Comparison of Polynomial and Radial Basis Kernel Functions based SVR and MLR in Modeling Mass Transfer by Vertical and Inclined Multiple Plunging Jets

S. Deswal, M. Pal

Abstract—Presently various computational techniques are used in modeling and analyzing environmental engineering data. In the present study, an intra-comparison of polynomial and radial basis kernel functions based on Support Vector Regression and, in turn, an inter-comparison with Multi Linear Regression has been attempted in modeling mass transfer capacity of vertical ($\theta = 90^O$) and inclined (θ multiple plunging jets (varying from 1 to 16 numbers). The data set used in this study consists of four input parameters with a total of eighty eight cases, forty four each for vertical and inclined multiple plunging jets. For testing, tenfold cross validation was used. Correlation coefficient values of 0.971 and 0.981 along with corresponding root mean square error values of 0.0025 and 0.0020 were achieved by using polynomial and radial basis kernel functions based Support Vector Regression respectively. An intra-comparison suggests improved performance by radial basis function in comparison to polynomial kernel based Support Vector Regression. Further, an inter-comparison with Multi Linear Regression (correlation coefficient = 0.973 and root mean square error = 0.0024) reveals that radial basis kernel functions based Support Vector Regression performs better in modeling and estimating mass transfer by multiple plunging jets.

Keywords—Mass transfer, multiple plunging jets, polynomial and radial basis kernel functions, Support Vector Regression.

I. Introduction

PLUNGING jets have wide applications in environmental and chemical engineering, including aeration and floatation in water and wastewater treatment, bubble floatation of minerals, oxygenation of mammalian-cell bio-reactors, biological aerated filter, fermentation, stirring of chemicals as well as increasing gas-liquid transfer, cooling system in power plants, plunging columns, breakers and waterfalls [1]-[7]. Plunging jet aeration/oxygenation system provides a simple and inexpensive mode of mass transfer and it is an attractive way to effect mass/oxygen transfer than conventional systems for various reasons [1], [7]-[9] such as simplicity in design, construction and operation; facilitation in the make-up of "closed" system, which enhance complete utilization of oxygen and volatile reactants; absence of compressor blower; absence of stirring devices because the water jet itself achieves

aeration and mixing; energetically attractive as a means of straightforward contacting mechanism in fouling or hazardous environments; and free from operational difficulties like clogging in air diffusers, limitations on the installation of mechanical aerators by the tank width, etc. Due to these potential advantages, there has been a growing interest in the aeration/oxygenation by plunging water jets in the last few years.

Numerous studies have been reported on air-water oxygen transfer by single plunging jets [10]-[18]. Empirical relationships between various jet parameters for estimating mass/oxygen transfer capacity have also been suggested in some of these studies. The simplest relationships for single water jets plunging vertically (i.e. jet impact angle, $\theta = 90^O$) as proposed by [19], [15] and [14] respectively are:

$$K_L A_{(20)} = 3.1 \times 10^{-4} + 4.85 \times 10^{-2} v_j^3 d_j^2 \qquad (1)$$

$$K_L A_{(20)} = 9 \times 10^{-5} P \qquad (2)$$

$$K_L a_{(20)} = 0.029 (P/V)^{0.65} \qquad (3)$$

where $K_L A_{(20)}$ is volumetric oxygen transfer factor at standard conditions (m^3/h); v_j is jet velocity at exit (m/s); d_j is jet diameter (m); P is jet power (W); $K_L a_{(20)}$ is volumetric oxygen transfer coefficient at standard conditions (1/s); and P/V is jet power per unit volume (kW/m^3).

Few of the studies have also been reported on air-water oxygen transfer by multiple plunging jets [20]-[22], and have suggested relationships between various jet parameters for estimating and predicting oxygen transfer by multiple plunging jets. The relationships for vertical multiple plunging jets ($\theta = 90^O$) as proposed by [20] and for inclined multiple plunging jets ($\theta = 60^O$) as proposed by [21] respectively are:

$$K_L a_{(20)} = 0.113 \, n^{0.84} \, v_j^{2.14} \, d_j^{1.53} \qquad (4)$$

$$K_L a_{(20)} = 0.103 \, n^{0.81} \, v_j^{2.11} \, d_j^{1.43} \qquad (5)$$

where, $K_L a_{(20)}$ is the volumetric mass/oxygen transfer

Dr. Surinder Deswal and Dr. Mahesh Pal are Professors in Civil Engineering Department of National Institute of Technology, Kurukshetra - 136119, Haryana, India (Phone: +91-1744-233356; fax: +91-1744-238050; e-mail: deswal.leo@gmail.com; mahesh.pal@nitkkr.ac.in).

coefficient at standard conditions (per sec) and n is the number of jets in multiple plunging jets oxygenation system.

Recently, [23] has used multi linear regression (MLR) approach and proposed a joint equation for estimating oxygen transfer capacity by multiple plunging jets, both vertical (θ = 90°) and inclined jets (θ = 60°), as under:

$$K_L a_{(20)} = 0.095\, I_f\; n^{0.82}\; v_j^{2.13}\; d_j^{1.48} \tag{6}$$

where, I_f is Inclination Factor. For vertical jets (θ=90°), I_f = 1; and for inclined jets (θ=60°), I_f = 1.29.

In last few years, computational techniques have been used successfully in civil and environmental engineering applications [24]-[32]. In this paper, an attempt has been made to utilize and check the applicability and performance of polynomial and radial basis kernel functions based on Support Vector Regression and, in turn, an inter-comparison with Multi Linear Regression in modeling mass transfer by vertical and inclined multiple plunging jets.

II. SUPPORT VECTOR REGRESSION

Support vector machines (SVMs) are classification or regression methods derived from statistical learning theory [33]. The SVMs classification methods are based on the principle of *optimal separation of classes*.

If the classes are separable – this method selects, from among the infinite number of linear classifiers, the one that minimize the generalization error, or at least an upper bound on this error, derived from structural risk minimization. Thus, the selected hyper plane will be one that leaves the maximum margin between the two classes, where margin is defined as the sum of the distances of the hyper plane from the closest point of the two classes [33].

If the two classes are non-separable, the SVMs try to find the hyper plane that maximizes the margin and at the same time, minimizes a quantity proportional to the number of misclassification errors. The trade-off between margin and misclassification error is controlled by a positive constant that has to be chosen beforehand. This technique of designing SVMs can be extended to allow for non-linear decision surfaces. This can be achieved by projecting the original set of variables into a higher dimensional feature space and formulating a linear classification problem in the feature space [33]. The support vector machines can be applied to regression problems and can be formulated as given below:

Vapnik [33] proposed Support Vector Regression (SVR) by introducing an alternative insensitive loss function (ε). This loss function allows the concept of margin to be used for regression problems. Purpose of the SVR is to find a function having at the most ε deviation from the actual target vectors for all given training data and have to be as flat as possible [34]. This can be put in other words as the error on any training data has to be less than ε. For a given training data with 'k' number of samples, represented by $(x_1, y_1),............,(x_k, y_k)$ a linear decision function can be represented by

$$f(x, \alpha) = \langle w, x \rangle + b \tag{7}$$

where $f(x, \alpha) \Rightarrow \alpha \in \Lambda$ (where Λ is a set of parameters used in the decision rule; for example, in a multilayer neural network, Λ is a set of weights of the network), 'x' is an N dimensional observed data vector, R is set of all real numbers, 'b' is the bias term that determine the offset of the hyperplane from origin and 'w' determines the orientation of hyperplane. Further, $\langle w, x \rangle$ represents the dot product in space R^N. A smaller value of 'w' indicates the flatness of (7), which can be achieved by minimizing the Euclidean norm [34] as defined by $\|w\|^2$. Thus, an optimization problem for regression can be written as:

$$\text{minimize } \frac{1}{2}\|w\|^2 \text{ subject to} \begin{cases} y_i - \langle w, x_i \rangle - b \ \le\ \varepsilon \\ \langle w, x_i \rangle + b - y_i \ \le\ \varepsilon \end{cases} \tag{8}$$

The optimization problem in (8) is based on the assumption that there exists a function that provides an error on all training pairs which is less than or equal to ε. In real life problems, there may be a situation like one defined for classification by [33]. Therefore, to allow some more error, slack variables ξ, ξ' can be introduced in (8), and the optimization problem defined above can be rewritten as:

$$\text{minimize } \frac{1}{2}\|w\|^2\ +\ C\sum_{i=1}^{k}\left(\xi_i\ +\ \xi_i'\right)$$

$$\text{subject to } y_i - \langle w, x_i \rangle - b \ \le\ \varepsilon + \xi_i$$

$$\langle w, x_i \rangle + b - y_i \ \le\ \varepsilon + \xi_i' \tag{9}$$

and $\xi_i, \xi_i' \ge 0$ for all $i = 1, 2,......, k.$

The parameter 'C' is determined by the user and determines the trade-off between the flatness of the function and the amount by which the deviations to the error more than ε can be tolerated. The optimization problem in (9) can be solved by replacing the inequalities with a simpler form by transforming the problem to a dual space representation using Lagrangian multipliers [35].

The Lagrangian is formed by introducing positive Lagrange multipliers $\lambda_i, \lambda_i', \eta_i, \eta_i'$ where i = 1,....,k and multiplying the constraint equations by these multipliers, and finally subtracting the results from the objective function (i.e. $\|w\|^2$). The Lagrangian for (9) can be written as:

$$L = \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{k}\left(\xi_i + \xi_i'\right) - \sum_{i=1}^{k}\lambda_i\left(\varepsilon + \xi_i - y_i + \langle w, x_i \rangle + b\right)$$
$$- \sum_{i=1}^{k}\lambda_i'\left(\varepsilon + \xi_i' + y_i - \langle w, x_i \rangle - b\right) - \sum_{i=1}^{k}\left(\eta_i\xi_i + \eta_i'\xi_i'\right) \quad (10)$$

The solution of this optimization problem can be obtained by locating the saddle point of the Lagrange function defined in (10). The Saddle points of (10) can be obtained by equating partial derivative of 'L' with respect to w, b, ξ_i and ξ_i' to zero. Thus, (7) can now be written as:

$$f(\mathbf{x}, \alpha) = \sum_{i=1}^{k}\left(\lambda_i' - \lambda_i\right)\langle \mathbf{x}_i, \mathbf{x} \rangle + b \quad (11)$$

The technique discussed above can be extended to allow for non-linear support vector regression by introducing the concept of the kernel function [33]. This is achieved by mapping the data into a higher dimensional feature space, thus performing linear regression in feature space. The regression problem in feature space can be written by replacing $\mathbf{x}_i \cdot \mathbf{x}_j$ in (11) with $\Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}_j)$, where $\Phi(\mathbf{x})$ is the mapping to the feature space.

$$K(\mathbf{x}_i, \mathbf{x}_j) \equiv \Phi(\mathbf{x}_i) \cdot \Phi(\mathbf{x}_j) \quad (12)$$

Regression function given in (11) can now be written as:

$$f(\mathbf{x}, \alpha) = \sum_{i=1}^{k}\left(\lambda_i' - \lambda_i\right)K(\mathbf{x}_i, \mathbf{x}) + b \quad (13)$$

TABLE I
VALUES OF USER-DEFINED PARAMETERS

Kernel	C	d	γ
Polynomial (poly)	25	2	--
Radial basis (rbf)	25	--	1

TABLE II
CORRELATION COEFFICIENT AND RMSE VALUES

Approach	Correlation coefficient	Root mean square error
MLR: (6) proposed by [23]	0.973	0.0024
SVR poly	0.971	0.0025
SVR rbf	0.981	0.0020

III. DATA SET AND METHODOLOGY

Data used in the present study is taken from two earlier studies [20] and [21] on mass transfer by multiple vertical (jet impact angle, θ = 90[O]) and multiple inclined (jet impact angle, θ = 60[O]) plunging jets respectively. The dataset consists of eighty eight experimental observations, forty four each for vertical and inclined multiple plunging jets, on different configurations in terms of jet diameter and number of jets (varying from 1 to 16).

Four input parameters, namely jet velocity at exit (v_j, in

m/s), jet diameter (d_j, in m), number of jets (n) and inclination factor (I_f) representing jet impact angle (θ, in degree) were used to predict volumetric mass/oxygen transfer coefficient at standard conditions ($K_L a_{(20)}$, in per sec) in the present study. These are the same input parameters as used in (6) derived by using Multi Linear Regression by [23].

Support Vector Regression (SVR) requires selection of a suitable kernel. The two most frequently used kernel functions namely, polynomial and a radial basis kernel function were used in present study for intra-comparison. The use of SVR requires setting of user-defined parameters such as regularisation parameter (C), kernel specific parameters (d and γ) and error-insensitive zone ε. Variation in error-insensitive zone ε found to have no effect on the predicted volumetric mass/oxygen transfer coefficient in present study so a default value of 0.0010 was chosen for all experiments [36]. The optimal values of parameters C, d and γ were obtained after several trials with the dataset. In order to test the performance of the used algorithm with both kernel functions, a ten-fold cross-validation was used. Correlation coefficient and root mean square error (RMSE) were used to compare the performance in the present study.

IV. RESULTS

Table I provides the optimal values of user-defined parameters; whereas, Table II provides the correlation coefficient and RMSE values using both kernels and (6). For intra-comparison of the performances of two kernel functions of SVR, as well as for inter-comparison with (6) proposed by [23], a graph between actual and predicted volumetric mass/oxygen transfer coefficient at standard conditions ($K_L a_{(20)}$, in per sec) is plotted in a way to show the scatter around a line of perfect agreement (i.e. a line at 45[O]). The performance of SVM_poly, SVM_rbf and MLR represented by (6) are shown in Fig. 1.
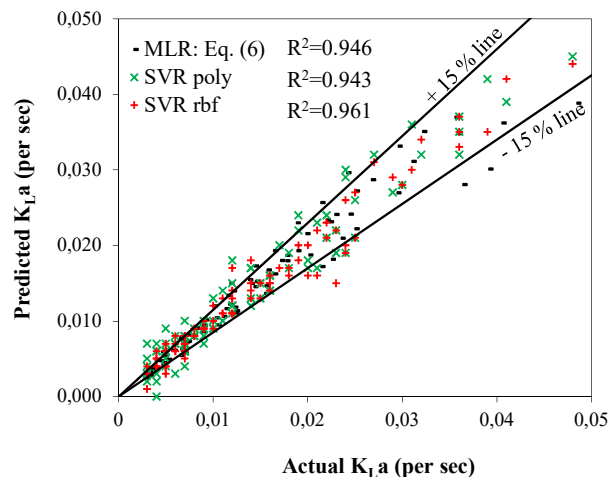

Fig. 1 Actual v/s predicted volumetric mass transfer coefficient

Results suggest effectiveness of both kernel functions in modeling and predicting volumetric mass/oxygen transfer coefficient with this dataset as majority of points are lying within ±15 % of the line of perfect agreement as shown in Fig. 1. A correlation coefficient of 0.971 (RMSE = 0.0025) and 0.981 (RMSE = 0.0020) was achieved with polynomial and radial basis function kernels respectively in comparison to a correlation coefficient of 0.973 (RMSE = 0.0024) by (6) as proposed by [23] (Table II). A coefficient of determination (R^2) of 0.943 and 0.961 was achieved with polynomial and radial basis function kernels respectively in comparison to a coefficient of determination of 0.946 by (6) and provided in Fig. 1. Further, Fig. 1 suggests that MLR, represented by (6), under-predict the volumetric mass transfer coefficient in comparison to SVR_{rbf} and over-predict in comparison to SVR_{poly} for this dataset. The average ratio of actual to predicted volumetric mass transfer coefficient of all experiments is 0.992 using (6), in comparison to 1.443 and 1.056 with polynomial and radial basis kernel function respectively. The statistical results indicate the applicability of SVR in predicting the overall mass transfer coefficient by multiple plunging jets (both vertical and inclined); however, radial basis kernel function works well in comparison to polynomial kernel function.

Fig. 2 represents the variation of actual and predicted overall mass transfer coefficient by multiple plunging jets with the number of test data. The first 44 test data numbers are for inclined multiple plunging jets and the rest 45 to 88 test data numbers are for vertical multiple plunging jets. It is evident from this plot that overall mass transfer coefficient predicted by radial basis kernel function of SVR is in good agreement with actual experimental values of both vertical and inclined multiple plunging jets in comparison with polynomial kernel function of SVR and MLR represented by (6) as proposed by [23].
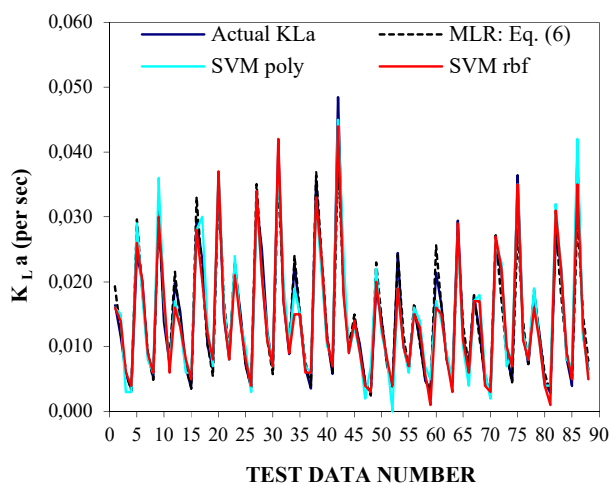

Fig. 2 Variation in predicted values by SVR in comparison to (6) and the actual values of overall oxygen transfer coefficient at standard condition (K_La) by vertical and inclined multiple plunging jets

V. CONCLUSION

Results from this study suggests that SVR is a powerful computational tool and can effectively be used in modeling and predicting overall oxygen mass transfer coefficient by multiple plunging jets, both vertical and inclined. The proposed modeling approach works quite well with radial basis kernel, while it works well with polynomial kernel. Thus, SVR can effectively be used in modeling physical processes like one predicting the overall oxygen mass transfer coefficient by plunging jets, within the range of input parameters used to train the model, rather than referring to costly experimental investigation.

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