

Mechanical Property Prediction of Investment Castings using Artificial Neural Network and Multivariate Regression Analysis

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Abstract

Mechanical properties of castings, such as ultimate tensile strength, yield strength and percentage elongation play an important role in their operational life. This is especially true of investment cast parts which are used with little post-casting operations. Computer-aided prediction of the mechanical properties, instead of destructive testing, can save considerable time and cost, and also provide better insight useful for process parameter optimization. In this work, two computational techniques: Artificial Neural Network (ANN) and Multivariate Regression (MVR) have been investigated to predict the mechanical properties of investment castings. For this purpose, real-life data from an industrial investment casting foundry producing stainless steel parts was obtained. This included 24 parameters (15 process parameters related to wax making, shell making, shell dewaxing and metal pouring; 9 related to chemical composition of alloy) from about 800 heats. Then Principal Component Analysis (PCA) was employed to reduce redundancy in the input data. The reduced data was used as input to ANN and MVR to predict mechanical properties. Three extensively established training algorithms: Back Propagation (BP), Momentum & Adaptive (MA) and Levenberg-Marquardt (LM) were used to train the network using a 75% of the input data, and the remaining data was used to test the networks. The MVR was also employed to predict mechanical properties using the same set of input data. The results of three different networks as well as MVR were compared. It was observed that both ANN and MVR successfully predicted the mechanical properties of investment casting, though MVR was found to be slightly more accurate. The proposed approach is easy to implement and use in industrial foundries, and can significantly improve the quality of investment castings in terms of their mechanical properties.

Keywords: Artificial Neural Network, Investment casting, Mechanical properties, Multivariate Regression, Principal Component Analysis.

1. Introduction

Investment casting is widely used to produce intricate parts with high dimensional accuracy and surface finish, usually in difficult-to-machine alloys, for automotive, aerospace, bio-medical, chemical, defense and other sectors. The process involves the following key steps (Fig. 1):

- *Wax pattern making:* Wax patterns are produced by injecting industrial wax into a die, then cleaned and assembled with gating system to make a tree.
- *Ceramic shell making:* The tree is alternately coated with a slurry (usually a mixture of zircon flour and colloidal silica) of fine and coarse sand particles to obtain a ceramic shell.
- *Ceramic shell dewaxing and preheating:* The shell is dried in a controlled environmental condition and then it is heated to melt out the wax.
- *Melting and pouring:* The casting alloy is melted and poured into the preheated shell. After metal solidification, the shell is broken to obtain the cast part.



Figure 1: Investment casting process

There are more than 200 industrial investment casting foundries in India, mainly producing industrial valves, pumps and machinery (Dave & Tamboli, 2012). Most of these foundries are located in Rajkot, Coimbatore, Belgaum and Kolhapur clusters. The investment castings usually have higher quality conformance criteria (dimensional accuracy, internal soundness and mechanical properties) compared to sand cast parts. There is an increasing emphasis on mechanical properties, including ultimate tensile strength, yield strength and percentage elongation since they affect the service life of cast components. The properties are checked using various destructive testing methods, which are expensive and take considerable time, especially when carried out on all samples of all batches. Hence prediction of the mechanical properties can not only save inspection time, but also enable optimizing the process parameters to achieve the

desired quality. The mechanical properties of investment castings are primarily governed by the chemical composition of the alloy and process parameters related to various process steps mentioned above. These parameters can be recorded and used for prediction of mechanical properties without carrying out destructive tests. The earlier research work in this area is reviewed next followed by our proposed approach.

2. Previous and Related Research Work

Several researchers have explored different techniques for predicting the effect of alloy composition and selected process parameters on mechanical properties, mainly for sand and die casting. The most widely used techniques include computer simulation, artificial neural networks and statistical methods, briefly reviewed here.

Casting simulation essentially involves modelling the physical phenomena such as flow, heat-transfer, solidification of metal/alloy, and phase transformation of castings in terms of governing equations (Ravi, 2010). These governing equations are differential in nature, and require numerical methods to solve and obtain the temporal (time-based) values of metal velocity as well as temperature. These values are used in various metallurgical models to predict the microstructure and mechanical properties of the castings. The accuracy of simulation is governed by the thermo-physical properties of cast metal and mold, as well as interface boundary conditions. These values are temperature dependent and are difficult to acquire for different metal-mold-process combinations. This essentially limits the application of simulation for prediction of properties. The earlier research in the area of predicting mechanical properties in castings using finite element method and finite difference method is summarized in table 1.

A few researchers have explored the application of artificial neural network (ANN) to predict casting properties. ANN is essentially a *data-driven* approach to predict the outputs while casting simulation is a *model-driven* approach (Partheepan, et al., 2011). An ANN consists of several *neurons* and *weights*. The basic function of a *neuron* is to accept signals (values) from an input data, multiply it with an assumed value of *weight*, sum up all weighted inputs values using a *summation function*, and transfer this information to output. The computed output is compared with the actual output to calculate the *network error*. If this error is more than the acceptable limit (user defined), then the weights are iteratively modified. Each iteration of weight modification is called an *epoch* and entire process is referred to as *training* of a network. The values of *weights* for which *network error* is the minimum are stored, and used for prediction during the *testing* of ANN. The training of a network affects its accuracy; thus a larger amount of input data helps in better training and accurate prediction. Different types of training algorithms used by earlier researchers for prediction of mechanical properties in sand castings and die castings are summarized in table 2.

Table 1: Mechanical property prediction using computer simulation

Researcher (Year)	Numerical Method	Alloy	Process	Input parameters	Output	Concluding Remarks
Seifeddine et al. (2006)	FDM	Al	PDC	SDAS, CR	YS, EL	Predicted results shows good agreement with actual results
Guo and Samonds (2007)	FEM	Ti	IC	Volume fraction	YS	Prediction was accurate
Seifeddine (2008)	FDM	Al	SC, GDC HPDC	SDAS, CR	YS, EL	Predicted results are comparable
Seifeddine and Svensson (2010)	FDM	Al	GDC	Iron content	TS	Prediction was accurate
Shabani & Mazahery (2011)	FEM	Al	SC	SDAS, CR	TS, YS, EL	Predicted results were accurate
Zhou et al., (2012)	FDM	CI	SC	CR	H	Cooling rate can be employed
Olofsson and Svensson (2012)	FDM	DI	SC	microstructure	RS	Predicted results show good agreement with actual results
Schneider et al., (2012)	FDM	Al	SC	SDAS, GS	YS	Simulation can be employed for prediction

Note: FDM: finite difference method; FEM: finite element method; Al: Aluminum; Ti: Titanium; CI: Cast iron; DI: Ductile iron; PDC: Pressure die casting; IC: Investment casting; GDC: Gravity die casting; SC: Sand casting; SDAS: Secondary dendrite arm spacing; CR: Cooling rate; GS: Grain Size; YS: Yield strength; EL: Elongation; TS: Tensile strength; H: Hardness; RS: Residual stress

Table 2: Mechanical property prediction using ANN

Researcher (Year)	Training algorithm	Alloy	Process	Input parameters	Output	Concluding Remarks
Calcaterra et al. (2000)	SLP and MLP	DI	SC	Process parameters (cooling rate & inoculation temperature), Chemical composition (% C, %Si, %Mn, %S, %P, %Cu, %Sn, %Ni, %Mo, %Mg & %Cr)	TS	MLP with one layer gives best results
Perzyk and Kochanski (2001)	BP	DI	SC	Process parameters (spheroidisation & pouring temperature), Chemical Composition (%Al, %Ti & %Sn)	TS,YS, EL	ANN shows good results
Dobrzanski et al. (2008)	KM	Al	GDC	Process parameter (cooling rate), Chemical Composition (%Si, %Cu, %Fe, %Mg and %Mn)	H, MH,YS,EL	ANN can accurately predict
Dobrzanski and Krol (2010)	BP	Al	GDC	Process parameter (cooling rate), Chemical Composition (%Al, %Zn, %Mn, %Si, %Cu, %Fe and %Mg)	H,SC,GS	ANN is showing accurate results
Emadi and Mahfoud (2011)	--	Al	SC, GDC	Process parameters (Aging temperature), Chemical Composition (%Si, %Na, %Sn & %Sb)	TS,YS	ANN is better than Multiple Regression
Krupinski and Tanski (2012)	BP	Mg	GDC	Chemical Composition (%Al, %Zn, %Mn, %Zr)	H,TS	ANN can be employed

Note: SLP: Single layer perceptron; MLP: multilayer perceptron; BP: Back propagation; KM: K mean; DI: Ductile iron; Al: Aluminum; Mg: Magnesium; SC: Sand casting; GDC: Gravity die casting; TS: Tensile strength; YS: Yield strength; EL: Elongation; H: Hardness; MH: Micro hardness; GS: Grain Size;

In the last few years, statistical techniques have been used for building empirical models correlate process parameters and mechanical properties. The relationship is established using the *least square method* that is used to fit a line through a number of observations. The relevant techniques include *linear regression*, *multiple regression* and *curve fitting*, which are very useful when input data is readily available. The regression analysis is however, unsuitable when the dataset consists of a large number of inputs and output parameters or when the relationships between inputs and outputs are non-linear. The previous research for prediction of mechanical properties of castings using empirical models through curve fitting and regression is summarized in table 3.

A more recent technique called Multi-Variate Regression (MVR), has drawn the interest of researchers due to its ability to establish relationships between multiple inputs and outputs. Noori et al. (2009, 2010) applied MVR to predict solid waste generation and river flow. Riad et al. (2011) predicted the initial setting time of concrete mixer using MVR. This technique however, does not appear to have been explored for metal casting property prediction, so far.

Table 3: Mechanical property prediction using statistical techniques

Researcher (Year)	Statistical technique	Alloy	Process	Input	Output	Concluding Remarks
Morinaga et al. (1998)	LR	Al	PDC	Orbital energy	TS, YS	Very easy to model
Goulart et al. (2006)	CF	Al	GDC	SDAS, Tip growth rate, Heat transfer coefficient, solidification time	TS, YS	SDAS is most significant parameter
Collini et al. (2008)	WR	CI	SC	Grain lamellas Size, Eutectic cell size, Inoculate content	TS, FS	Graphite content is most significant variable
Costa et al. (2010)	MR	DI	SC	Graphite nodules' size, shape and microstructure	FS	Predicted with good accuracy
Pucher et al. (2011)	MR	Al	GDC	%Si, %Cu, %Mg, %Mn	TS	Can be employed to predict
Shabani and Mazahery (2011)	CF	Al	SC	SDAS	TS, YS, EL	excellent match with actual results
Shinde et al. (2012)	MR	DI	SC	Copper addition, Thickness of casting	TS, YS, H	Copper content is important parameter
Dong et al. (2012)	CF	Al	GDC	SDAS, Cooling rate	TS, YS, H	Analytical correlation can be used

Note: LR: Linear regression; CF: Curve fitting; WR: Weibull regression; MR: Multiple regression; Al: Aluminum; CI: Cast iron; DI: Ductile iron; PDC: Pressure die casting; GDC: Gravity die casting; SC: Sand casting; TS: Tensile strength; YS: Yield strength; FS: Fatigue strength; EL: Elongation; H: Hardness

Both ANN and MVR require large input data to develop the mathematical models for prediction. At the same time, the data should be free from redundancy to get reasonably accurate prediction. In this context, Principal Component Analysis (PCA) can be used for redundancy reduction without loss of information (Fodor, 2002). The applications of PCA in various domains have been reported in various technical literatures. Lorenz (1989) introduced the usefulness of PCA in production engineering for selection of the most suitable tap tool to cut thread on a nut. Mehrjoo & Bashiri, (2013) developed PCA based decision support system to plan the production in an

automotive industry. Ransing, et al. (2013) developed PCA based mathematical model to identify noise free correlations amongst data in metal casting domain. However, the application of PCA has not been explored for investment castings so far.

This work attempts automatic prediction of mechanical properties using foundry shop floor data, using Artificial Neural Network and Multi-Variate Regression; Principal Component Analysis is employed to reduce the redundancy in input data. The relevant mathematical models are described next, followed by industrial data collection and mechanical property prediction. Finally, these models are compared in terms of their accuracy of prediction.

3. Mathematical Model Development

The proposed methodology is shown in figure 2. The data related to process parameters and chemical composition of alloy was collected and the redundancy of input data was reduced by PCA. After that, ANN and MVR models were used to predict mechanical properties. The modeling of ANN included selection of controlling parameters for network while modeling of MVR is about the computation of the coefficients for the empirical model. The PCA as well as modelling of ANN and MVR are described here.

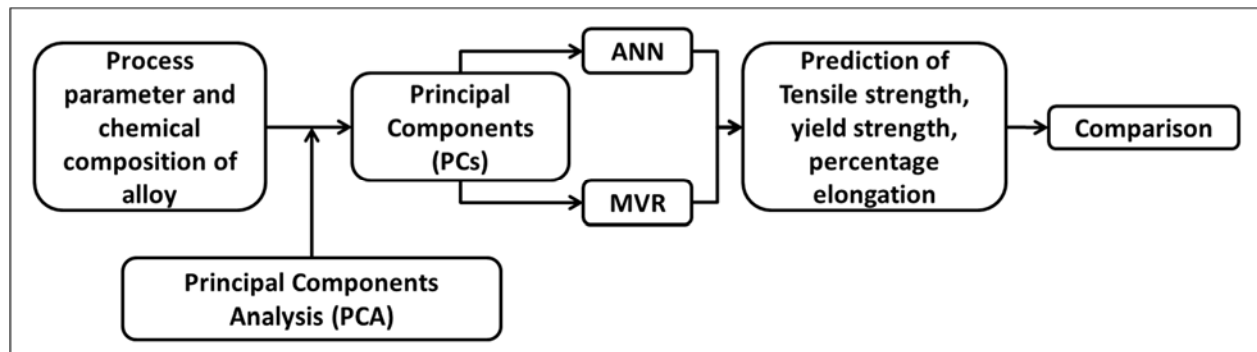


Figure 2: Methodology for prediction of mechanical properties in investment castings

3.1 Principal Component Analysis

Principal Component Analysis (PCA) reduces the redundancy in input data by determining the Principal Components (PCs) from a given data set and then appropriate PCs are chosen for further analysis. These PCs are selected in such a way that the useful information remains nearly unchanged. In general, the input data can be represented by a matrix (X), given by:

$$X = n \times q \dots\dots\dots \text{Eq.(1)}$$

where, n = observations = 1580, q = input variables = 24, giving $X = 1580 \times 24$ in this work.

The matrix X can be pre-processed in two ways to derive the PCs: *covariance matrix* (each element of X is divided by the square root of each observation of n), and *correlation matrix* (each variable is divided by its *norm*, that is, the square root of the sum of all squared elements of each variable). Most of the statistical packages employ the correlation matrix to derive PCs (Abdi & Williams, 2010). The *correlation matrix* (R) is further used to compute *eigen values* (amount of variation in input data) using equation (2).

$$|R - I\lambda| = 0 \dots\dots\dots \text{Eq.(2)}$$

where, R = correlation matrix = 1580 x 24; I = unit matrix = 1580 x 24; λ = eigen value = vector of 1580 x 1

For each *eigen value* λ , there exists a vector a such that $Ra = \lambda a$, where a is called an *eigen vector* of R , which is associated with the *eigen value* λ . These *eigen vectors* are further used to derive PCs using equation (3):

$$PC_i = a_1X_1 + a_2X_2 + a_3X_3 + \dots\dots\dots + a_iX_q \dots\dots\dots \text{Eq.(3)}$$

where, X = input variables; i = specific PCs = 1 to 24; a_i = Eigen vector = 24 x 1; q = Specific input variable = 24

In this work, 24 PCs (equal to the number of input variables, described in a later section) were derived using equation (3). It is important to decide the appropriate number of PCs to consider for further analysis that reduce redundant information in the data set. They are selected on the basis of *Kaiser's rule*, which implies retaining the PCs whose eigen values are greater than one (Ransing, et al., 2013). The ten PCs were selected on the basis of *Kaiser's rule* and were retained for further analysis.

3.2 Artificial Neural Network

The basic architecture of ANN is shown in figure 3. It comprises three layers including one hidden layer. The number of neurons in the hidden layer was kept equivalent to the number of retained PCs.

As mentioned earlier, the training algorithm plays an important role in modelling of ANN. Three training algorithms including Back propagation (BP), Momentum & Adaptive (MA) and Levenberg-Marquardt (LM) were tested in this work. These were chosen as their learning capability and prediction accuracy were already established in other published technical literatures (Saini & Soni, 2002; Karunakar & Dutta, 2007; Saini, 2008). The basic characteristic of these algorithms are not discussed here for the sake of brevity.

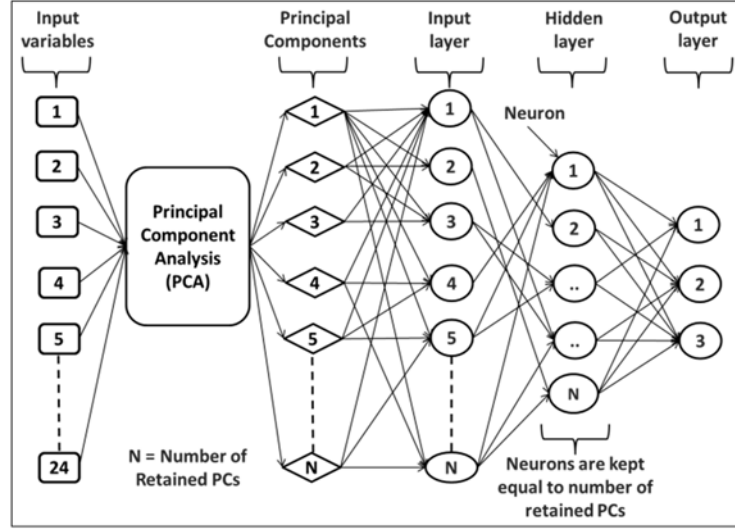


Figure 3: ANN network fed by principal components

Other controlling parameters included the following: the *transfer function* kept as a *hyperbolic tangent sigmoid*; the maximum number of *epochs* was restricted to 10000; the *learning rate* was set as 0.25 and the *network error goal* was taken as 1×10^{-5} . Out of the total number of observations (1580), 75% were used for *training*, and the remaining were used for *testing* the model. The training was stopped when either of these conditions was met: the maximum number of *epochs* is reached, or the *network error goal* is achieved.

3.3 Multi-variate Regression

The MVR is also referred to as multivariate multiple regression, where multi-variate refers to the output variables, and multiple refers to the input variables (Noori et al., 2009). The general form of input matrix X and output matrix Y for modelling the present problem are given in equations (4) and (5).

$$X = \begin{pmatrix} X_{11} & X_{12} & X_{1q} \\ X_{21} & X_{22} & X_{2q} \\ \vdots & \vdots & \vdots \\ X_{n1} & X_{n2} & X_{nq} \end{pmatrix} \dots \dots \dots Eq.(4)$$

$$Y = \begin{pmatrix} Y_{11} & Y_{12} & Y_{1p} \\ Y_{21} & Y_{22} & Y_{2p} \\ \vdots & \vdots & \vdots \\ Y_{n1} & Y_{n2} & Y_{np} \end{pmatrix} \dots \dots \dots Eq.(5)$$

where, Y = casting defects; Y_1 = ultimate tensile strength, Y_2 = yield strength, Y_3 = percentage elongation; p = number of output variables = 3; n = total number of observations = 1580; X = process parameters and chemical composition; q = number of input variables = 24.

The weights ($\beta_1, \beta_2, \dots, \beta_p$) were calculated from experimental data in a such way that it minimized the error (ε) between output (Y) and input variables (X). These coefficients were used to develop the empirical model, which was tested for prediction with the help of inputs using equation (6).

$$Y = \beta X + \varepsilon \dots\dots\dots \text{Eq.(6)}$$

The collection of industrial data for training and testing the ANN models, and the results of defect prediction are presented next.

4. Foundry Data Collection and Property Prediction

Shop floor data was collected from an investment casting foundry situated near Rajkot (India), which mainly produces ASTM A351 (stainless steel) alloy castings. In this work, data of about 800 heats was acquired along with the values of process parameters as well as the chemical composition of the alloy (charge composition). The actual data represented 1580 observations, since almost two batches of shells were used for each heat. The foundry also measured the mechanical properties (ultimate tensile strength, yield strength and percentage elongation) for each batch, by casting sample test bars (figure 4) along with the castings in each batch, and testing each sample bar on a universal testing machine as per ASTM A370. The total data set comprises 24 input parameters and three output parameters. The list of input parameters and their range of values as well as standard deviation (SD) is given in table 4.

As mentioned earlier, Principal Component Analysis was employed to reduce the complexity of data using correlation matrix. The eigen values were calculated using equation (2) and (3). The Principal Components whose eigen values were greater than one were retained, and are listed in table 5. Ten PCs, whose eigen values were greater than one, were retained for further analysis. The selected PCs explained more than 99% of total variations. The component loading, a matrix containing the eigen vectors of PCs was calculated (not shown here for the sake of brevity). The component loadings related to specific PCs were multiplied with the values of the respective input variables to get the scores related to corresponding PCs. All 24 variables were considered to calculate the score of each PC. In this way, original input variable matrix (1580 x 25) was reduced to PCs' matrix (1580 x 10). This matrix was further used as input for ANN and MVR. The range of values of the 10 PCs considered as an input is also given in table 5, along with their standard deviation.



Figure 4: Sample test bar

Table 4: Range of input parameters

No.	Parameters	Notation	Minimum	Maximum	SD
1.	Time Taken for Injection (sec)	TTI	0.69	10.42	1.61
2.	Press Room Temperature (°C)	PRT	14.8	21.6	1.2
3.	Press Room Humidity (%)	PRH	56.0	90.0	8.3
4.	Viscosity of Primary Slurry (sec)	VPS	18.6	26.5	1.1
5.	pH of Primary Slurry	PHPS	9.0	9.6	0.1
6.	Primary Coating Room Temperature (°C)	PCRT	18.7	24.3	1.3
7.	Primary Coating Room Humidity (%)	PCRH	9.5	82.0	8.6
8.	Viscosity of Secondary Slurry (sec)	VSS	9.4	11.5	0.3
9.	Shell Making Process Duration (days)	PD	2.0	9.00	1.0
10.	Secondary Coating Room Temperature (°C)	SCRT	19.6	26.4	1.4
11.	Secondary Coating Room Humidity (%)	SCSH	54.5	90.0	7.5
12.	Shell Weight before Dewaxing (kg)	SWBD	5.5	11.9	1.0
13.	Shell Weight after Dewaxing (kg)	SWAD	3.9	9.1	0.8
14.	Metal Preparation Time (minutes)	MPT	22.0	317.0	18.3
15.	Tapping Temperature (°C)	TT	1548.0	1580.0	5.6
16.	Nickel-extra (%)	NE	0.001	0.6	0.060
17.	Carbon (%)	C	0.040	0.0	0.010
18.	Manganese (%)	MN	0.560	1.4	0.080
19.	Silicon (%)	SI	1.010	1.5	0.060
20.	Sulphur (%)	S	0.001	0.010	0.010
21.	Phosphorous (%)	P	0.030	0.040	0.010
22.	Chromium (%)	CR	18.00	18.54	0.10
23.	Nickel (%)	NI	8.00	8.80	0.09
24.	Molybdenum (%)	MO	0.10	0.40	0.03

Out of the total 1580 observations, data corresponding to 1185 observations (75% of data) were used for training the ANN and MVR models. The remaining 395 observations (25% of data) were used for testing the models. The data is initially normalized (between -1 and 1) to avoid dimensionality conflict amongst input and output. The normalized data set is fed into the ANN and MVR for training. The output data is reconverted into the original form after testing. The predicted results from the models are compared with the actual results. The code for PCA, ANN and MVR was written and executed in MATLAB environment.

Table 5: Eigen values and range of retained PCs

Components	Eigen values and their contribution			Range of PCs		
	Eigen values	Proportion	Cumulative	Minimum	Maximum	SD
PC1	337.783	0.580	0.580	35.78	330.31	18.37
PC2	108.6	0.186	0.766	-84.27	-17.54	10.48
PC3	59.2741	0.101	0.868	69.09	141.98	7.70
PC4	35.8689	0.061	0.930	251.87	323.45	6.13
PC5	30.3931	0.052	0.982	1522.45	1553.56	5.52
PC6	2.93234	0.005	0.987	-13.26	12.08	1.77
PC7	2.13695	0.003	0.990	42.25	63.14	1.52
PC8	1.58196	0.002	0.993	-2.79	9.07	1.28
PC9	1.23228	0.002	0.995	0.81	10.78	1.12
PC10	1.00222	0.001	0.997	-7.24	0.31	1.00

The four models, including three ANN models (BP, MA and LM) and MVR were compared for their prediction capability. They were all tested on the same set of data, and the error for each model was calculated. Then the Root Mean Squared Error (RMSE) was calculated using equation (7) for all models. This signifies the performance of prediction, which is considered to be better if the value of RMSE is low. The values of RMSE for all models are represented in figure 5 (a) and (b). The performance of MVR in prediction of properties was found to be relatively better than ANN models.

$$RMSE = \sqrt{\frac{(Y_1 - y_1)^2 + (Y_2 - y_2)^2 + \dots + (Y_n - y_n)^2}{n}} \dots \dots \dots Eq(7)$$

where, $y_1, y_2, y_3 \dots y_n =$ actual values; $Y_1, Y_2, Y_3, \dots Y_n =$ predicted values

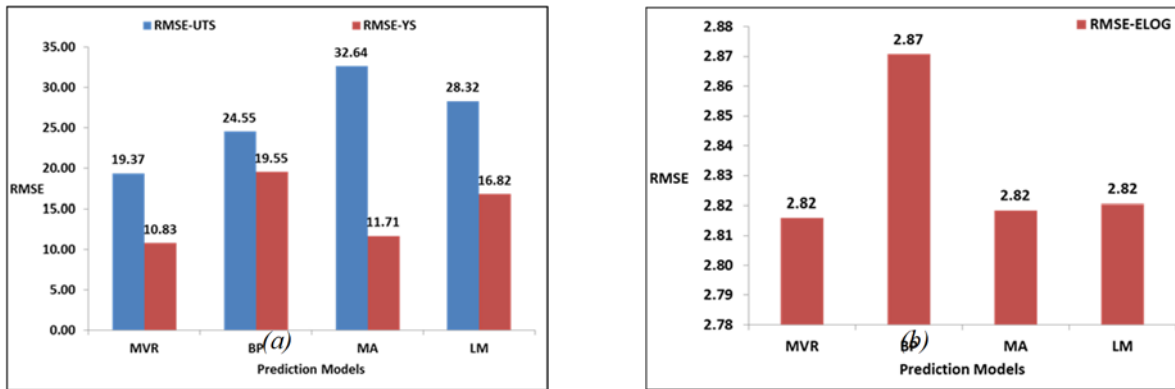


Figure 5: Prediction of UTS, YS and ELOG using ANN and MVR techniques

5. Conclusion

This work has successfully demonstrated the feasibility of predicting the mechanical properties of stainless steel investment castings using either artificial neural network or multivariate regression model. The large amount of shop-floor data obtained from an industrial foundry helped in evolving better mathematical models with improved prediction accuracy. The redundancy in input data was reduced by principal component analysis (using *correlation matrix*). The Root Mean Squared Error (RMSE) enabled comparing the different models. It was observed that MVR model yielded better results than ANN models. Among ANN models, the Levenberg-Marquardt training algorithm gave better results than others. The performance of ANNs can be further improved by tuning the transfer function, momentum rate, learning rate and error goal.

In conclusion, both ANN and MVR techniques can be used for predicting the mechanical properties using industrial data related to process parameters and chemical composition of alloy. This approach, instead of destructive test, can save valuable cost and time. Unlike simulation tools, these models are easy to use by shop-floor engineers and are expected to benefit even small and medium foundries. We hope this work will lead to greater interest and academia-industry collaborations in this field.

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