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Research article

Triboinformatic Modeling of Wear in Total Knee Replacement Implants Using Machine Learning Algorithms

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A B S T R A C T

Pin-on-disk (PoD) tests, the most prevalent studies, are being carried out in order to evaluate tribological behaviour of different bearing materials. However, the comparison of results obtained from the PoD tests is very difficult. In this present study, several machine learning models were developed and trained and then these trained machine learning models were validated by quantifying forecasting error against the experimental data reported in literature. These machine learning based models can be utilized as alternative solution of PoD trials in order to minimize time consumption and experiment complexity.

1. INTRODUCTION

Tribology is a science of friction, wear and lubrication, present in the bodies which has relative motion with each other [1]. The tribological behaviors are not only limited to mechanical systems but also this phenomenon finds an application in the field of biomedical engineering. Since the human body comprises of several joints and these joints finds different kind of articulations with their mating parts. In recent decade, a separate domain, bio-tribology, has been introduced in order to deal with such kind of wear phenomenon, present in medical and biological systems [2]. The bio-tribology emerges as an interesting area of research, includes biomechanics, biochemistry, physiology and pathology. It has wide range of applications into the biomechanical system including total joint arthroplasties viz. knee and hip, artificial hearts and dental implants as there is friction and wear come into existence [3]. The artificial joints are composed of two bodies which are in contact with each other so that they can function as a natural joint [4]. Total knee replacement (TKR) is very popular surgical treatment for knee osteoarthritis and is a very successful technique for pain relief and restoring subject's normal physical activities [5]. Nowadays, total knee replacements are being carried out more frequently on younger, obese, and physically more active individuals [6-11]. A typical TKR prosthesis composed of a metallic femoral and tibial component, and a polymer insert in between them. In the simple walking, the TKR insert is subjected to rolling along with sliding and an axial force transferred from body weight [12]. Under the action of complex motion, insert material generates wear debris as number of cycles progresses. These wear debris induces inflammatory tissues response as well as implant loosening and hence leads to implant failure. The exact prediction of wear in implants is a very complex job. The wear in artificial implants is a long term phenomenon as it requires number of millions of cycles and largely depends on joint kinematics and kinetics of individuals. The kinematics and kinetics changes person to person because they have different gait cycles and bodyweight. Several attempts have been made by researchers all over the globe to predict the wear behavior of insert material through different, intro studies, wear models, computational modelling and machine learning approaches.

In vitro studies have given us an insight how different types of articulation affect the wear performance of insert material [13]. These in vitro studies includes pin-on-plate and the pin-on-disk trials which are used in screening and exploring the effect of various above discussed parameters on the wear characteristics and wear mechanism of orthopedic bearing materials. Pin-on-disc (PoD) wear studies are prevalent approaches for quantifying, comparing, and ranking wear of various polymer based bearing materials [14]. Pin-on-disk is a very well-known and widely used for wear quantification and composed of fixed pin and rotating disk. The force is applied orthogonally to the rotating disk with the help of pin at a certain distance from axis of rotation as shown in Fig. 1 [15]. Though, the in-vitro study is very important to evaluate the wear behavior of insert material and knee prosthesis geometry, but these studies involves high cost associated with experimentation.

Computational wear modelling could be a possible approach to overcome the shortcoming of In-vitro studies. The Archard's law and its modified version have been used for preclinical wear performance evaluation which are primarily based on sliding distance, contact area, wear factor, and contact stress [16-19].

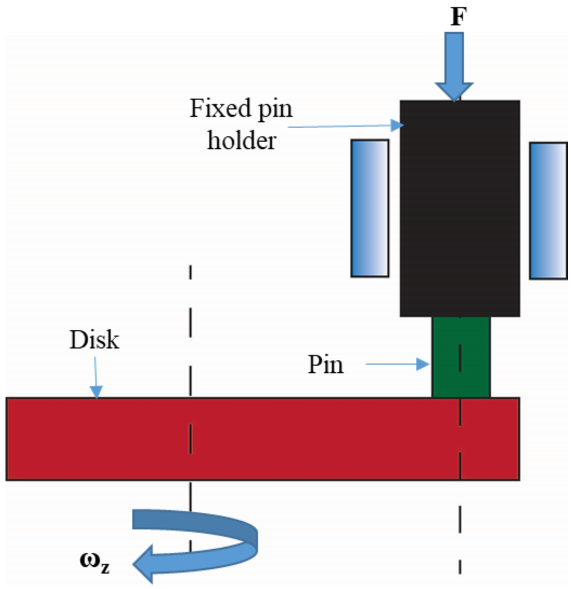

Fig. 1. Scheme of pin-on-disc. F is the applied load, on a rotating disc at speed ω_z, at a distance from the rotation axis.

Abdelgaied et al. [19] have developed and validated a wear model which is based on cross-shear ratio and has potential to simulate a wide range of physical activities viz. standard walking, deep squatting, and stair ascending. Another important modelling approach being considered these days by the scientists, engineers and researchers in the field of wear modelling is Machine learning. Though, there are enough works on computational modelling of wear in TKRs, but hardly any study has been conducted on prediction of wear in TKRs using machine learning based models.

Machine learning (ML) based models have been successfully implemented in the field of material science and healthcare systems. Machine learning based models have a potential to solve more complex and time consuming problems in a very efficient way and has a wide range of applications including mechanical and tribological characteristics estimation, image classification, estimation of hardness of cast iron, heart-rate estimation, fatigue detection associated with physical activities, breast cancer detection etc.

[20-22]. ML based models were also proposed to classify wear particles isolated from malfunctioned knee shoulder and hip arthroplasties implants [23, 24]. ML approaches also capable of prediction wear rate in UHMWPE bearing material used in knee replacement and hip replacement implants [25, 26]. The current study is based on hypothesis that machine learning based models have great potential in prediction of the linear depth of total knee replacement (TKR) implants if implemented correctly.

2. MATERIALS AND METHODS

2.1 Test specimen

The details of the test specimen selected for current study are given in Table.1

Table 1. The details of test specimen taken for study [19].

Insert material	UHMWPE (GUR 1020)
Radiation dose	5Mrad
Size	3
Thickness	10mm
Femoral Component	cobalt-chromium
TKR type	DePuy Sigma fixed bearing

2.2 Wear model

This wear model given for estimating linear wear depth is described as volumetric wear (W), where wear is proportional to apparent contact area (A) and sliding distance (S) under a specified pressure range. The wear volume is given as:

$$W = A \times S \times C \tag{1}$$

The linear wear depth can be written as:

$$\delta = S \times C \tag{2}$$

Where C is a non-dimensional wear coefficient.

Clinical and experimental observations reveal that articulating surface wear depends on the cross-shear ratio (CS) and contact stresses acting on the same articulating surface [27, 28]. Therefore, the non-dimensional wear coefficient can be described as a function of cross-shear ratio and non-dimensional contact stresses (P/E).

$$C = fun\left(CS, \frac{P}{E}\right) \tag{3}$$

Where E is modulus of elasticity of the polyethylene wearing material.

The linear wear depth, formulated from eq. 2, is given as:

$$\delta = S \times C\left(fun\left(CS, \frac{P}{E} \right) \right) \tag{4}$$

$$CS = \frac{E_{cross-shear}}{E_{total}} \tag{5}$$

The work done by Abdelgaid et al. 2018 established a relationship among wear coefficient, cross-shear ratio (CS) and non-dimensional contact stresses (P/E) as described in equation 6.

$$C = 10^{-9} \times \left[\begin{array}{c} 1.47 \times (1 - \exp(-116.21 \times CS)) \times \\ \left(0.84 + 450.23 \left(\left(\frac{P}{E} \right)^{1.49} \right) \right) \end{array} \right] \tag{6}$$

2.3 Data acquisition and feature selection

The raw dataset was generated in Microsoft excel spreadsheet by using equation 2. The ranges of all input parameter at which the data is generated are directly taken from data reported in reference number [19]. The various statistical parameters viz. mean, maximum (max), minimum (min), and standard deviation (SD) of raw input features and target, have been given in Table 2. The standard deviation shows how close the data set values are to the mean value of the particular dataset used for training. The SD of given dataset is calculated as the square root of variance by determining each data point's deviation relative to the mean.

Table 2. Statistical parameters of wear variable and δ (nm).

No. of instan-ces		P/E (--)	S (mm)	CS (--)	δ (nm)
10×10^3	Mean	0.074	19.1	0.07	50.4
	Max	0.142	28.0	0.18	137.0
	Min	0.007	10.0	0.01	20.5
	SD	0.039	8.0	0.06	33.8

For current work 10x10[3] instances are created and 70% of the dataset is used for training and rest 30% for testing of the machine learning models. The Pearson's correlation coefficient is computed to know the correlation of features with each other. Figure 2 shows the correlation among all the input features.

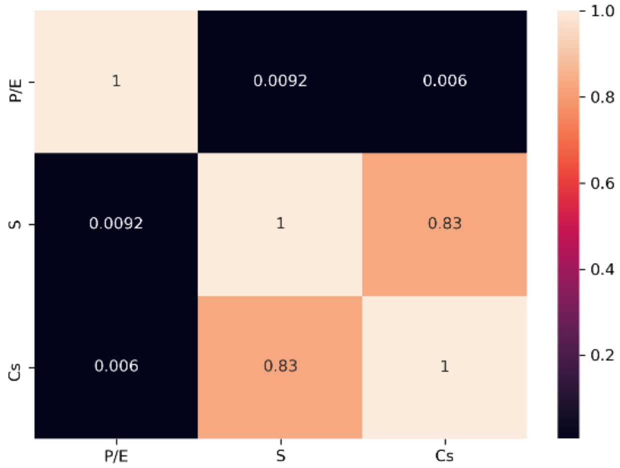

Fig. 2. Heatmap depicting correlation among all input attributes.

In Fig. 2, there are no robust correlations among all the input features as correlation coefficient between them is below 0.9. Therefore, in this study all the input features were taken into account for machine learning model building.

2.4 Machine learning approaches

In this current research work, four types of machine learning based approaches viz. Multivariate linear regression (MVR), Ridge regression, Lasso regression, ANN and random forest regression are trained with input features and correlation between input features and target is evaluated. At last, the predictions are computed from these trained models. The training and testing of models is performed on python 3.0 and its inbuilt scikitlearn toolkit [29]. The flow chart of machine learning pipeline used in this study is shown in Fig. 3.

If regression includes one dependent variable and numerous independent variables it is referred as multiple linear regression (MLR).

The MLR correlates dependent variable (Y) to a function of independent variable (X) and constant coefficients (β) as described by equation given below [30].

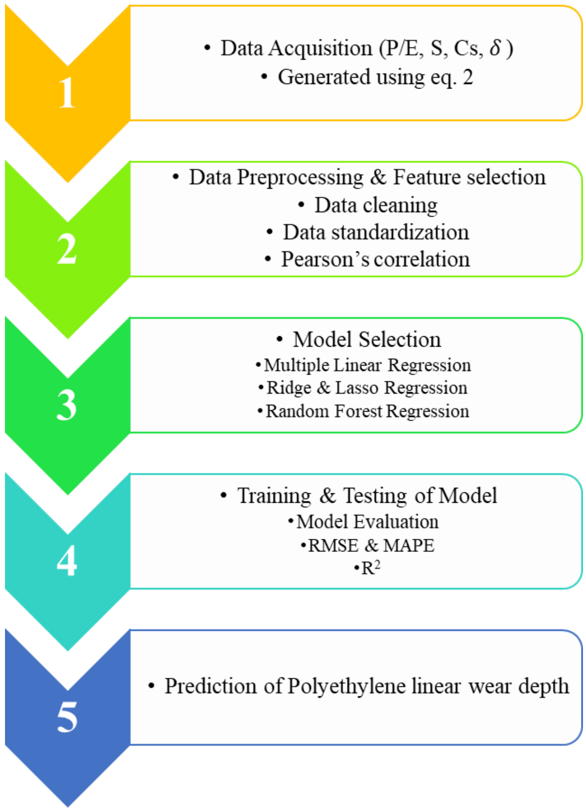

Fig. 3. A typical machine learning pipeline containing all the steps which are explained in section 2.

$$y = \beta_0 + \sum_{i=1}^{n} \beta_i x_i \quad (7)$$

and when given m instances of each x_i, named as x_{ij}, and respective instances y_j, the β_i parameters are selected to minimize residual sum of squares (RSS) given as follows:

$$RSS = \sum_{j=1}^{m} \left(\beta_0 + \sum_{i=1}^{n} \beta_i x_{ij} - y_j \right)^2 \quad (8)$$

This allows researchers to see if a multiple linear regression model can capture the relationship between operating factors and polyethylene linear wear depth.

Ridge regression improves upon multiple linear regression by including a penalty parameter proportional to the square of the magnitude of the coefficients. The ridge regression minimizes

$$RSS + \lambda \sum_{j=1}^{m} \beta_j^2 \text{ for } \lambda > 0 .$$

Lasso has a propensity to limit the number of input variables that influence the values of the target variable [31]. It typically makes coefficients equal to zero, in contrast to Ridge, which never does so. The LASSO regression minimizes $RSS + \lambda \sum_{j=1}^{m} \left| \beta_j \right|$ and otherwise LASSO works same as ridge regression. The merit of LASSO over ridge regression is that some coefficient values in it are kept zero for larger values of λ.

ANN establishes a relationship between the input features and target PE wear rate by means of neurons which are functional unit of ANN model [32]. One of the ANN architecture used in current study has been shown in Fig. 4 as shown below.

In order to improve ANN model, the hyper parameters viz. number of hidden layers, learning rate activation function and optimizers etc., are fine tuned.

A Random Forest (RF) model uses several decision trees rather than single decision to determine the polyethylene linear wear depth.

In this technique, the resultant variances is low as compared to single decision tree model because each tree in random forest are perfectly trained on that dataset.

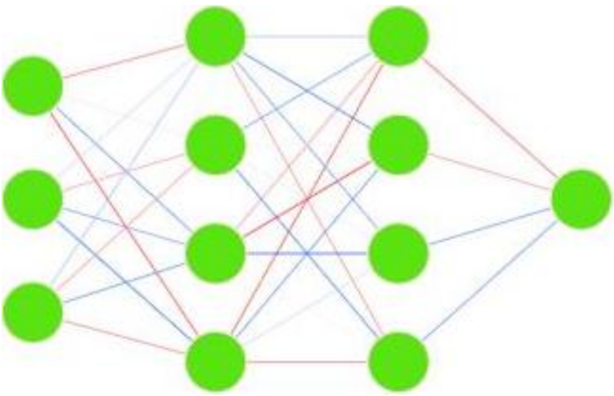

Fig. 4. The schematics of 3-4-4-1 ANN structure.

Therefore the target variable has dependence on multiple decision trees instead of single decision tree. The prediction (y) in RF model is computed by taking the mean of predictions of n regression trees (P_n) as given by equation 9.

$$y = \frac{1}{n} \sum_{i=1}^{n} P_n(x) \tag{9}$$

Random forest model is also optimized by tweaking and tuning hyper parameters viz. the maximum depth, number of leaves per node and pruning [14].

2.5 Cross-Validation

The ten-fold cross validation is applied to compute the error in prediction of polyethylene wear depth using machine learning models. The dataset is randomly divided into n number of equal subsets, called folds and then, n-1 subsets are used to train the machine learning based models and one remaining subset is used for cross-validation of that model. This procedure is repeated n times in order to make it possible that the model is validated for each subset of data at least once. In cross validation, the model is validated with the dataset that is not the part of training of the model. The schematics of cross validation has been shown in Fig. 5.

Fig. 5. The depiction of cross validation.

2.6 Model performance criteria

The machine learning based model performance is calculated on the basis of the following error functions and the square of the correlations coefficient [33].

The mathematical expression of mean absolute percentage error can be given as follows:

$$MAPE = \frac{1}{N} \sum_{i=1}^{N} \left| \frac{O_i - C_i}{O_i} \right| \tag{10}$$

The root mean square error is defined as:

$$RSME = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (C_i - O_i)^2} \tag{11}$$

And the mathematical expression of Square of the correlation coefficient (R^2) can be given as:

$$R^2 = 1 - \frac{\sum_{i=1}^{n} \left(O_i - C_i \right)^2}{\sum_{i=1}^{n} \left(O_i - \bar{O}_i \right)^2} \tag{12}$$

3. RESULTS AND DISCUSSION

The descriptive statistics of entire dataset generated using eq. 2 is presented in Table 2 as described in section 2.3 and different machine learning based approaches are implemented to train and test the dataset as described in section 2.4.

Table 3. The overall polyethylene linear wear depth dataset, utilized to calculate the prediction error of each machine learning technique employed here (*3, 4, 1 shows the number of nodes in input hidden and output layer respectively).

Method	MAPE (%)	RSME	R^2
MLR	30.67	10.85	0.89
Ridge	29.00	10.26	0.90
Lasso	27.40	10.35	0.90
ANN(3-4-4-1)	23.00	13.07	0.77
ANN(3-5-5-1)	21.00	14.10	0.79
ANN(3-6-6-1)	19	10.06	0.81
Random Forest	0.13	0.07	0.99

Table 3 shows the model evaluation parameters viz. MAPE, RSME and R^2 of the machine learning based approaches which are implemented in current work, based on the entire polyethylene linear wear depth dataset. It is found that random forest regression yield lowest forecasting error (MAPE< 1%) as compared to other machine learning based models. Thus, the random forest predicts the polyethylene linear wear depth within 0.13% prediction error range for a new data with all input features that are used for training and testing of this particular model. Furthermore, this random forest model outperform to predict the new dataset as compared to other machine learning based model used in this research work. Figure 6 shows the comparison between predicted and actual values of linear wear depth based on wear model described in section 2.2, using ridge (Fig. 6a) and random forest (Fig. 6b) machine learning approaches. It is observed that as the value of actual polyethylene linear wear depth reaches 18 nm (indicated in region (i & ii) in Fig. 6(a)), the predicted linear wear depth deviates from the actual values by 8 to 58% in case of ridge regression model but the prediction thrThe reason behind this behaviour of random forest model is that it is composed of several decision trees whose predictions are aggregated into final polyethylene linear depth.

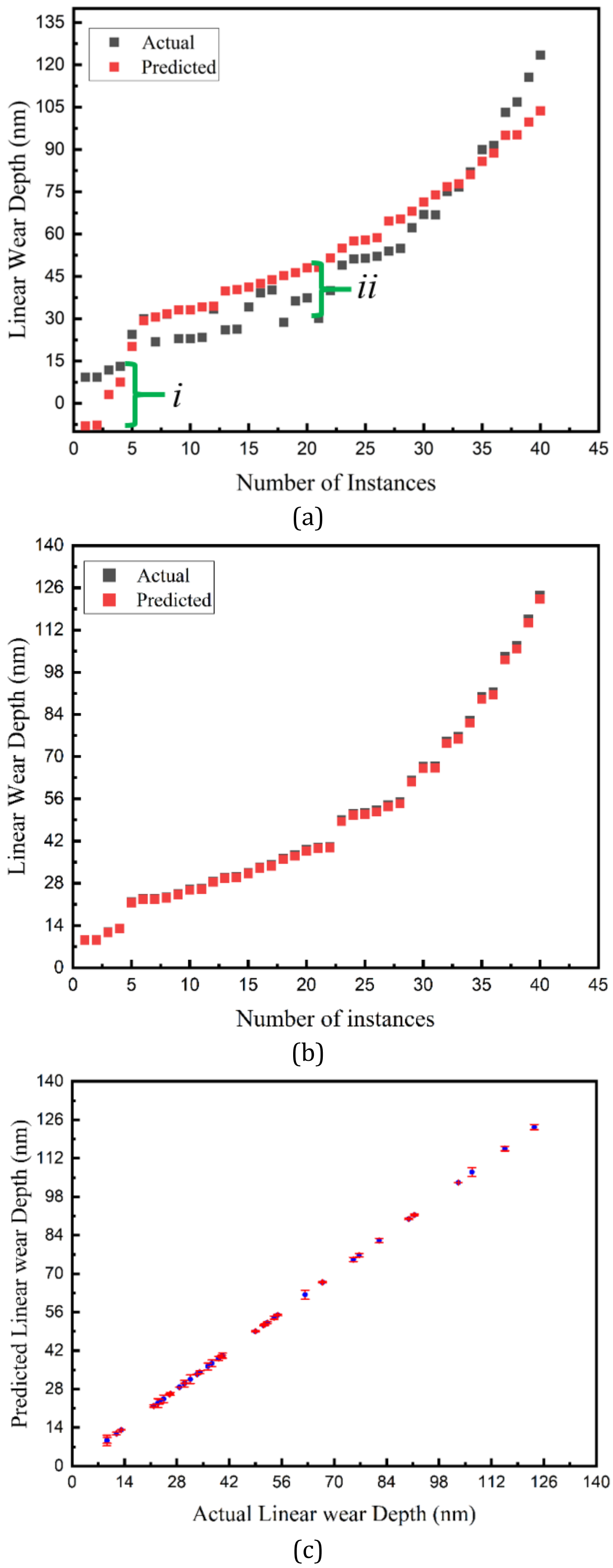

Fig. 6. A comparison between predicted values of target evaluated using (a) Ridge regression (b) Random forest regression and (c) showing the prediction error for the corresponding actual polyethylene linear depth.

The representation of decision tree in random forest model has been shown in Fig. 7. As shown in Fig. 7, random forest regression model split the input features and uses the subset of input parameters in each decision tree and the inputough random forest regression model is found in line with the actual polyethylene wear depth with an error less than 1% as shown in Fig. 6(b).

Uses the multiple trees in forest. Each node of decision tree represents an operating variable and takes a decision on the basis of that operating parameter whether it is less than or equal to, and or greater than the specified value at that particular node. It is found that "cross-shear ratio" is the most significant feature in random forest decision tree for forecasting the polyethylene linear wear depth. Random forest regression tree considers Cs as an effective features over all other features on which the polyethylene linear wear depth is dependent. Furthermore, it is also found that for a C_s greater than 0.29, the polyethylene linear wear depth is dominated by the non-dimensional contact stress and hence this is the dominating deciding features.

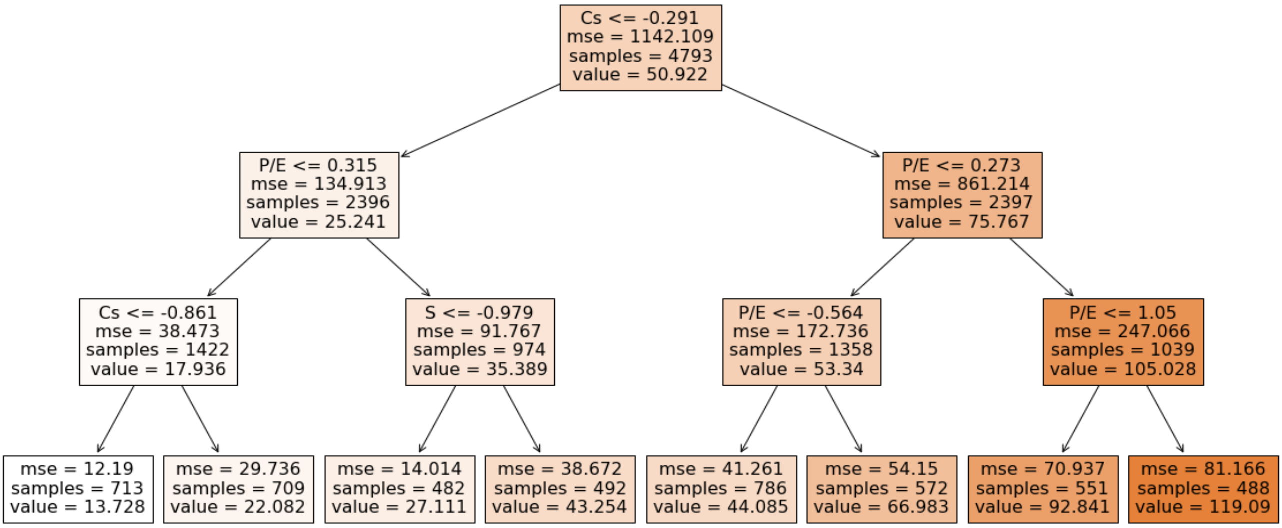

Fig. 7. The diagram showing how input feature split into random forest regression tree, and ultimately predicts values of the target features.

Similarly, this interpretation of decision tree can be applied to each level of decision tree in random forest regression and an understating can be developed about how random forest regression model interprets dataset and predict the target feature.

ANN modeling has also a potential to predict the polyethylene linear wear depth for a given input feature but these are computationally expensive as compared to random forest regression model. The primary reason of its being computationally expensive is that there always tweaking among hyper parameters viz. number of hidden layer optimization function and activation function, to predict the polyethylene linear wear depth.

4. CONCLUSION

In the current work, the linear wear depth δ is predicted using machine learning techniques for TKRs using 3 input variables (P/E, S, and CS) and δ as an output variable. It is found that the random forest regression model is more suitable to predict polyethylene linear wear depth in context to total knee replacement (TKR) and shows the relative importance of PoD test input features to polyethylene linear wear depth. This gives an insight for designing and optimizing PoD wear screening tests and these operating feature should be incorporated in PoD experimental test as per their relative importance to the polyethylene rate. The polyethylene linear wear depth is predicted with dataset i.e. not included in training dataset using tenfold cross-validation. This illustrates that model accurately predicts the polyethylene linear wear depth for the dataset which is unknown for the machine learning model. Therefore, the machine learning based models can be used as alternative solutions to these PoD experimental studies to save time as well as cost associated with these PoD based experimental studies.

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