impact machining of Ti64 on surface finish, checked alterations obtained in machining, and analyzed material characterizations in the material piece and diverse types of tooling used in the study. Ramesh et al. [2007], in their article “Modeling for Prediction of Surface Roughness in Machining of Ti64 Alloy Using Response Surface Methodology”, proposed a prediction model in which he included parameters such as progress, speed, and depth of cut to determine their effects in turning the titanium and achieving the surface quality parameter response.

Kopac et al. [2002] used an experimental Taguchi design to determine the optimal machining parameters for the best surface finish in traditional turning. The design of the Taguchi method was used to identify the impact of various parameters and investigate how using these parameters in combination of them helps to control the variation. They found that the roughness increased with increasing cutting speed. Krain et al. [2007] evaluated the effects of changes in the feed rate and the thickness of the chip by changing the radius of the cutting tool, as well as the material and geometry of this phenomenon, and its impact on the life and wear of the tool in the milling of Inconel 718.They showed that no single material or geometry could give the best results. Rico et al. [2005] used the Surface Response methodology and neural networks to predict roughness in machined steel. The authors developed a model for predicting the temperature and roughness of the cutting tool for machining steel 1018. Pawadea et al. [2007] showed in their article “Effect of Machining and Cutting-edge Geometry Parameters on Surface Integrity of High-speed Turned Inconel 718” that high-speed cutting and a low feed rate, as well as a moderate depth of cutting through the use of delicate angles of cut can ensure the generation of residual compression efforts when machining. Molinari et al. [2002] were devoted to comprehensive studies of chips produced during the milling of Ti-6Al-4V, analyzing the process of orthogonal cutting produced at different speeds, and the transformation of adiabatic shear banding. They found that, at lower speeds, the chips became rougher; this way likely due to thermomechanical limitations, which generate adiabatic shear banding and behave differently at high speeds.

It appears that a considerable amount of work has been done in the optimization of machining parameters, based on different criteria such as tool wear, vibration, surface roughness, unit cost, etc. [Pawadea et al., 2007; Krain et al., 2007; Kopac et al., 2002]. Currently, artificial intelligence (AI) based on modeling has emerged as a new trend in modeling for machining operations [Morales et al., 2007]. The use of heuristic methods to predict models of surface roughness is very limited, thus emphasis is laid on the development of a surface roughness prediction model. In this paper, a new technique, Estimation of Distribution Algorithms, is proposed and implemented to efficiently and robustly optimize multiple machining parameters simultaneously for the case of milling titanium.

1.2 Artificial Neural Networks (ANNs)

Neural networks are computational paradigms that simulate some of the human brain properties, including rational capacities such as association, recognition of shapes and even behavioral patterns. Prediction is an important property of neural networks. Neural networks are non-linear mapping systems that consist of simple processors, called neurons, linked by weighted connections. Each neuron has inputs and generates an output resulting from stored information and the processes in the hidden layers. The output signal of a neuron is fed to other neurons as input signals via interconnections. Since the capability of a single neuron is limited, complex functions can be formed by connecting many neurons. It is widely reported that in the structure of a neural network, as shown in Figure. 1, the representation of data, normalization of inputs/outputs, and appropriate selection of activation functions have strong influence on the effectiveness and performance of the trained neural network [He et al., 2001; Egiazaryan, 2007]. Some merits of ANN applications are high accuracy and adaptability, historical data management, and noise suppression.

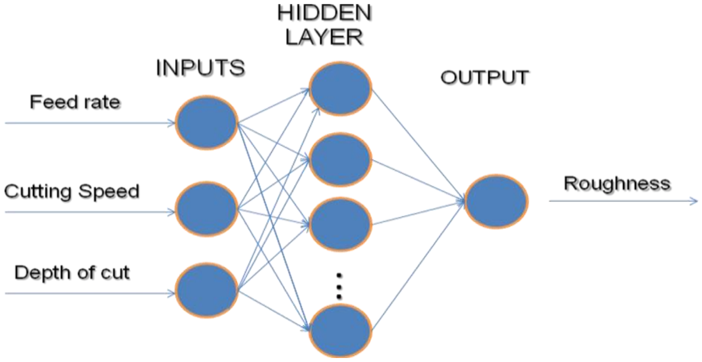

Figure 1: Typical multi-layered feed-forward ANN.

There are several neural networks [Morales et al., 2007; He et al., 2001; Pawadea et al., 2007; Krain et al., 2007]. This research shows that a perceptron with a backpropagation learning rule is the network most used to predict parameters. To develop this research, a multilayer perceptron with backpropagation learning rule was used. The Backpropagation Neural Network (BPNN) consists of three layers of neurons: input layer, hidden layer, and output layer (Figure 1). The input layer receives external information such as the adjustable process parameters (see in Table 1). The output layer transmits the data and thus corresponds to various individual outputs. In this study, there was only one neuron in the output layer. The BPNN also incorporates hidden layers of neurons that do not interact with the outside world, but assist in performing nonlinear feature extraction on the data provided by the input and output layers. Here, the number of the hidden layers was obtaining by experimental design [Byungwhan et al., 2005]. Backpropagation (BP) is based on searching a surface for errors (error as a function of ANN weights) using gradient descent for points with minimum error. Each BP interaction comprises two sweeps: forward activation to produce a solution and backward propagation of the computed error to modify the weights. This starts at the input layer, where each input node transmits the value received forward to each hidden node in the hidden layer. The collective effect on each of the hidden nodes is summed up by performing the dot product of all the values of the input nodes and their corresponding interconnection weights.

Once the net effect at one hidden node is determined, the activation at that node is calculated using a transfer function (e.g., sigmoidal function) to yield an output between 0 and +1. The amount of activation obtained represents the new signal to be transferred forward to the subsequent layer. The same procedure of calculating the net effect is repeated for each hidden node and for all hidden layers. The net effects calculated at the output nodes are consequently transformed into activations using a transfer function. The activations are only calculated at the output node [Basheer et al., 2000].

The weights represent the synapse and determine the performance of the neural network. The learning rule is used to update these weights. Several learning rules can be considered; however, the backpropagation learning rule with momentum is commonly used [Haykin, 1999; Freeman et al., 1991]. The following equations illustrate the implementation of the backpropagation learning rule considering only a multilayer Perceptron with I inputs, M neurons in the inner layer, and one output Y_N. The activation function used is a sigmoidal one (Equation 1):

$$f_a(x) = 1/(1+\exp(x))^{-x} \ . \tag{1}$$

Two operations are defined: the activation and the training of the neural network. The objective is the adjustment of the weights of every layer (matrices W_M and W_o) to minimize the error between the desired response (represented in vector Y_D) and the response of the neural neuron (Y_N) considering the same input vector (X). The first step of the activating the inner neurons that it is made using Equations 2 and 3:

$$N_M(m) = \sum_{i=1}^{I} W_M(m,i) \cdot X(i) \, , \tag{2}$$

$$R_M(m) = f_a(N_M(m)) \, . \tag{3}$$

There is only one output Y_N so the activation of a single neuron is required (Equations 4 and 5):

$$N_O(m) = \sum_{m=1}^{M} W_O(m) \cdot R_M(m) \, , \tag{4}$$

$$\mathbf{Y_M} = \boldsymbol{fa(N_O)} . \tag{5}$$

The training of the neural network is made by adjusting the inner (W_M) and output weights (W_O). First, the error between the desired output Y_D and the output of the neural network Y_N is calculated (Equation 6). The adjustment of the weight is made using Equation 7. The calculation of the momentum requires the values of the weights before the adjustment, and this calculation is made using Equation 8.

$$\partial_O = (Y_{Dp} - Y_{Np}) f_a^{'}(N_O) \, , \tag{6}$$

$$W_O(m) \leftarrow W_O(m) + \eta \partial_O N_M(m) + \alpha W_{OA}(m) \, , \tag{7}$$

$$W_{OA}(m) = \eta \partial_O N_M(m) \, , \tag{8}$$

The internal weights require an error signal that can be calculated using Equation 9. This calculation requires a derivative of the activation function (Equation 10). The inner weights are actualized using Equation 11 and the weights before the adjustment is required can be determined using equation 12.

$$\partial_m(m) = f_a^{'}(N_m(m)) \cdot \partial_O \cdot W_O(m) \, , \tag{9}$$

$$f_a^{'}(x) = f_a(x)(1 - f_a(x)) \, , \tag{10}$$

$$W_M(m,i) \leftarrow W_M(m,i) + \partial_m X(i) + \alpha W_{MA}(m,i) \, , \tag{11}$$

$$W_{MA}(m) = \eta \partial_m (m) X(i) \,. \tag{12}$$

The learning parameter η and the momentum parameter α must be adjusted by experience or using an experimental design. A pair of patterns (X_P, Y_{NP}) is considered, where Y_{NP} is the output of the neural network generated by the input pattern X_P and the desired output pattern is Y_{Dp}. Following Equations 6 to 12 per a pair of patterns p, all the weights are adjusted until an error measurement is minimized (Equation 13).

$$EG = (1/2)\sqrt{(\sum_{p=1}^{N_P}(Y_{Dp} - Y_{Np})^2)} \,. \tag{13}$$

1.3 Estimation of Distribution Algorithms (EDA).

The evolutionary estimation of normal distribution function parameters (Evonorm) [Torres-Treviño, 2006], is an easy implementation of an estimation of distribution algorithms (EDAs) [Larranaga, 2002] where the crossover and mutation operators are substituted by an estimation of a distribution function to represent a population of fittest solutions (Table 1). The number of selected individuals to generate a new population (PS) is lower than the number of individuals of the original population (P). A global fitness MFE is determined by considering the sum of the normalized values of the evaluation functions. A mean (MN) and a standard deviation (SD) are calculated per parameter considering the selected population. The population is assumed to have many independent variables, so an estimation of the mean and standard deviation is made per variable. A new population is generated using a normal random generator considering the mean and standard deviation calculated per decision variable. Considering a probability of 50%, the calculated mean (MN) is used. The other 50% used is the best solution found.

```
1) Create basic population P
2) Evaluation(P) -> (MFE,Ix)
3) Selection(P,MFE) -> PS
4) Calculation(PS) ->  (MN,SD)
5) Generation(MN,SD,Ix) -> P
6) if end condition not satisfied go to step (2)
```

Table 1: Evonorm algorithm for global optimization.

The calculation and the generation procedures require detailed explanation. The population of selected individuals is considered from a sample of a population used to determine the parameters of normal distribution functions. The mean and the standard deviation of the sample are calculated from the sample for every decision variable. The generation procedure creates a new population using the mean and the standard deviation recalculated per decision variable. Table 2 shows the algorithm in pseudo-code for generating a population. It is appropiate to use a set of calculated parameters for normal distribution functions in every decision variable. The vectors MN and SD store the mean and standard deviation, respectively, calculated in a previous procedure from the selected population. The size of the vector is equal to the number of decision variables. The constant NTI indicates the number of individuals to be evaluated and NTIS indicates the number of individuals to be selected; usually, NTIS < NTS. The number of decision variables is represented in NTPr. The population is represented by a matrix P with NTI rows and NTPr columns that represent the decision variables. The individuals selected are represented in the matrix PS. Two distribution functions are used. The first one is a uniform distribution function represented by u.

This function generates random numbers between 0 and 1. The second distribution function is a normal one N(μ, σ). This function uses two parameters, a mean ($\mu = MN_{pr}$) and a standard deviation ($\mu = SD_{pr}$).

```
for k=1, NTI
   for pr=1,NTPr
      if u > 0.5 then
         P(k, pr) = N(MN(pr), SD(pr))
      else
         P(k, pr) = N(Ix(pr), SD(pr))
      end of condition
   end of cycle
end of cycle
```

Table 2: Generation of a new population

1.4 Surface Roughness

In everyday life, as well as in the industry, the degree of roughness of a surface is very crucial. Sometimes, it is necessary to have very high values of roughness; at other times, it is undesirable because the surface of the product may require a better appearance or the lowest surface friction possible as it is in contact with another surface. Smoother surfaces minimize wear on materials. Surface roughness is the set of irregularities on the actual surface, conventionally defined within a section where the shape and undulation errors have been eliminated [González et al., 2006]. To measure the roughness of parts, an electronic instrument sensitivity micrometer, called a roughness meter, is used to quickly determine the roughness of surfaces. There are several parameters that reflect the measurement of roughness, such as Ra, Ry, and Rz. The most common one is Ra, computed from the arithmetic mean [González et al., 2006] of the absolute values of the distance profile roughness of the line of the length measurement see Figure 2 and Equation (14).

$$Ra = \frac{1}{N}\sum_{i=0}^{N}|Data| \tag{14}$$

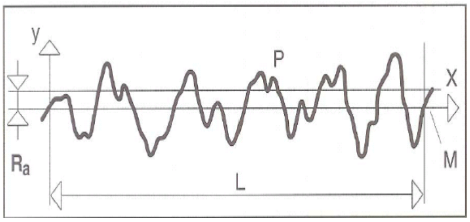

Figure 2: Graphic Ra for measuring roughness

2 Development

2.1 Experimental design and statistical analysis

We first determined the parameters to be taken into account for the cut, including the ranges for the depth of machining, the feed rate, and speed, which would be the input of statistical analysis. The machining was done on a Vertical Machining Center Bridgeport VMC 760(Figure 3) using rectangular pieces of titanium (Ti 6Al-4V) sized 125 x 47 x 22 mm. The tool used was an endmill coated with Aluminum Titanium Nitride (AlTiN) with 4 cutting edges and a 3/8" diameter (Figure 4). The milling was carried out over a length of 47 mm, using an experimental design with 3 factors and 3 levels (see Table 3), giving a total of 27 experiments with 3 runs. To determine roughness, measurements were made using a ZEISS Profilometers Surfcom 1500 SD2 with automatic controls, shown in Figure 5.

Condition	**Units**	**Level 1**	**Level 2**	**Level 3**
Speed	**m/min**	70	80	90
Feed	**mm/rev**	0.11	0.13	0.15
Depth	**mm**	0.50	1.00	1.50

Table 3. Machining parameters used for the test

Figure 3: Vertical Machining Center Bridgeport VMC 760.

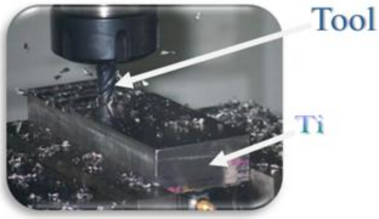

Figure 4: The material and the tool used in the test.

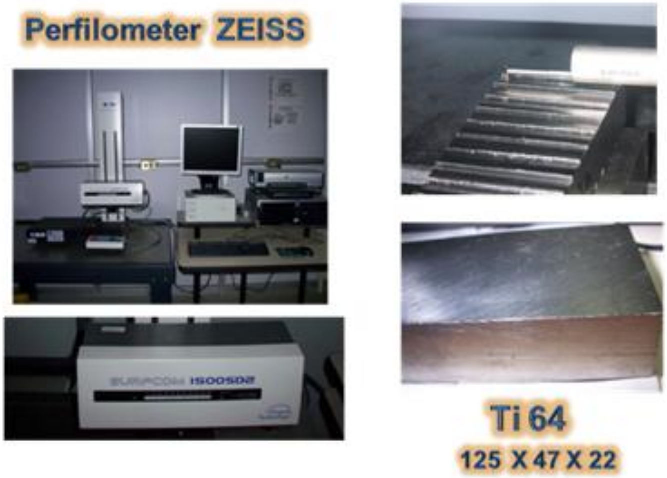

Figure 5: Profilometer Surfcom 1500SD2.

In the past, some methods have been used to check the impact of machining parameters on the surface finish quality. Though the processes previous researchers utilized are similar, they all differ slightly in their implementation. All of the relevant literature includes some kind of experimental design that allows for an organized approach to quantifying the effects of a finite number of parameters. Some experiments were full-factorial designs with a small number of factors, while others were fractional factorial designs meant to screen factors for impact. In this test, we used a three-factor full factorial design to determine the effects of speed, feed, and depth of cut on surface roughness in finish milling. Three replicates for each factor level combination were performed in order to account for variability in the process. Table 4 shows values of roughness of the 27 combinations of parameters obtained in the tests, which were used to create the regression model that represents the machine under study. The main purpose of this study is to determine the best parameters for the machining of titanium alloy 6AL-4V, considering the optimization of roughness at the time of the machining of this material.

Test	Design of experiment			Replies		
	Speed	Feed	Depth	1 Roughness	2 Roughness	3 Roughness
1	1	1	1	0.8669	0.8472	0.8794
2	1	1	2	0.8442	0.8586	0.8644
3	1	1	3	0.9383	0.8520	0.9043
4	1	2	1	0.8188	0.8796	0.8265
5	1	2	2	0.9369	0.8541	0.8512

Table 4: A sample of the results obtained in the test

After completing the experiments, we conducted an analysis of variance (ANOVA) to determine the differences in surface quality between various runs using Minitab® . In addition to degrees of freedom (DF), mean square (MS), and F-ratio, p-values associated with each factor level and interactions are presented. In Table 5 along with the crucial observed p-values. For surface roughness generation, most of the factors are apparently significant; only the p-value for feed and the interaction of feed and depth are statistically insignificant.

Source	DF	MS	F	P-value
Speed	2	0.1547	266.390	0.000
Feed	2	0.0014	2.330	0.107
Depth	2	0.0021	3.570	0.035
Speed*Feed	4	0.0022	3.730	0.009
Speed*Depth	4	0.00|	4.120	0.006
Feed*Depth	4	0.0013	2.280	0.073
Speed*Feed*Depth	8	0.0026	4.410	0.000
Error	54	0.0006		
Total	80			

Table 5: ANOVA table for Ra surface roughness.

The regression analysis technique using least squares estimation was applied to obtain the coefficients of the exponential model by using the experimental data to generate the next models. The regression model considered only the variables without interaction between them. Table 6 shows the model generated parameters. Upon further analysis, we found that the VIF values were good but the R-Sq (adj) had a low value. This means that the model fit is not satisfactory.

Predictor	Coef	SE Coef	T	P	VIF
Constant	1.35323	0.06219	21.76	0.000	
Speed	-0.00021	0.00002	-11.43	0.000	1
Feed	0.06490	0.29540	0.22	0.827	1
Depth	0.00260	0.01182	0.22	0.826	1
S = 0.0434111		R-Sq = 62.9%		R-Sq(adj) = 61.5%	

Table 6. Results of the regression model analyzing the roughness versus speed, feed, and depth

The next step was to analyze the model using the interaction between the factors and generate the multiple lineal regression model suggested. As shown in Table 7, for parameters obtained with the model, the R-Sq(adj) improved but the VIF values are very problematic. This means that the fit of the real data is inefficient.

Predictor	Coef	SE Coef	T	P	VIF
Constant	-1.2021000	0.85390000	-1.41	0.164	
Speed	0.0024358	0.00043470	5.60	0.000	1217.80
Feed	-15.2420000	6.82800000	-2.23	0.029	1185.10
Depth	-1.0003000	0.62900000	-1.59	0.116	6284.30
Speed * Speed	-0.0000006	0.00000007	-8.61	0.000	768.20
Speed * Feed	0.0031960	0.00201800	1.58	0.118	1121.70
Speed * Depth	0.0004754	0.00024480	1.94	0.056	6622.50
Feed * Feed	30.1600000	17.18000000	1.76	0.083	508.00
Feed * Depth	10.4300000	4.78200000	2.18	0.033	6817.50
Depth * Depth	-0.0600300	0.02748000	-2.18	0.032	49.00
Speed*Feed* Depth	-0.0043600	0.00186800	-2.33	0.022	7197.80
S = 0.0291520	R-Sq = 84.8%			R-Sq(adj) = 82.6%	

Table 7. Results of regression model analyzing roughness versus all interactions of the factors

Using the real data in the generated models, the first model shows a good fit; however, the second model that uses interactions shows poor performance. Thus, it is necessary to use another kind of modeling. The Neural Network is proposed.

2.2 Neural Network Backpropagation

To build the network, it is important to identify the following parameters: (1) The set of training patterns, input, and target; (2) A value for the learning rate; (3) A criterion that terminates the algorithm; (4) A methodology to update weights; (5) The nonlinearity function; (6) Initial weight values; and (7) Learning moments. To develop this research, a multilayer perceptron with a backpropagation learning rule was used. Some of variables used were the following: Tinp = Neurons of the input layer and bias; Tmid = Neurons of the hidden layer; Tout = Neurons of the output layer; eta = Constant learning; and alpha = Moment. The parameter values were obtained via an experimental design. Table 8 shows the best results obtained in the tests used to train the network.

Tinp	Tmid	Tout	eta	alpha	Ntepochs	error4
3+1	25	1	0.900	0.550	10000	0.009

Table 8. Results with the best values for the variables used in the Neural Network.

The input parameters were speed, feed and depth of cut. The output value was the surface roughness value. After performing different tests to train the network and obtain the best configuration graph, the results between experimental data and training data using the best neural network parameter (Figure 6) show that the network output data is reliable and corresponds closely to the real data.

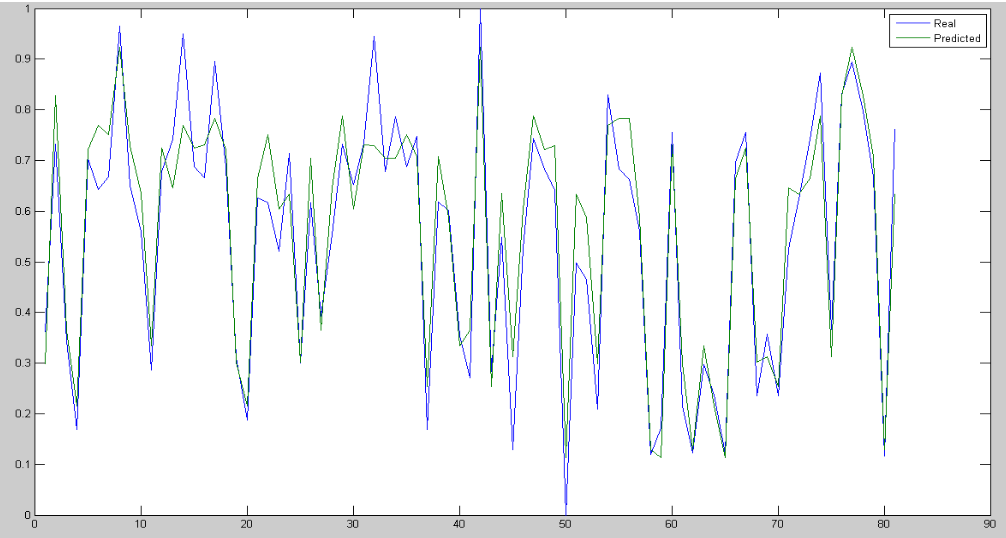

Figure 6. Graph of real values of experimentation versus trained data obtained from Neural Network Backpropagation

3 Discussion and Results

3.1 Parameter optimization using EDA integrated with neural network

In order to search for optimal process parameter sets to satisfy demands, a neural network model of surface roughness was integrated with Estimation of Distribution Algorithms. Figure 7 shows the integrated optimization scheme. In this graph, EDA is initiated by randomly generated particles that are optimum solution candidates within the range of inputs. The Backpropagation Neural Network model predicts surface roughness values for each of the particles. The most crucial part of optimization problems is the definition of objective functions. Predicted roughness is used in the calculation of the objective function that the EDA tries to minimize. In this paper, the objective is to be able to optimize the cutting conditions such as feed, speed, and depth of cut, in order to minimize the surface roughness of machined equipment, thereby satisfying customer requirements and obtaining maximum productivity.

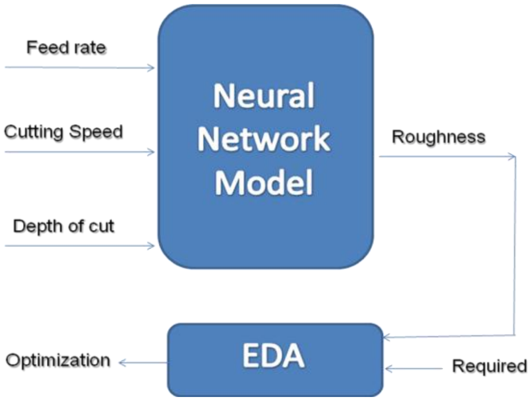

Figure 7. PSO based on Neural Network Optimization Graph.

The ranges of the variables used in the EDA are shown in Table 9. Furthermore Table 10 shows the best machining conditions, assuming that the minimum roughness is to be selected as optimal according to the prediction model of the backpropagation neural network and optimization based on Estimation of Distribution Algorithms.

NTPr	NTI	NTIS	NTGen
3	50	10	100

Table 9. Variable values used in the EDA.

Speed	Feed	Depth	Ra
2865	353	0.5	0.703

Table 10. Near optimal parameters of the machining process.

4 Conclusions and Future Works

This work presented a new approach to optimizing cutting conditions in the titanium machining process, considering speed, feed, and depth cut. Using a neural network as an objective function to define the parameters to optimize (in this case, minimize), an algorithm for EDA was developed and used to robustly and efficiently determine the optimum cutting conditions. The advantage of this method is that once the results obtained are optimized to reduce the roughness, and these values are entered into a machine as parameters. It is important to keep working on techniques to improve these methodologies. Research is currently being done to integrate multi-objective optimization algorithms considering the different variable combinations and constraints involved in the parts being machined. The analysis of different types of materials in different conditions within the process (such as superalloys) is necessary because some types of materials have poor machinability and require expensive processes to machine.

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