

Prediction of Superconducting Transition Temperatures for Fe- Based Superconductors using Support Vector Machine

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Abstract
Quench for materials that can persistently carry electrical current without loss of power is confined to low temperatures. The future dream of room temperature superconductors is hampered by the absence of unique theory that fully explains superconductivity as well as high cost of the equipment involved in the characterization of the potential samples. Support vector machine (SVM) is hereby proposed to predict the superconducting transition temperature of any family of iron-based superconductors at ambient pressure using lattice parameters of the samples. Accuracy of over 99% obtained in our developed model is not only creating an efficient and low cost way of predicting transition temperature but also makes lattice parameter a premise through which full understanding of superconductivity can be grown.
Keywords: Iron-based superconductor, Support vector machine, correlation coefficient and superconducting transition temperature

1. Introduction

The trend of accidental discovery of superconductivity in mercury in 1911 in Leiden University by the Dutch Physicist, K. Onnes extended to the recently discovered iron based superconductors of high critical superconducting temperature (T_c). Heike Kamerlingh Onnes was investigating the behavior of the residual resistivity of high purity mercury when accidentally discovered superconductivity. More recently; Hideo Honoso of Toyko Institute of technology desired to fabricate transparent semiconductor, he stumbled on a new type of superconducting material; the Iron based (Kamihara et al. 2008). Since the advent of superconductivity in 1911, no theoretical explanation was available that fully describe the new phenomenon. Not until 1957 when three physicist came up with a theory known as BCS theory (Bardeen, Leon 1957) which explains that the ability of electrons to pair results into a new state called superconductivity. The formation of cooper pair is heavily affected by thermal energy in the lattice and magnetism, meanwhile at high temperature, the tendency of forming cooper pair is low. The issue of superconductivity remained confined into low temperature until emergency of high temperature superconductivity in copper oxide. Surprisingly, superconductivity was discovered in 1986 in oxides which are known to be insulators(K.A.Muller 1986). The insulator that shows this superconductivity is a sheet of copper and oxygen termed cuprate. They are non-conventional in the sense that they do not follow BCS theory and they are of high transition temperature. The cuprate made the entire world realized that the magnetism is not only hostile to superconductivity but plays a key role in Cooper pairing. Applications of superconductors, such as magnetic levitation train would have revolutionized the world of electronics if we have materials that can super-conducts at room temperature. Recently, optimism and hope of reaching room temperature in superconductivity came into existence when iron based superconductor was discovered. What amazed the entire scientist on these iron based superconductors being the fact that ferromagnetism in iron can hinder the formation of cooper pairs which is the main background of superconductivity. Locally polarized spins present in ferromagnetic materials(such as iron) whose magnetic field is liable to distorts the formation of cooper pairs, appeared to be a setback to Dirk Johrendt and his group when they suspected superconductivity in ferromagnetic materials ($SrRh_2P_2$ and $SrCo_2P_2$) in the mid-1990(Day 2009). The ability of ferromagnetic based material to super-conduct was made public by Hideo Hosono in 2008(Kamihara et al. 2008). However, several families(Day 2009) of this kind of superconductor with promising high critical temperature emerged on daily basis.

Support vector machine is an algorithm that works on the platform of artificial intelligence. It has been widely deployed in several fields of study for prediction. In oil and gas industries, it has excellent performance in the prediction of permeability of carbonate reservoirs(Olatunji et al. 2014) as well as other properties of crude oil(Olatunji 2010). It is employed in medical field for identification of skin diseases(Olatunji & Arif 2013) as well as predicting prostate cancers(Shini et al. 2011). Application of SVM and other tools of artificial intelligence is not left out in materials characterization (Swaddiwudhipong et al. 2005), predicting software maintainability of object oriented systems(Olatunji & Hossain 2012), handwritten recognition(Mahmoud & Olatunji 2009), forecasting stock prices(Olatunji 2013),predicting correlation properties of crude oil(Olatunji et al. 2011),estimation of atomic radii(O. Owolabi et al. 2014),predicting compressive concrete strength(O. Akande et al. 2014) and to mention but few.

The uniqueness of this research work is that it adopts a simple model (support vector regression) through which the superconducting transition temperatures (T_c) of any kind of high temperature iron-based superconductors are accurately determined at ambient pressure without carry out transport or magnetic measurements. The model will also enhance intelligent researchers that are incapacitated to acquire equipment to carry out low temperature researches as well as serving as premise through which the full understanding of superconductivity can be grown.

2. Proposed method

Support vector machine is a kind of artificial intelligence system that learns from experiences. Statistical leaning theory (Vapnik 1995)forms the basis of support vector machines(SVM). SVM is widely used for classification and regression. Classifications are made using SVM based on a principle that employs optimal separation of classes. If the classes under consideration are not separable, SVM adopts hyper-plane that maximizes the margin as well as minimizes a parameter which has direct influence on misclassification errors(Gupta 2007).

Support vector regression, as proposed by Vapnik(C. Cortes & Vapnik 1995), introduces ε- insensitive loss function which permits the application of the concept of margin for regression problems. The main goal of SV regression is to search for a flat function which at most, deviated from the actual target vector by ε for all training data under the consideration. For simplicity, the equation (1) represents a linear function for training data $(x_1, y_1),............(x_n, y_n)$ set with n number of samples.

$$f(x) = \langle w, x \rangle + d \quad .... (1)$$

Where $w \in P$, $d \in R$ and $\langle w, x \rangle$ represents the dot product in space of the P input.

Minimization of the Euclidean norm $\|w\|^2$ ensures the flatness of the equation (1). Therefore, optimization attained in SV regression can be represented as

$$\text{Minimize } \frac{1}{2}\|w\|^2 \text{ as subject to } \begin{Bmatrix} y_i - \langle w, x_i \rangle - d \le \varepsilon \\ \langle w, x_i \rangle + d - y_i \le \varepsilon \end{Bmatrix} \quad .... (2)$$

The above equation holds on the basis of the existence of a function which gives rise to an error that is less than ε for all training pairs. For the purpose of creating a room for another kind of error that may arise in real life problems, slack variables (ξ, ξ') are introduced. The equation (2) can further be written as

$$\text{Minimize } \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}(\xi_i + \xi_i')$$

$$\begin{Bmatrix} y_i - \langle w, x_i \rangle - d \le \varepsilon + \xi \\ \langle w, x_i \rangle + d - y_i \le \varepsilon + \xi_i' \end{Bmatrix} \quad \xi_i, \xi_i' \ge 0 \quad .... (3) \quad \text{For all } i = 1, 2......n$$

The regularization factor C is determined by the user and it measures the trade-off between the flatness of the generated function and the amount to which the deviation from the target that are larger than ε is tolerated.

Equation (3) can be transferred to a dual space representation using Langrangian multiplier. To execute this, the constraint equation is multiplied by Langrangian multiplier ($\lambda_i, \lambda_i', \eta_i, \eta_i' i = 1,.......n$) and then subtracted from the objective function ($\frac{1}{2}\|w\|^2$). Therefore, the equation becomes,

$$L = \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}(\xi_i + \xi_i') - \sum_{i=1}^{n}\lambda_i(\varepsilon + \xi_i - y_i + \langle wx_i \rangle + d) - \sum_{i=1}^{n}\lambda_i(\varepsilon + \xi'_i + y_i - \langle wx_i \rangle - d) - \sum_{i=1}^{n}\left(\eta_i \xi_i + \eta'_i \xi^i{}_i\right) \quad .... (4)$$

In order to obtain the solution to the above optimization problem, the saddle points are located by equating the derivatives of Lagrangian in equation (4) (with respect to w, d, ξ_i and ξ') to zero. Therefore,

$$w = \sum_{i=1}^{n} \left(\lambda^{i} - \lambda\right) x_{i}$$

$$\eta_i = C - \lambda_i \quad , \; \eta_i = C - \lambda^{i}{}_{i} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.. (5)$$

The optimization problem is maximized by putting equation (5) in equation (4). We have

$$-\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\lambda_i{}' - \lambda_i\right)\left(\lambda_j{}' - \lambda_j\right)\left(x_j - x_i\right) - \varepsilon\sum_{i=1}^{n}\left(\lambda_i{}' + \lambda_i\right) + \sum_{j=1}^{n} y_i\left(\lambda_i{}' - \lambda_i\right) \ldots\ldots\ldots\ldots\ldots(6)$$

Subject to $\sum_{j=1}^{n}\left(\lambda_i{}' - \lambda_i\right) = 0$ and $0 \le \lambda_i{}', \lambda_i \le C$

Equation (1) can therefore be modified by utilizing the solutions (λ^{i} and λ) obtained from equation (8). The modified equation becomes

$$f(x) = \sum_{i=1}^{n}\left(\lambda_i{}' - \lambda_i\right)\langle x_i , x\rangle + d \ldots\ldots\ldots\ldots\ldots (7)$$

Non-linear functions are treated in support vector regression by adopting the concept of kernel functions(C. Cortes & Vapnik 1995). This kernel function enhances SV regression to perform the linear regression in feature space by mapping the data into high dimensional space. It is easy to write the regression problem in feature space by replacing x_j and x_i in equation (6) by $\Phi(x_i)$ and $\Phi(x_j)$

The optimization problem becomes,

$$-\frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n}\left(\lambda_i{}' - \lambda_i\right)\left(\lambda_j{}' - \lambda_j\right)K(x_i . x_j) - \varepsilon\sum_{i=1}^{n}\left(\lambda_i{}' + \lambda_i\right) + \sum_{j=1}^{n} y_i\left(\lambda_i{}' - \lambda_i\right)$$

Subject to $\sum_{j=1}^{n}\left(\lambda_i{}' - \lambda_i\right) = 0$ and $0 \le \lambda_i{}', \lambda_i \le C$ …………………….. (8)

Where $K(x_i . x_j) = \Phi(x_i).\Phi(x_j)$

The regression function now becomes

$$f(x) = \sum_{i=1}^{n}\left(\lambda_i{}' - \lambda_i\right)K(x_i , x) + d \ldots\ldots\ldots\ldots (9)$$

The transformation of datasets into hyper-plane is carried out by the kernel function (Olatunji 2010). The complexity of the final solution is governed by the structure of high-dimensional feature space which is determined by the variables of the kernel. Hence, the variables of the kernel need to be accurately computed. Polynomial, Linear ,Gaussian and Sigmoid are the most commonly used kernel functions in the literature(Mahmoud & Olatunji 2009).

$$K(\vec{x}_i , \vec{x}_j) = (\vec{x}_i \cdot \vec{x}_j + 1)^{d} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (10)$$

$$K(\vec{x}_i , \vec{x}_j) = \exp\left(-\gamma \left\|\vec{x}_i - \vec{x}_j\right\|^{d}\right) \ldots\ldots\ldots\ldots\ldots\ldots\ldots (11)$$

The polynomial kernel function is represented in the equation (10) with degree d. This polynomial kernel function becomes linear function when d=1. Equation (11) is the Radial Basis Function (RBF) kernel (also known as Gaussian) with parameter γ (Mahmoud & Olatunji 2009)(Olatunji & Hossain 2012)(Cortes & Vapnik 1995)(Olatunji 2010)

Other kernel functions that are obtainable in the literatures are

Linear: $K(x_i, x_j) = x_i{}^{T} x_j$ and sigmoid: $K(x_i, x_j) = \tanh(\gamma x_i{}^{T} x_j + r)$ with $\gamma, r, and\ d$ kernel parameters.

3.0 Empirical Study

3.1 Data set description

The actual data (obtained experimentally) employed in this research work was drawn from literatures(Johnston 2010)(Yadav, Anil K 2014). Total number of thirty-three data set was used for both training and testing as presented in table1 with indication of quenched samples using liquid nitrogen by Q. The adoption of this few data sets was due to the efficiency of SV regression model which is known to be highly stable and performs accurately and excellently for few data sets(Shin et al. 2005). The adopted actual data set comprises the true representatives of different families of polycrystalline iron based superconductors (11-type, 111-type, 122-type and 1111-type) prepared using different methods. The lattice parameters of the dataset were obtained from room temperature x-ray diffraction of the iron based superconductor and the superconducting transition temperatures were drawn from transport measurements performed on the samples at ambient pressure. Statistical analysis of the data set is shown in table2 and3. The correlation coefficients between the predictors (lattice parameters) and the target (superconducting transition temperature) is not magnificent in such a way that one may thing that the superconducting transition temperature is not likely to be estimated from lattice parameters. SV regression helps in studying both linear and non-linear relationship between the predictors and the target so as to draw virtual relation through which unknown targets can be accurately predicted. High accuracy of the trained system on the basis of coefficient of correlation to predict superconducting temperature gives assurance of the existence of virtual relationship between the predictors and the target which may be difficult to achieve using any conventional relation.

Table1: The Data set

Iron-based superconductors	a(A^0)	c(A^0)	T_c(K)
$LaFeAsO_{0.89}F_{011}$	4.028	8.713	28.0
$LaFeAsO_{0.86}F_{014}$	4.025	8.695	20.0
$LaFe_{0.89}Co_{0.11}AsO$	4.035	8.713	14.3
$SmFeAsO_{0.93}F_{0.07}$	3.393	8.482	35.0
KFe_2As_2	3.842	13.838	3.6
$SrFe_{1.8}Co_{0.2}As_2$	3.928	12.303	19.0
$SrFe_{1.4}Ru_{0.6}As_2$	3.992	12.064	19.3
$SrFe_{1.3}Ru_{0.7}As_2$	4.005	12.009	19.3
$SrFe_{1.3}Ru_{0.8}As_2$	4.011	11.984	17.6
$Ba_{0.89}K_{0.11}Fe_2As_2$	3.949	13.088	2.5
$Ba_{0.82}K_{0.18}Fe_2As_2$	3.937	13.155	25.4
$Ba_{0.7}K_{0.3}Fe_2As_2$	3.919	13.263	36.4
$Ba_{0.6}K_{0.3}Fe_2As_2$	3.915	13.294	38.6
$Ba_{0.56}K_{0.44}Fe_2As_2$	3.907	13.335	36.8
$Ba_{0.38}K_{0.062}Fe_2As_2$	3.887	13.506	29.6
$Ba_{0.29}K_{0.71}Fe_2As_2$	2.880	13.569	14.6
$Ba_{0.15}K_{0.8}Fe_2As_2$	3.852	13.735	8.9
$Ba_{0.1}K_{0.9}Fe_2As_2$	3.848	13.793	8.9
LiFeP	3.692	6.031	6.0
$FeNi_{0.02}Se$	3.774	5.519	5.0
$FeCo_{0.02}Se$	3.771	5.522	6.0
$Fe_{1.01}Se$	3.768	5.521	8.2
$Fe_{1.01}Se$ (Q)	3.771	5.520	9.0
$FeMn_{0.04}Se$	3.770	5.522	10.0
$FeMn_{0.04}Se$ (Q)	3.775	5.527	10.0
$FeCr_{0.02}Se$	3.773	5.524	10.5
$FeCr_{0.02}Se$(Q)	3.767	5.519	10.8
$FeV_{0.02}Se$	3.772	5.5242	9.5
$FeV_{0.02}Se$ (Q)	3.772	5.5205	11.2
$FeV_{0.03}Se$ (Q)	3.776	5.508	9.2
$FeV_{0.05}Se$ (Q)	0.0	0.0	0.0
$FeT_{0.02}Se$	3.773	5.525	8.0
$FeV_{0.01}Se$ (Q)	3.770	5.180	11.0

Table2: Statistical Analysis of the data set

	Mean	Median	Standard Deviation
a(A^o)	3.70	3.78	0.70
c(A^o)	8.94	8.70	3.90
T_c(K)	15.20	10.80	10.64

Table3: Correlation between each pair of the attributes of the dataset

	a and T_c	c and T_c
Correlation coefficient	0.28	0.52

3.2.1 Description of the experiment

This research work was conducted using MATLAB environ. For the purpose of facilitating efficient computation, the data set was reshuffled, normalized and then partitioned into training and testing phase in the ratio of 8 to 2(that is, 80%training and 20% testing) respectively. The training datasets were then applied to train the SVM model used in predicting the superconducting transition temperature of the testing datasets.

3.2.2 Working principle of SV regression

Support vector regression adopts kernel trick to generate function that relates the predictors to the target through which unknown targets are predicted. It works on the principle of artificial intelligence (that is, leaning from experiences). During the training period, SV regression takes some input parameters (such as hyper-parameter λ , regularization factor C, kernel –option and epsilon ε) by which the chosen kernel function generates a relation between the predictor and the target. The hyper-parameter guides SVM to adopt hyper-plane that maximizes the margin as well as minimizes a parameter which has direct influence on likely errors between the actual and the predicted values(Gupta 2007). The epsilon ε represents the maximum tolerable deviation of the predicted values from the actual values. The SV regression under the training is allowed to see the target for each data so as to adjust the generated function until the function is generalized for any kind of predictors of similar properties. The user defines and adjusts these input parameters until maximum obtainable correlation is achieved between the actual and the predicted values. The regularization factor C (defined by the user) dictates the trade-off between the flatness of the generated function and amount to which the deviations that are larger than ε is tolerated. The input parameters that give the optimum correlation are referred to as the optimum parameters and the SV regression system is said to be well trained and can be tested before being used.

The trained system needs to be tested in order to ascertain its efficiency. In this case, the target values will not be shown to the trained system and high correlation between the actual and the predicted values measures the accuracy and efficiency of the system.

In the case of our trained system, accuracies of over 98% and 99% were obtained for both training and testing dataset. The High performance obtained in testing our system confers confidence in the developed system and can therefore be used to predict the superconducting transition temperature of all sort of iron-based superconductors at ambient pressure.

3.2.3 Optimum parameter search strategy using polynomial kernel

3.2.3 .1 Regularization factor: Optimum parameters were searched for using all searching parameters. For the polynomial kernel, the effect of regularization factor is depicted in fig1.

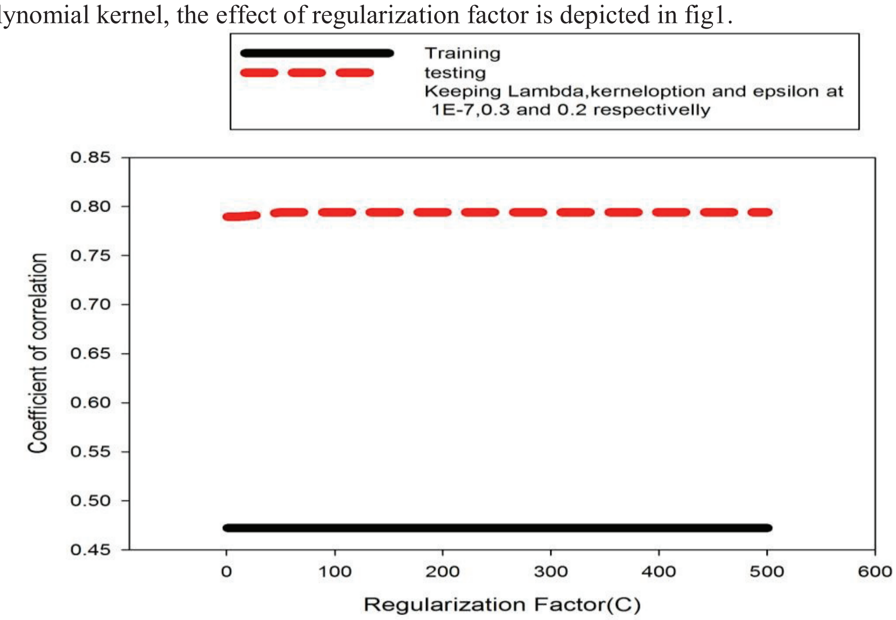

Fig 1:The trend of Variation of regularization factor with coefficient of correlation between the actual and predicted superconducting transition temperature while training and testing our model using Polynomial Kernel

The coefficient of correlation between the actual and the predicted transition temperature (while training the system) rises slightly as the value of regularization factor increases. It attains maximum value at 79.4% with which it maintains until the value of regularization factor reaches 500.The value of regularization factor could not be increased further because of high computation involved which was manifested by long period of time for execution.

In the case of coefficient of correlation while testing our system, it maintains a constant value of 47.2% for the whole of the computation.

3.2.3.2 Hyper-parameter (λ): The effect of hyper-parameter on the coefficient of correlation between the actual and the predicted value was also investigated and presented in fig2.

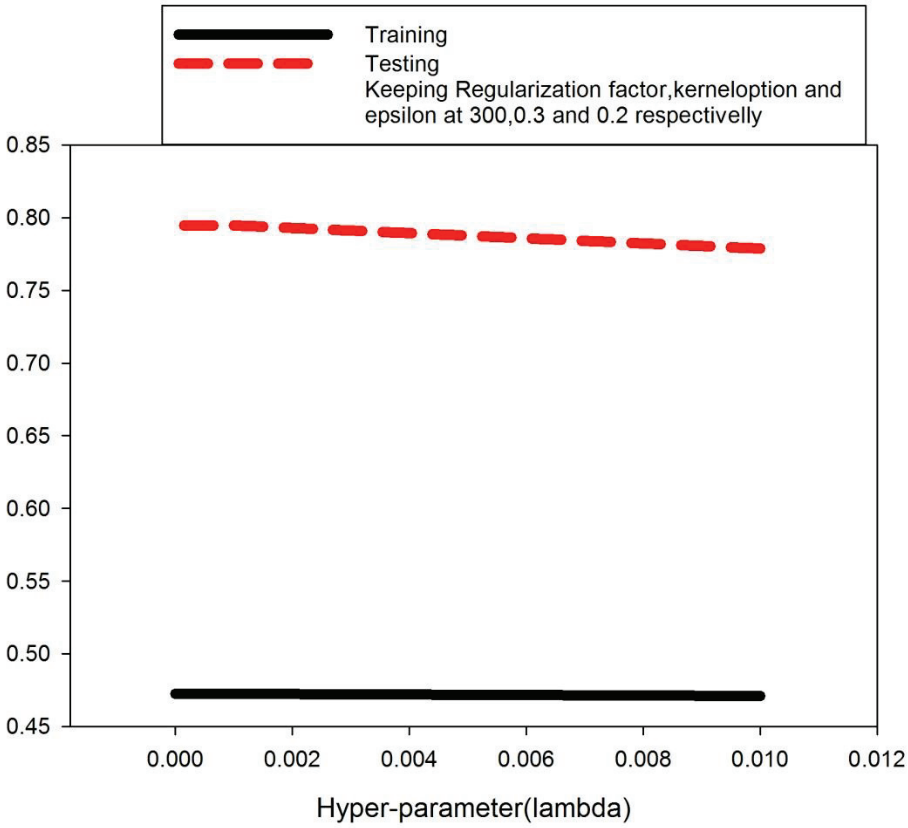

Fig 2:The trend of Variation of lambda with coefficient of correlation between the actual and predicted superconducting transition temperature while training and testing our model using Poly Kernel

Figure 2 shows the decrease in the coefficient of correlation for the training dataset as hyper-parameter increases. Hyper-parameter has a slight influence on the testing dataset as can be seen from the figure. It can be seen from the graph that the best hyper-pane was selected by SV regression for optimum performance when the hyper-parameter was defined as 0.001.

3.2.3.3 Epsilon (ε): The variation of epsilon with the coefficient of correlation for both training and testing dataset is represented in the figure 3.

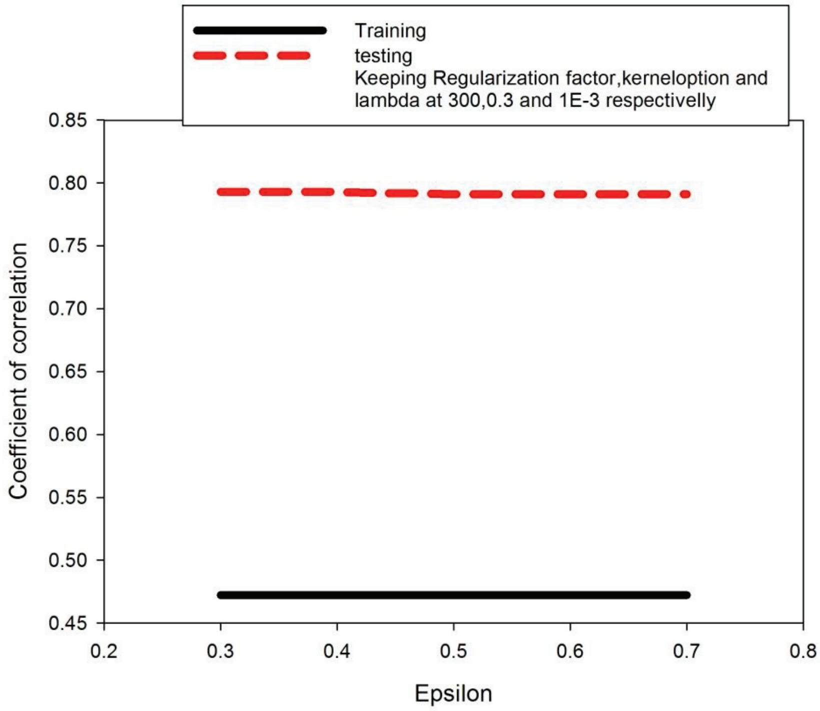

Fig 3:The trend of Variation of epsilon with coefficient of correlation between the actual and predicted superconducting transition temperature while training and testing our model using Poly Kernel

The variation of epsilon with the performance of the system is not really significant as can be seen from the figure. This means that the maximum allowable deviation of the predicted temperature from the actual temperature (which gives the system an optimum performance while using polynomial kernel) occurs at a value of 0.2.

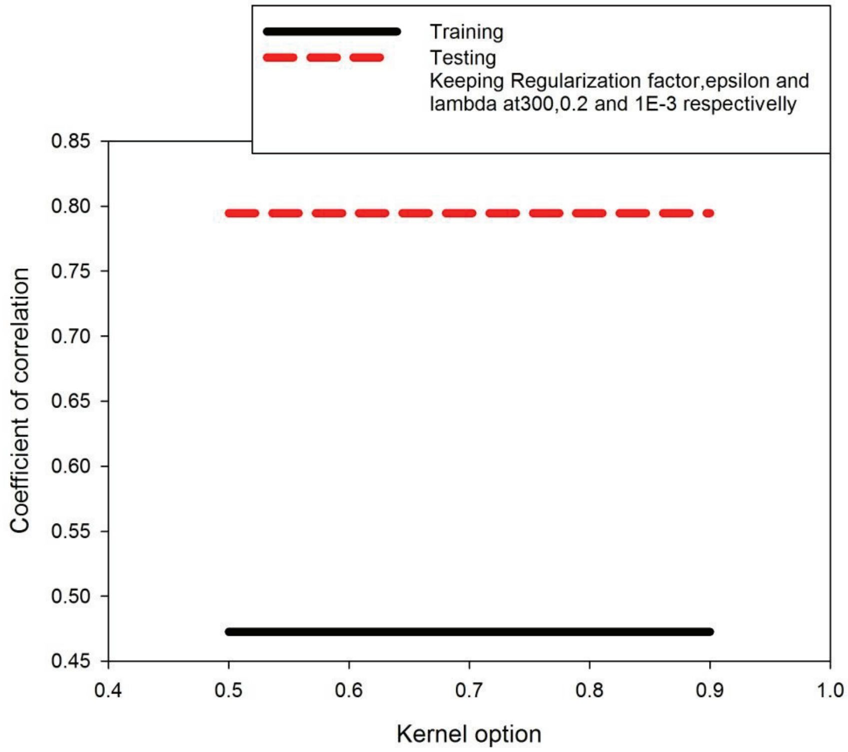

Fig 4:The trend of Variation of kernel option with coefficient of correlation between the actual and predicted superconducting transition temperature while training and testing our model using Poly Kernel

3.2.3.4 Kernel option: Presentation of the variation of kernel option with the performance of the system is shown in figure4. This variation is not strongly significant as can be figured out in the graph.

3.3 Optimum parameter search strategy using Gaussian kernel

3.3.1 Regularization factor: The trend of the variation of regularization factor on the performance of the system using Gaussian kernel is illustrated in figure5. During the training and testing period of the system, the performance of the system attains optimum value when the value of regularization factor gets to 1400. The coefficient of correlation (which determines the performance of the system) while training and testing the system maintains constant value after leaving the maximum point. Among factors that are unique to this model is that the model performs better while testing the system as can be seen in all the figures.

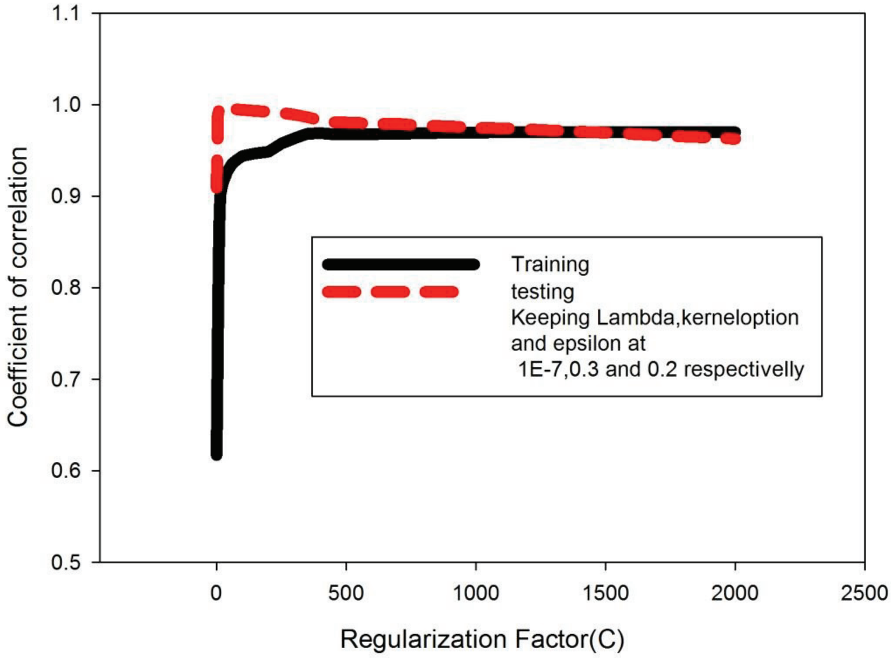

Fig 5:The trend of Variation of regularization factor with coefficient of correlation between the actual and predicted superconducting transition temperature while training and testing our model using Gussian Kernel

3.3.2 Hyper-parameter (λ *)*: Figure6 shows the effect of hyper-parameter on the performance of the system. The performance (as spelt out from the coefficient of correlation) increases to its maximum value and begins to decrease. During the training, SV regression selects the best hyper-plane that minimizes the error. The optimum performance is attained when the value of hyper-parameter was set at 0.01.

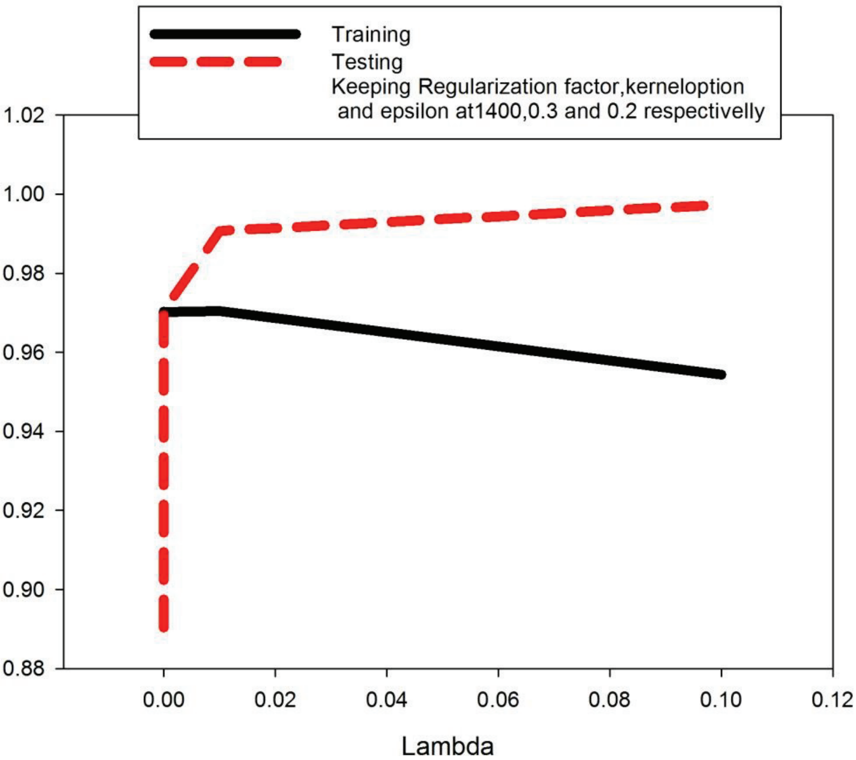

Fig 6:The trend of Variation of lambda with coefficient of correlation between the actual and predicted superconductingtransition temperature while training and testing our model using Gussian Kernel

3.3.3 Epsilon (ε): For the purpose of comprehending the influence of the amount to which the deviation from ε is being tolerated, figure7 is presented in order to figure out the effect.

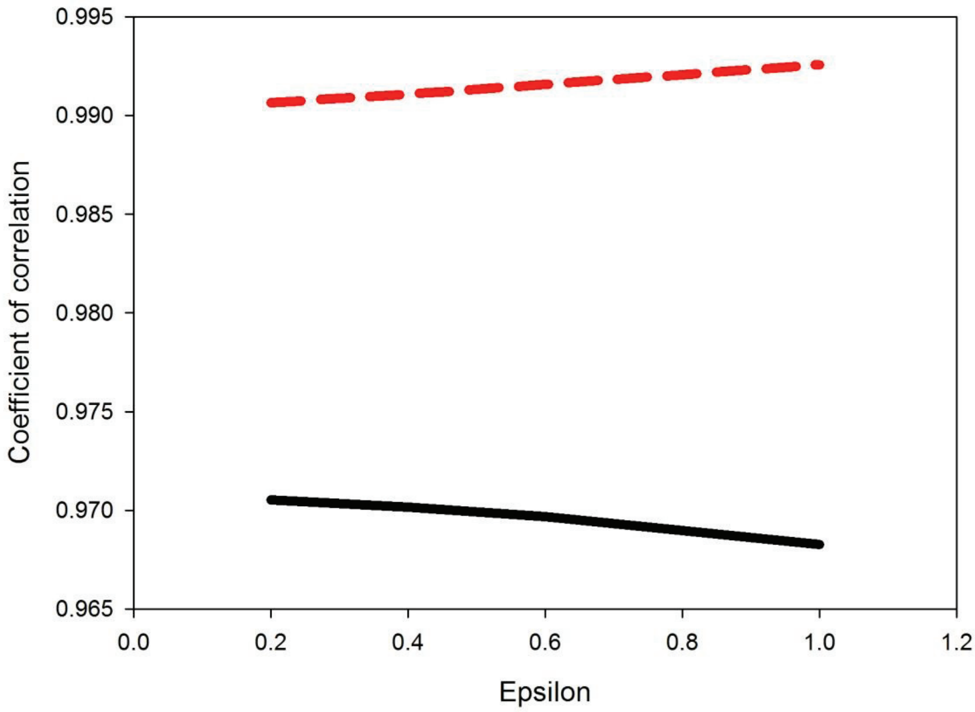

Fig 7:The trend of Variation of epsilon with coefficient of correlation between the actual and predicted superconducting transition temperature while training and testing our model using Gussian Kernel

The performance of the system increases as the epsilon decreases and attain the optimum value at 0.2. In the same vein, our system performs well while testing than training.

3.3.4 Kernel option: The influence of the kernel option is illustrated in figure8. The performance of the system rises as the kernel option decreases. The optimum value was attained in the system when the kernel option was set to 0.079.

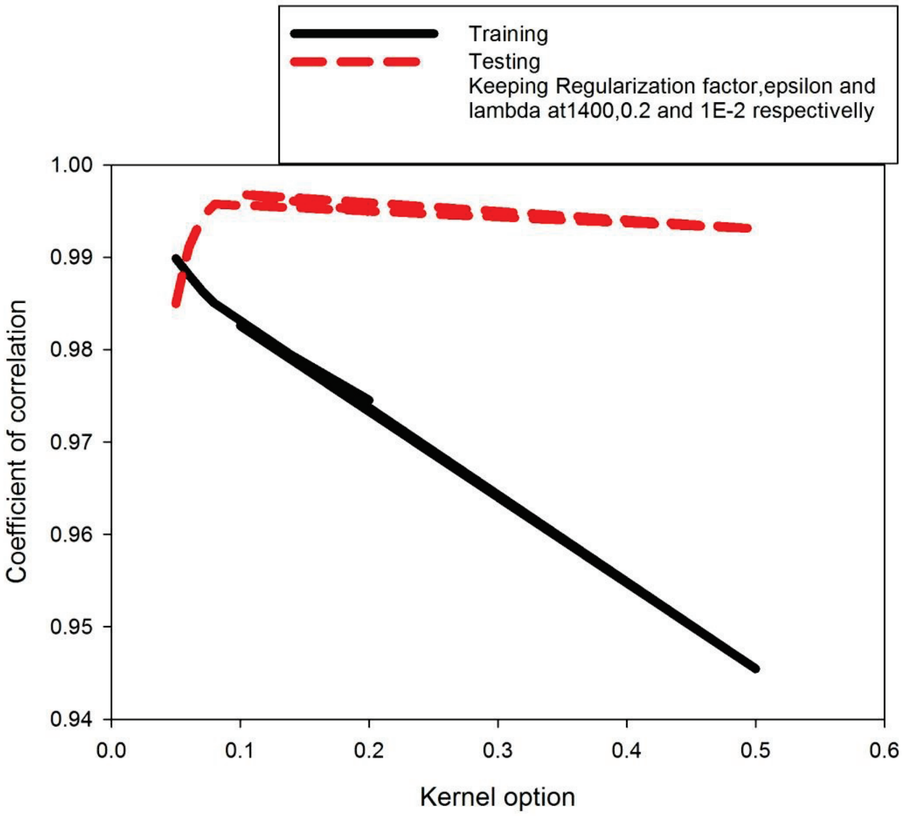

fig 8:The trend of Variation of kernel option with coefficient of correlation between the actual and predicted superconductingtransition temperature while training and testing our model using Gussian Kernel

Based on the above parameters search, the SV regression parameters that give optimum performance to our system are presented in table4.

Table4: Optimum parameters for SV Regression model

C	1400
Lambda	1.00E-02
Epsilon(ε)	0.2
Kernel option	0.07
Kernel	Gaussian

3.4 Performance quality measures

Excellent performance of our trained and tested system is characterized by low root mean square error (rmse) and very high correlation coefficient (cc) between the actual and predicted transition temperatures. The quality of the adopted model in this research work was determined by invoking equations (12), (13) and (14).

$$cc = 1 - \left[\sum_1^n \left\{\frac{T_{act} - T_{pre}}{T^2{}_{act}}\right\}^2\right] \qquad (12)$$

$$rmse = \sqrt{\frac{1}{n}\left[\sum_1^n \left\{\frac{T_{act} - T_{pre}}{T^2{}_{act}}\right\}^2\right]} \qquad (13)$$

$$Ea = \sum_1^n \left\{\frac{T_{act} - T_{pre}}{n}\right\}^2 \qquad (14)$$

Where T_{act} , T_{pre} represent the actual and predicted superconducting transition temperature respectively. The number of available data point is represented by n.

4. Result and discussion

The actual superconducting transition temperatures were compared with the transition temperatures predicted by the trained SV regression model and the presentation of the comparison is shown graphically in figure 9 and 10. High performance was recorded while testing the model. The model makes it easy to effectively predict superconducting transition temperature of polycrystalline iron based superconductor at ambient pressure. The table5 presents the actual and predicted transition temperature obtained while training and testing the developed model.

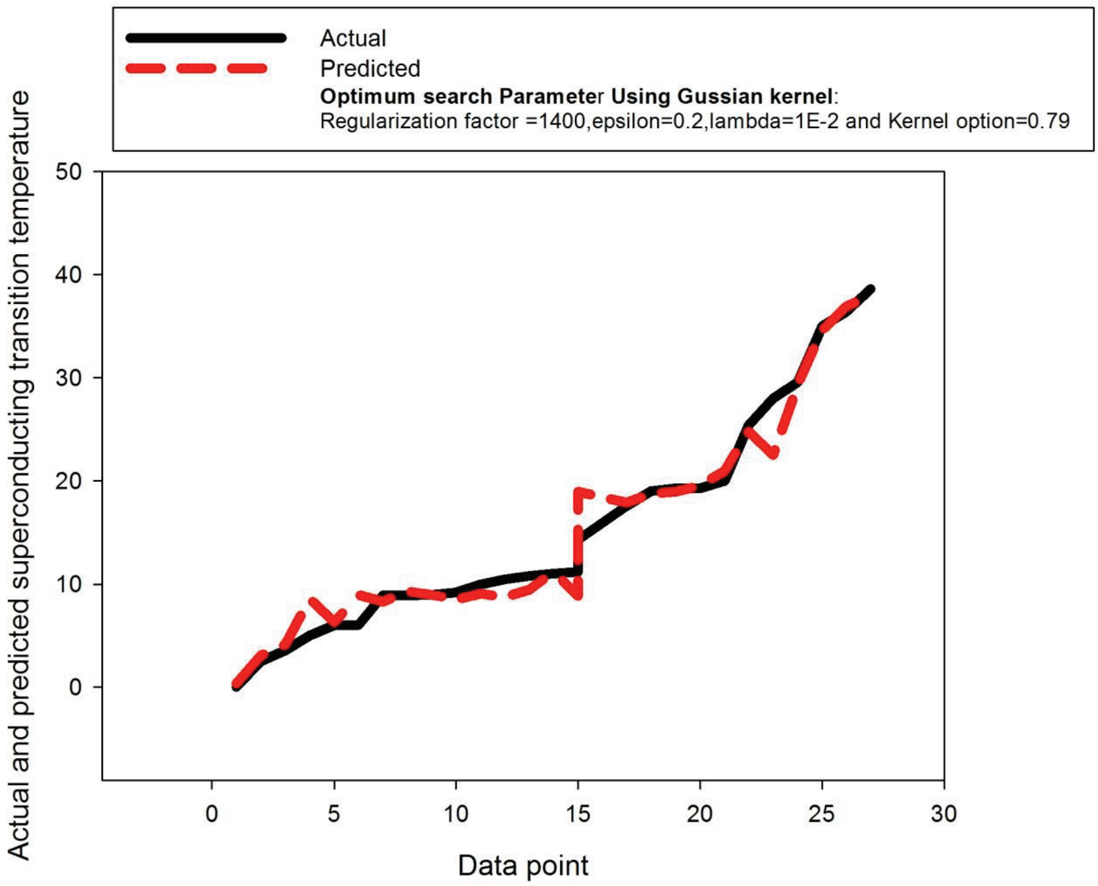

Fig 9:Actual and predicted superconducting transition temperature while training our model

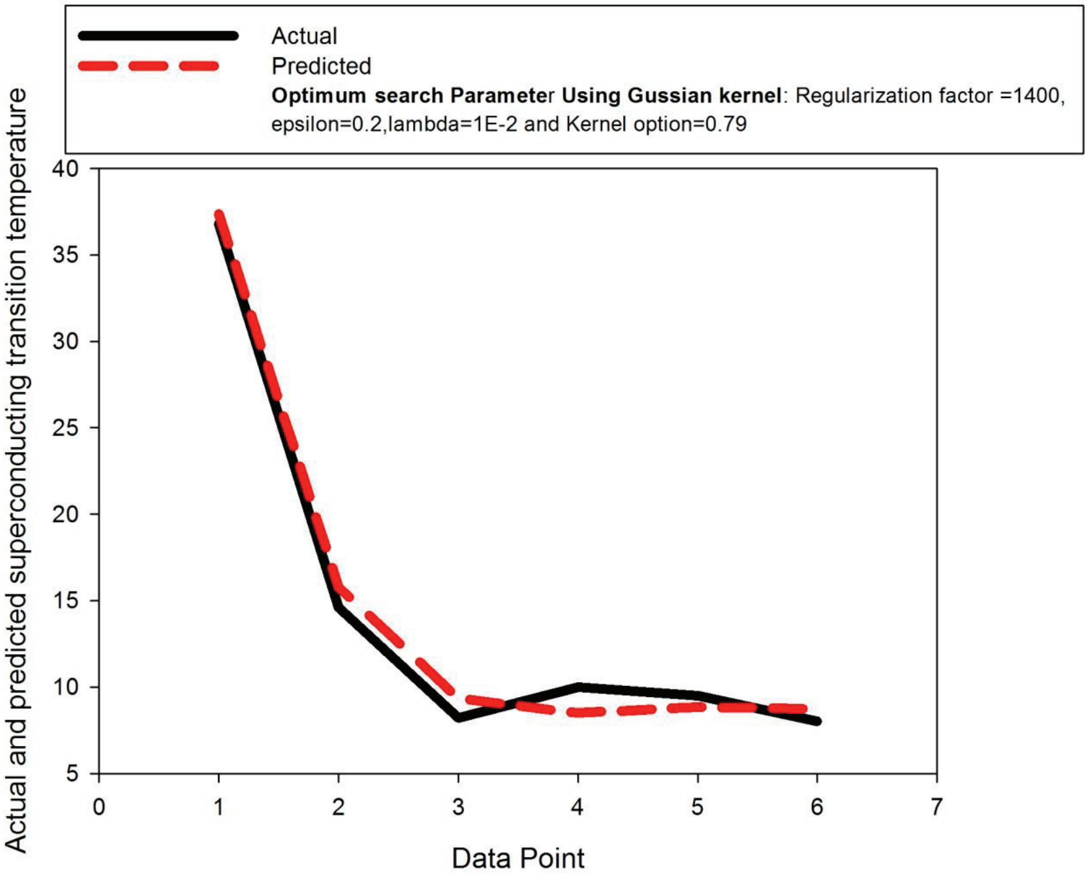

Fig 10:Actual and predicted superconducting transition temperature while testing our model

Table5: Actual and predicted superconducting transition temperatures for polycrystalline iron-based superconductors at ambient pressure

Training dataset		
	Actual Transition temperature(K)	Predicted Transition temperature(K
$LaFeAsO_{0.86}F_{014}$	20	21.0
$SrFe_{1.8}Co_{0.2}As_2$	19	18.8
$LaFeAsO_{0.89}F_{011}$	28	22.9
$Ba_{0.89}K_{0.11}Fe_2As_2$	2.5	3.0
$SrFe_{1.3}Ru_{0.7}As_2$	19.3	19.0
$FeV_{0.02}Se$ (Q)	11.2	8.8
LiFeP	6	6.3
$Ba_{0.82}K_{0.18}Fe_2As_2$	25.4	24.9
$FeCo_{0.02}Se$	6	9.0
$Fe_{1.01}Se$ (Q)	9	9.0
$FeCr_{0.02}Se$	10.8	9.6
$FeCr_{0.02}Se$	10.5	8.7
$FeNi_{0.02}Se$	5	8.6
$SmFeAsO_{0.93}F_{0.07}$	35	34.6
$FeV_{0.05}Se$ (Q)	0	0.4
$Ba_{0.7}K_{0.3}Fe_2As_2$	36.4	36.8
$Ba_{0.15}K_{0.8}Fe_2As_2$	8.9	8.4
$FeV_{0.03}Se$ (Q)	9.2	8.5
$Ba_{0.38}K_{0.062}Fe_2As_2$	29.6	29.3
$SrFe_{1.3}Ru_{0.8}As_2$	17.6	17.9
$Ba_{0.1}K_{0.9}Fe_2As_2$	8.9	9.3
$LaFe_{0.89}Co_{0.11}AsO$	14.3	18.7
KFe_2As_2	3.6	4.1
$SrFe_{1.4}Ru_{0.6}As_2$	19.3	19.4
$Ba_{0.6}K_{0.3}Fe_2As_2$	38.6	38.1
$FeV_{0.01}Se$ (Q)	11	11.2
$FeMn_{0.04}Se$	10	9.1
Testing data set		
$Ba_{0.56}K_{0.44}Fe_2As_2$	36.8	36.1
$Ba_{0.29}K_{0.71}Fe_2As_2$	14.6	16.0
$Fe_{1.01}Se$	8.2	9.3
$FeMn_{0.04}Se$ (Q)	10	8.4
$FeV_{0.02}Se$	9.5	8.8
$FeT_{0.02}Se$	8	8.6

The correlation coefficients between the actual and predicted transition temperatures were presented in table6. Low root mean square errors are also presented as obtained. The obtained high accuracies on the performance of the model suggest that the developed model is an excellent model for predicting superconducting transition temperature of any family of iron-based superconductor using the lattice parameter obtained from room temperature x-ray diffraction analysis of the samples. This reduces the cost incurred in acquiring low temperature cryostats as well as time it takes to execute the characterization. The lattice parameters for prediction are easily obtainable from common x-ray diffraction machines.

Table6: Results

	Training data set	Testing data set
Coefficient of correlation	98.65%	99.42%
Root mean square error	1.74	1.104

5. Conclusions and recommendation

SV regression model was used to predict the transition temperature of iron-based superconductors and very high accuracy was obtained while training and testing the model. The obtained accuracy indicates that there exist a strong relation between lattice parameters and the superconducting temperature from which the full understanding of superconductivity can be drawn. Hence, this model is recommended in predicting transition temperature of any kind of iron-based superconductors at ambient pressure.

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