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Model of Least Square Support Vector Machine (LSSVM) for Prediction of Fracture Parameters of Concrete

Kulkrni Kallyan S.,[1)] Dookie Kim,[2)] S. K. Sekar,[3)] and Pijush Samui[4)]

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Abstract: This article employs Least Square Support Vector Machine (LSSVM) for determination of fracture parameters of concrete: critical stress intensity factor (K^s_{Ic}) and the critical crack tip opening displacement ($CTOD_c$). LSSVM that is firmly based on the theory of statistical learning theory uses regression technique. The results are compared with a widely used Artificial Neural Network (ANN) Models of LSSVM have been developed for prediction of K^s_{Ic} and $CTOD_c$, and then a sensitivity analysis has been performed to investigate the importance of the input parameters. Equations have been also developed for determination of K^s_{Ic} and $CTOD_c$. The developed LSSVM also gives error bar. The results show that the developed model of LSSVM is very predictable in order to determine fracture parameters of concrete.

Keywords: least square support vector machine (LSSVM), fracture mechanics, artificial neural network (ANN), support vector machine (SVM).

1. Introduction

Application of Linear Elastic Fracture Mechanics (LEFM) for concrete was introduced previously, but it was not valid for cementitious material. Several different non-linear fracture mechanics approaches have been developed for the concrete modeling. These approaches involve size effect model,[1] crack band model,[2] fictitious crack model,[3] two parameter model,4 peak load method[5] and etc. In addition, several methods also have been presented to determine the fracture parameters of concrete like experimental technique,[1,3-5] and regression models.[2,6,7] All the above methods have their own advantages and disadvantages.8 Recently, Ince8 introduced Artificial Neural Network (ANN) for predication of fracture parameters of concrete. He has used backpropagatation ANN with three layers: one input layer, one hidden layer with four neurons and one output layer. Two bias neurons were also connected to the hidden and output layers.[8] Each has a constant value of 1.8 The value of learning rate is 0.35. The value of momentum factor is 0 for first 100 training and 0.9 for the rest. The ANN has converged at 15,000 iterations. However, the ANN has the following limitations:

1) ANN does not provide information about the relative importance of the various parameters.[9]

2) ANN has some inherent drawbacks such as slow convergence speed, less generalizing performance, arriving at local minimum and over-fitting problems.

3) The knowledge acquired during the training of the model is stored in an implicit manner and hence it is not easy to come up with reasonable interpretation of the overall structure of the network.[10]

This paper examines the potential of least-square support vector machine (LSSVM) to predict the fracture parameters of concrete. The LSSVM is a statistical learning theory that adopts a least-squares linear system as a loss function instead of the quadratic program in original support vector machine (SVM).[12] It is closely related to Gaussian processes and regularization networks. It requires solving a set of only linear equations (linear programming), which is much easier and computationally very simple.

The paper has the following aims:

1) To investigate the feasibility of LSSVM for predicting fracture parameters of concrete.

2) To compute the error of predicted data.

3) To compare the performance of developed LSSVM with other available methods for determination of fracture parameters of concrete.

2. LSSVM model

LSSVM models are an alternate formulation of SVM regression[13] proposed by Suykens et al.[14] Consider a given training set of N data points $\{x_k, y_k\}_{k=1}^N$ with input data $x_k \in R^N$ and output $y_k \in r$ where R^N is N-dimensional vector space and r is the one-dimensional vector space. The three input variables of the LSSVM model to predict concrete fracture parameters are water-cement ration (w/c), maximum size of aggregate (d_{max}) and characteristic strength (f_{sc}). The output of the LSSVM model is the

[1)]Structural Engineering, VIT University, Vellore, India.
[2)]Department of Civil Engineering, Kunsan National University, Kunsan, Jeonbuk, Korea.
[3)]Director, Centre for Disaster Mitigation and Management, VIT University, Vellore, India.
[4)]Centre for Disaster Mitigation and Management, VIT University, Vellore, India. Email: pijush.phd@gmail.com.

critical stress intensity factor (K_{Ic}^{s}) and the critical crack tip opening displacement ($CTOD_c$). Therefore, in this paper, $x = [w/c, d_{\max}, f_{sc}$ and $y = [K_{Ic}^{s}, CTOD_c$. In feature space, LSSVM models take the form

$$y(x) = w^T \varphi(x) + b \quad (1)$$

where the nonlinear mapping, $\varphi(x)$, maps the input data into a higher-dimensional feature space; $w \in R^N$; $b \in r$; w is an adjustable weight vector; b is the scalar threshold. In LSSVM for function estimation, the formulation of optimization problem as follows

$$\text{Minimize } \frac{1}{2}w^T w + \gamma \frac{1}{2} \sum_{K=1}^{N} e_k^2 \quad 2(a)$$

$$\text{Subjected to } y(x) = w^T \varphi(x_k) + b + e_k, k = 1, \cdots, N \quad 2(b)$$

where φ is the regularization parameter, determining the trade-off between the fitting error minimization and smoothness and e_k is error variable. The Lagrangian, $L(w, b, e, \alpha)$, for the above optimization problem (2) is

$$L(w, b, e, \alpha)$$

$$\frac{1}{2}w^T w + \gamma \frac{1}{2} \sum_{K=1}^{N} e_k^2 - \sum_{K=1}^{N} \alpha_K \{ Y_K (w^T \varphi(X_K) + b) - 1 + e_K \} \quad (3)$$

with α_k is a Lagrange multiplier. The conditions for optimality are given by

$$\frac{\partial L}{\partial w} = 0 \Rightarrow w = \sum_{k=1}^{N} \alpha_k [\varphi(x_k)]$$

$$\frac{\partial L}{\partial b} = 0 \Rightarrow \sum_{k=1}^{N} \alpha_k = 0$$

$$\frac{\partial L}{\partial e_k} = 0 \Rightarrow \alpha_k = e_k, k = 1, \cdots, N$$

$$\frac{\partial L}{\partial \alpha_k} = 0 \Rightarrow w^T \varphi(x_k) + b + e_k - y_k = 0 \quad (4)$$

After elimination of e_k and w, the solution is given by the following set of linear equations

$$\begin{bmatrix} 0 & 1^T \\ 1 & \Omega + \gamma^{-1} I \end{bmatrix} \begin{bmatrix} b \\ \alpha \end{bmatrix} = \begin{bmatrix} 0 \\ y \end{bmatrix} \quad (5)$$

where $y = [y_1, \cdots, y_N]$, $1 = [1, \cdots, 1]$, $\alpha = [\alpha_1, \cdots, \alpha_N]$ and Mercer's theorem is applied within the Ω matrix, $\Omega = \varphi(x_k)^T$, $\varphi(x_1) = K(x_k, x_l)$, k, $l = 1, \cdots, N$ and $K(x_k, x_l)$is the kernel function. Choosing $\gamma > 0$ ensures the matrix is invertible.

$$\Phi = \begin{bmatrix} 0 & 1^T \\ 1 & \Omega + \gamma^{-1} I \end{bmatrix} \quad (6)$$

Then the analytical of α and b is given by

$$\begin{bmatrix} b \\ \alpha \end{bmatrix} = \Phi^{-1} \begin{bmatrix} 0 \\ y \end{bmatrix} \quad (7)$$

The Gaussian kernel has been used for the analysis what is given by

$$K(x_k, x_l) = \exp\left\{ -\frac{(x_k - x_l)(x_k - x_l)^T}{2\sigma^2} \right\}, k, l = 1, 2, \cdots, N \quad (8)$$

where σ is the width of Gaussian kernel.The resulting LSSVM model:

$$y(x) = \sum_{k=1}^{N} \alpha k(x_k, x) + b \quad (9)$$

3. Details of LSSVM

The above-mentioned methodology has been implemented to predict critical stress intensity factor (K_{Ic}^{s}) and the critical crack tip opening displacement ($CTOD_c$). This study uses the database collected by Ince.8 For developing LSSVM, the data have been divided into two sub-sets: a training dataset to construct the model, and a testing dataset to estimate the model performance. This study uses the same training and testing dataset as used by Ince.8 In this paper, data are normalized against their maximum values. In this study, a sensitivity analysis has been done to extract the cause and effect relationship between the inputs and output of the LSSVM model. The basic idea is that each input of the model is offset slightly and the corresponding change in the output is reported. The procedure has been taken from the work of Liong et al.11 According to Liong et al,[11] the sensitivity(S) of each input parameter has been calculated by the following formula

$$S(\%) = \frac{1}{N} \sum_{j=1}^{N} \left(\frac{\%\text{change in ouput}}{\%\text{change in input}} \right)_j \times 100 \quad (10)$$

where N is the number of data points. The analysis has been carried out on the trained model by varying each of input parameter, one at a time, at a constant rate of 20%. In the present paper, training, testing and sensitivity analysis of LSSVM have been carried out using MATLAB.

4. Results and discussions

Different combinations of σ and γ values are tried to yield the best performance of LSSVM model. The coefficient of correlation (R) is the main criterion that is used to evaluate the performance of the LSSVM model. For good model, the value of R is close to one. For $CTOD_c$, the design values of γ and σ is 150 and 1 respectively. Figure 1 shows the performance of training and testing data of LSSVM model for prediction of $CTOD_c$. For K_{Ic}^{s}, the design values of γ and σ is 100 and 5 respectively. Figure 2 shows the performance of training and testing data of LSSVM model for prediction of K_{Ic}^{s}. The value of R is close to one for both $CTOD_c$

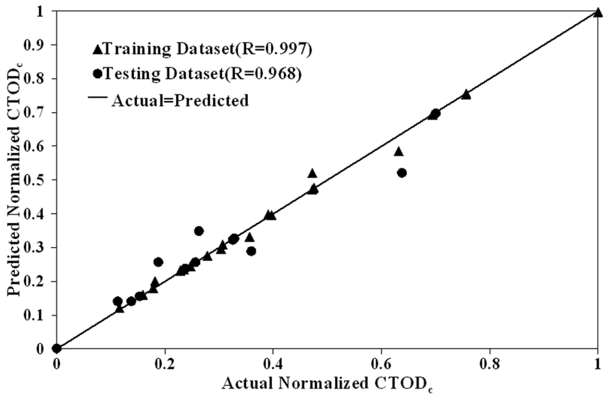


Fig. 1 Performance of training / testing dataset for ($CTOD_c$) prediction.

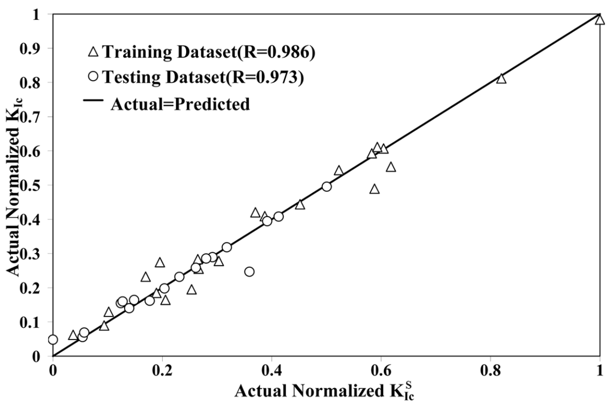


Fig. 2 Performance of training/testing dataset for (K_{Ic}^S) prediction.

as well as K_{Ic}^s . The following equation (by putting, $K(x_k, x) = \sum_{k=1}^{N} \exp\left\{-\frac{(x_k-x)(x_k-x)^T}{2\sigma^2}\right\}$, $N = 22$, $\sigma = 5$ and $b = -0.0130$ in Eq. (9)) has been developed for the prediction of K_{Ic}^s based on the developed LSSVM model.

$$K_{Ic}^s = \sum_{k=1}^{22} \alpha \exp\left\{-\frac{(x_k-x)(x_k-x)^T}{50}\right\} - 0.0130 \qquad (11)$$

Similarly for prediction of $CTOD_c$ (by putting, $K(x_k, x) = \sum_{k=1}^{N} \exp\left\{-\frac{(x_k-x)(x_k-x)^T}{2\sigma^2}\right\}$, $N = 22$, $\sigma = 1$ and $b = 0.2574$ in equation 9), the following equation has been developed.

$$CTOD_c = \sum_{i=1}^{22} \alpha \exp\left\{-\frac{(x_i-x)(x_i-x)^T}{2}\right\} + 0.2574 \qquad \text{(Eq.12)}$$

Figures 3 and 4 show the value of Lagrange multipliers [Alpha (α)] for ($CTOD_c$) and (K_{Ic}^s) respectively. For K_{Ic}^s, fig. 5(a) and (b) depict the 95% error bar of training and testing data respectively. For $CTOD_c$, Fig. 6(a) and (b) illustrate the 95% error bar of training and testing data respectively. The predicted error bar can be used to determine whether differences are statistical significant. For prediction of K_{Ic}^s and $CTOD_c$, the determination of error bar on the prediction point is important to estimate the corresponding risk. The developed LSSVM model has been applied on a new

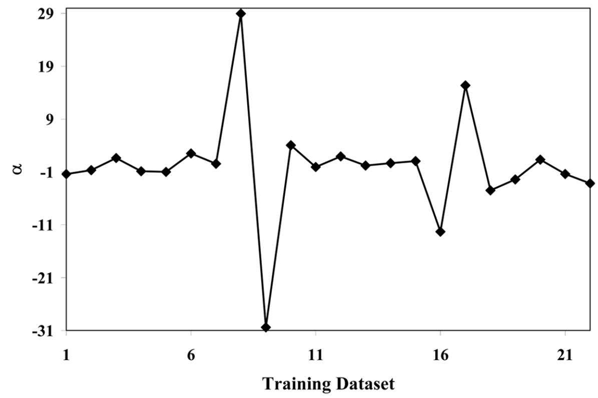


Fig. 3 Values of alpha (α) for $CTOD_c$.

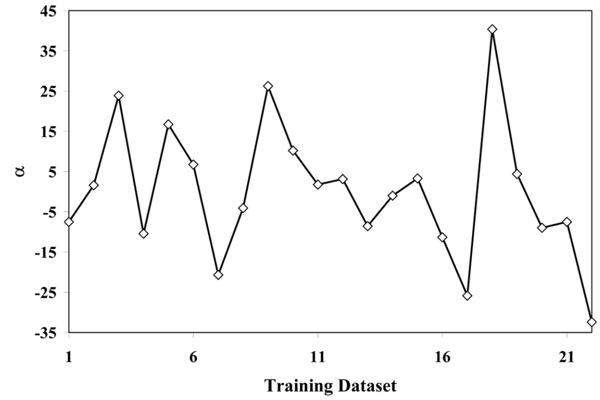
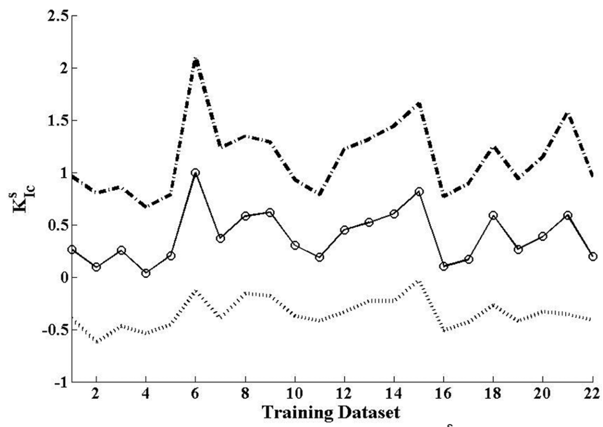
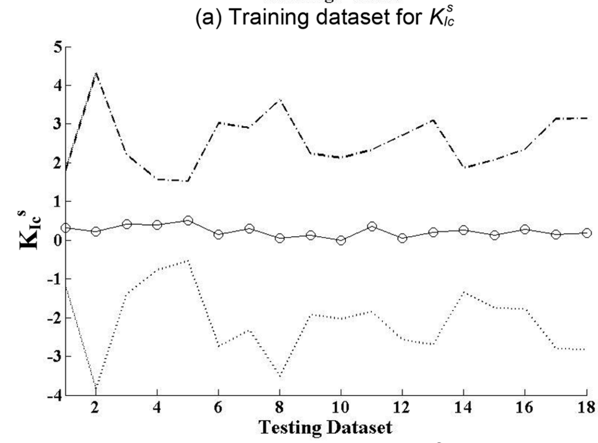


Fig. 4 Values of alpha (α) for K_{Ic}^S.

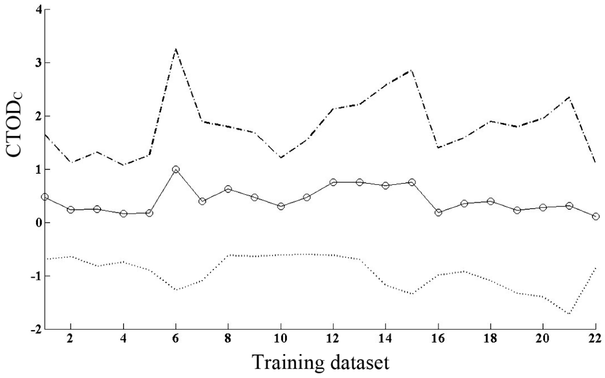


(a) Training dataset for K_{Ic}^s

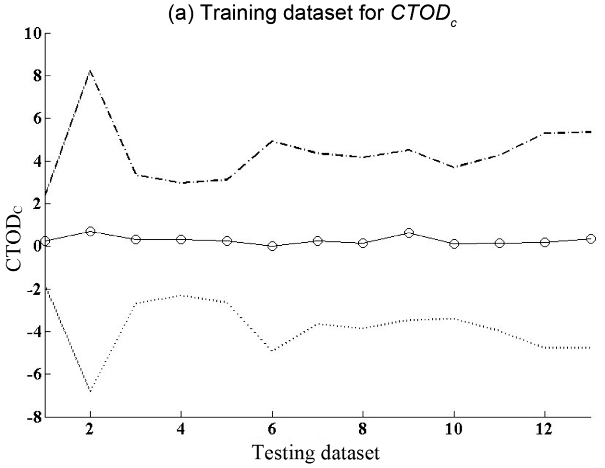


(b) Testing dataset for K_{Ic}^s

Fig. 5 95% error bar.



(a) Training dataset for $CTOD_c$



(b) Training dataset for $CTOD_c$

Fig. 6 95% error bar.

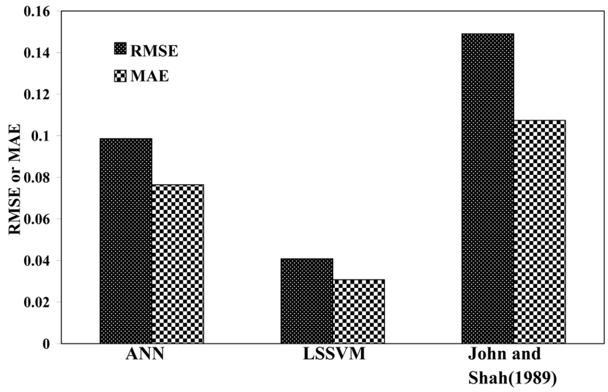


Fig. 7 Comparison between different methods for prediction of K^S_{Ic}.

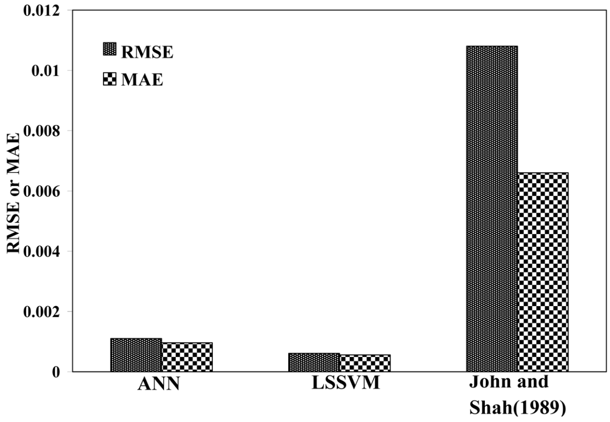


Fig. 8 Comparison between different methods for prediction of $CTOD_c$.

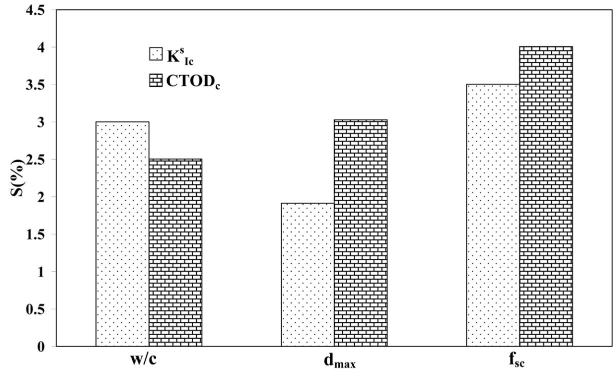


Fig. 9 Sensitivity analysis of input parameters.

dataset for prediction of K^s_{Ic} and $CTOD_c$. The new dataset has been collected from the work of Ince.8 Figures 7 and 8 show the comparative study between ANN, LSSVM and regression model developed by John & Shah6 for the new dataset. The comparison has been carried out in terms of root mean square error (RMSE) and mean absolute error (MAE). The performance of the LSSVM is better than the ANN and regression model (John & Shah).6 The use of the structural risk minimization principle in defining cost function provided more generalization capacity with the LSSVM compared to the ANN, which uses the empirical risk minimization principle. ANN uses large number of controlling parameters such as the number of hidden layers, number of hidden nodes, learning rate, momentum term, number of training epochs, transfer functions, weight initialization methods, etc. Whereas, LSSVM uses only two parameters (γ and σ). The developed LSSVM gives error bar of predicted K^s_{Ic} and $CTOD_c$. However, ANN does not give error bar.

Figure 9 presents the results of sensitivity analysis. For K^s_{Ic}, f_{sc} has the most significant effect on the predicted K^s_{Ic} followed by w/c and d_{max}. Sensitivity analysis also shows that f_{sc} has the most significant effect on the predicted $CTOD_c$ followed by d_{max} and w/c.

5. Conclusions

This study has shown that applied LSSVM for prediction of K^s_{Ic} and $CTOD_c$ of concrete is better than the available methods. LSSVM's most important advantage is that it leads to global (and often unique) nonlinear model that can be calculated easily. LSSVM has the additional advantage of error bar that yields confidence interval. The results indicate that the proposed method provides prediction reliability, accuracy and suppose to have promising potential for practical use. User can use the developed equation for prediction of K^s_{Ic} and $CTOD_c$ of concrete. In summary, it can be concluded that the LSSVM is a robust model for prediction of K^s_{Ic} and $CTOD_c$ of concrete.

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