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SCIENTIFIC PAPER

UDC 537.314:621.3.012.1:621.315.2

THE SUPPORT VECTOR REGRESSION WITH THE PARAMETER TUNING ASSISTED BY A DIFFERENTIAL EVOLUTION TECHNIQUE: STUDY OF THE CRITICAL VELOCITY OF A SLURRY FLOW IN A PIPELINE

This paper describes a robust Support Vector regression (SVR) methodology, which can offer a superior performance for important process engineering problems. The method incorporates hybrid support vector regression and a differential evolution technique (SVR-DE) for the efficient tuning of SVR meta parameters. The algorithm has been applied for the prediction of critical velocity of the solid-liquid slurry flow. A comparison with selected correlations in the literature showed that the developed SVR correlation noticeably improved the prediction of critical velocity over a wide range of operating conditions, physical properties, and pipe diameters.

Key words: support vector regression; differential evolution; slurry critical velocity.

Conventionally, two approaches, namely *phenomenological* (first principles) and *empirical*, are employed for the slurry flow modeling. The advantages of a phenomenological model are: (i) it represents a physico-chemical phenomenon underlying the process explicitly and (ii) it possesses the extrapolation ability. Owing to the complex nature of many multi-phase phase slurry processes, the underlying physico-chemical phenomenon is seldom fully understood.

Also, the collection of the requisite phenomenological information is costly, time-consuming and tedious and therefore the development and the solution of the phenomenological process models have considerable practical difficulties. These difficulties necessitate the exploration of the alternative modeling formalisms.

In the last decade, *the artificial neural networks* (ANNs) and more recently, *the support vector regression* (SVR) have emerged as two attractive tools for non-linear modeling, especially in situations where the development of phenomenological or conventional regression models becomes impractical or cumbersome. In recent years, the support vector regres-

sion (SVR) [1-3] which is a statistical learning theory based machine learning formalism is gaining popularity over ANN due to its numerous attractive features and a promising empirical performance.

The main difference between conventional ANNs and SVM lies in the risk minimization principle. The conventional ANNs implement the empirical risk minimization (ERM) principle to minimize the error on the training data, while SVM adheres to the Structural Risk Minimization (SRM) principle seeking to set up an upper bound of the generalization error [1-3].

This study is motivated by a growing popularity of the support vector machines (SVM) for regression problems. Although the foundation of the SVR paradigm was laid down in the mid 1990s, its chemical engineering applications such as fault detection [4,5] have emerged only recently.

However, many SVM regression application studies are performed by "expert" users having good understanding of SVM methodology. Since the quality of SVM models depends on a proper setting of SVM meta-parameters, the main issue for practitioners trying to apply the SVM regression is how to set these parameter values (to ensure good generalization performance) for a given data set. Whereas the existing sources on SVM regression give some recommendations on the appropriate setting of SVM parameters, there are clearly no consensus and contradictory opinions.

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Paper received: May 7, 2008.

Paper revised: August 29, 2008.

Paper accepted: September 8, 2008.

Conventionally, various deterministic gradient based methods [6] are used for optimizing a process model. Most of these methods however require that the objective function should be smooth, continuous, and differentiable. The SVR models can not be guaranteed to be smooth, especially in regions wherein the input-output data (training set) used in model building is located sparsely. In such situations, an efficient optimization formalism known as Differential Evolution (DE), which is lenient towards the form of the objective function, can be used. In the recent years, DEs that are members of the stochastic optimization formalisms have been used with a great success in solving problems involving very large search spaces. The DEs were originally developed as the genetic engineering models mimicking population evolution in natural systems. Specifically, DE like a genetic algorithm (GA) enforces the “survival-of-the-fittest” and “genetic propagation of characteristics” principles of the biological evolution for searching the solution space of an optimization problem. DE has been used to design several complex digital filters [7] and to design fuzzy logic controllers [8]. DE can also be used for parameter estimations, *e.g.* Babu and Sastry [9] used DE for the estimation of the effective heat transfer parameters in trickle-bed reactors using radial temperature profile measurements. They concluded that DE takes less computational time to converge, compared to the existing techniques, without compromising with the accuracy of the parameter estimates.

In the present paper, SVR formalism is integrated with the differential evolution to arrive at modeling and optimization strategies. The strategy (henceforth referred to as “SVR-DE”) use an SVR as the non-linear process modeling paradigm, and the DE for optimizing the meta-parameters of the SVR model so that an improved prediction performance is realized. To our knowledge, the hybrid involving SVR and DE is being used for the first time for the chemical process modeling and optimization. In the present work, we propose a hybrid support vector regression-differential evolution (SVR-DE) approach for tuning the SVR meta parameters and illustrate it by applying it for predicting the critical velocity of the solid liquid flow.

SUPPORT VECTOR REGRESSION (SVR) MODELING

Support vector regression (SVR) is an adaptation of a recent statistical learning theory based classification paradigm, namely “support vector machines” [3]. The SVR formulation follows structural risk minimization (SRM) principle, as opposed to the empirical risk minimization (ERM) approach which is

commonly employed within statistical machine learning methods and also in training ANNs. In SRM, an upper bound on the generalization error is minimized as opposed to the ERM, which minimizes the prediction error on the training data. This equips the SVR with a greater potential to generalize the input-output relationship learnt during its training phase for making good predictions for new input data. The SVR is a linear method in a high dimensional feature space, which is nonlinearly related to the input space. Though the linear algorithm works in the high dimensional feature space, in practice it does not involve any computations in that space due to the usage of kernels; all necessary computations are performed directly in the input space. In the following, the basic concepts of SVR are introduced. A more detailed description of SVR can be found elsewhere [1,10-12].

Support vector regression: at a glance

Consider a training data set $g = \{(x_1, y_1), (x_2, y_2), \dots, (x_P, y_P)\}$, such that $x_i \in \mathcal{V}^N$ is a vector of input variables and $y_i \in \mathcal{V}$ is the corresponding scalar output (target) value. Here, the modeling objective is to find a regression function, $y = f(x)$, such that it accurately predicts the outputs $\{y\}$ corresponding to a new set of input-output examples, $\{(x, y)\}$, which are drawn from the same underlying joint probability distribution, $P(x, y)$, as the training set. To fulfill the stated goal, SVR considers the following linear estimation function:

$$f(x) = \langle w, \phi(x) \rangle + b \quad (1)$$

where w denotes the weight vector; b refers to a constant known as “bias”; $f(x)$ denotes a function termed *feature*, and $\langle w, \phi(x) \rangle$ represents the dot product in the feature space, ℓ , such $\phi: \mathcal{X} \rightarrow \ell$, $w \in \ell$. In SVR, the input data vector, x , is mapped into a high dimensional feature space, ℓ , *via* a nonlinear mapping function, ϕ , and a linear regression is performed in this space for predicting y . Thus, the problem of non-linear regression in lower dimensional input space \mathcal{V}^N is transformed into a linear regression in the high dimensional feature space, ℓ . Accordingly, the original optimization problem involving non-linear regression is transformed into finding the flattest function in the feature space ℓ and not in the input space, x . The unknown parameters w and b in Eq. (1) are estimated using the training set, g . To avoid over-fitting and thereby improving the generalization capability, the following regularized functional involving summation of the empirical risk and a complexity term w^2 is minimized:

$$R_{\text{reg}}[f] = R_{\text{emp}}[f] + \lambda |w|^2 = \sum_{i=1}^P C[f(x_i) - y_i] + \lambda |w|^2 \quad (2)$$

where R_{reg} and R_{emp} denote the regression and empirical risks, respectively; w^2 is the Euclidean norm; C is a cost function measuring the empirical risk, and $\lambda > 0$ is a regularization constant. For a given function, f , the regression risk (test set error), $R_{reg}[f]$, is the possible error committed by the function f in predicting the output corresponding to a new (test) example input vector drawn randomly from the same sample probability distribution, $F(x, y)$, as the training set. The empirical risk, $R_{emp}[f]$, represents the error (termed "training set error") committed in predicting the outputs of the training set inputs. The minimization task described in Eq. (2) involves: (i) the minimization of the empirical loss function $R_{emp}[f]$ and (ii) obtaining as small a w as possible, using the training set g . The commonly used loss function is the "e-insensitive loss function" given as [2]:

$$C(f(x) - y) = |f(x) - y| - \varepsilon, \text{ for } |f(x) - y| \geq \varepsilon, \tag{3}$$

otherwise: $C = 0$

where ε is a precision parameter representing the radius of the tube located around the regression function (see Figure 1); the region enclosed by the tube is known as "e-intensive zone". The SVR algorithm attempts to position the tube around the data as shown in Figure 1.

The optimization criterion in Eq. (3) penalizes those data points whose y values lie more than ε distance away from the fitted function, $f(x)$. In Figure 1, the size of the stated excess positive and negative deviations are depicted by ζ and ζ^* , which are termed "slack" variables. Outside of the $(-\varepsilon, \varepsilon)$ region, the slack variables assume non-zero values. The SVR fits $f(x)$ to the data in a manner so that: (i) the training error is minimized by minimizing ζ and ζ^* and (ii) w^2 is mini-

mized to increase the flatness of $f(x)$ or to penalize over the complexity of the fitting function. Vapnik [2] showed that the following function possessing the finite number of parameters can minimize the regularized function in Eq. (2):

$$f(x, \alpha, \alpha^*) = \sum_{i=1}^P (\alpha_i - \alpha_i^*) K(x, x_i) + b \tag{4}$$

where α_i and $\alpha_i^* (\geq 0)$ are the coefficients (Lagrange multipliers) satisfying $\alpha_i \alpha_i^* = 0, i = 1, 2, \dots, P$ and $K(x, x_i)$ denotes the so-called "kernel" function describing the dot product in the feature space. The kernel function is defined in terms of the dot product of the mapping function as given by

$$K(x_i, x_j) = \langle \phi(x_i), \phi(x_j) \rangle \tag{5}$$

The advantage of this formulation (Eqs. (4) and (5)) is that for many choices of the set $\{\phi_i(x)\}$, including infinite dimensional sets, the form of K is analytically known and very simple. Accordingly, the dot product in the feature space $i \dots \ell$ can be computed without actually mapping the vectors x_i and x_j into that space (i.e., computation of $\phi(x_i)$ and $\phi(x_j)$). There are several choices for the kernel function K (refer Table 1); the two commonly used kernel functions, namely, radial basis function (RBF) and n^{th} degree polynomial are defined below in Eqs. (6) and (7), respectively.

$$K(x_i, x_j) = \exp\left(\frac{|x_i - x_j|^2}{2\sigma^2}\right) \tag{6}$$

$$K(x_i, x_j) = (1 + (x_i, x_j))^n \tag{7}$$

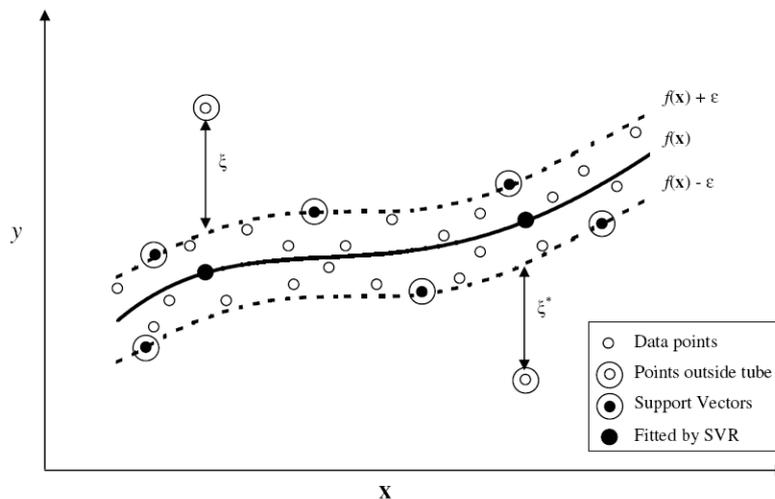


Figure 1. A schematic diagram of the support vector regression using e-insensitive loss function.

In Eq. (4), the coefficients α_i and α_i^* are obtained by solving following quadratic programming problem.

Maximize:

$$R(\alpha^*, \alpha) = -0.5 \sum_{i,j=1}^P (\alpha_i^* - \alpha_i)(\alpha_j^* - \alpha_j) K(x_i, x_j) - \varepsilon \sum_{i=1}^P (\alpha_i^* + \alpha_i) + \sum_{i=1}^P y_i (\alpha_i^* - \alpha_i)$$

subject to constraints:

$$0 \leq \alpha_i, \alpha_i^* \leq C, \forall i$$

and

$$\sum_{i=1}^P (\alpha_i^* - \alpha_i) = 0 \quad (8)$$

Having estimated α , α^* and b , using a suitable quadratic programming algorithm, the SVR-based regression function takes the form:

$$f(x, w) = f(x, \alpha, \alpha^*) = \sum_{i=1}^P (\alpha_i^* - \alpha_i) K(x_i, x) + b \quad (9)$$

where, vector w is described in terms of the Lagrange multipliers α and α^* . Owing to the specific character of the above-described quadratic programming problem, only some of the coefficients, $(\alpha_i^* - \alpha_i)$ are non-zero and the corresponding input vectors, x_i , are called support vectors (SVs). The SVs can be thought of as the most informative data points that compress the information content of the training set. The coefficients α and α^* have an intuitive interpretation as forces pushing and pulling the regression estimate $f(x)$ towards the measurements, y_i . In Eq. (9), the bias parameter, b , can be computed as follows:

$$b = \begin{cases} y_i - f(x_i), & b=0-\varepsilon \\ y_i - f(x_i), & b=0+\varepsilon, \text{ for } \alpha_i, \alpha_i^* \in (0, C) \end{cases}$$

where, x_i and y_i denote the i^{th} support vector and the corresponding target output, respectively.

In the SVR formulation, C and ε are two user-specified free parameters; while C represents the trade-off between the model-complexity and the approximation error, ε signifies the width of the ε -insensitive zone used to fit the training data. The stated free parameters together with the specific form of the kernel function control the accuracy and the generalization performance of the regression estimate. The procedure of a judicious selection of C and ε is explained by Cherkassky and Mulier [13].

Performance estimation of SVR

It is well known that SVM generalization performance (estimation accuracy) depends on a good setting of meta-parameters C and ε and kernel parameters, such as kernel type, a loss function type and the kernel parameters. The problem of the optimal parameter selection is further complicated by the fact that SVM model complexity (and hence its generalization performance) depends on all five parameters.

Selecting a particular kernel type and kernel function parameters is usually based on the application-domain knowledge and also should reflect the distribution of the input (x) values of the training data. Parameter C determines the trade off between the model complexity (flatness) and the degree to which deviations larger than ε are tolerated in optimization formulation. For example, if C is too large (infinity), then the objective is to minimize the empirical risk only, not regarding the model complexity part in the optimization formulation.

Parameter ε controls the width of the ε -insensitive zone, used to fit the training data [2,13]. The value of ε can affect the number of support vectors used to construct the regression function. The bigger ε , the fewer support vectors are selected. On the other hand, bigger ε values result in more “flat” estimates. Hence, both C and ε values affect the model complexity (but in a different way).

To minimize the generalization error, these parameters should be properly optimized.

The existing practical approaches to the choice of C and ε can be summarized as follows:

- Parameters C and ε are selected by users based on a priori knowledge and/or user expertise [2,13,14]. Obviously, this approach is not appropriate for non-expert users. Based on the observation that support vectors lie outside the ε -tube and the SVM model complexity strongly depends on the number of support vectors, Schölkopf [14] suggests the control of another parameter ν (*i.e.*, the fraction of points outside the ε -tube) instead of ε . Under this approach, the parameter ν has to be user-defined. Similarly, Mattera and Haykin [15] propose to choose ε value so that the percentage of support vectors in the SVM regression model is around 50 % of the number of samples. However, one can easily show examples when optimal generalization performance is achieved with the number of support vectors larger or smaller than 50 %.

- Smola et al. [16] proposed asymptotically optimal ε values proportional to noise variance, in agreement with general sources on SVM [2,13]. The main practical drawback of such proposals is that they do

not reflect the sample size. Intuitively, the value of ε should be smaller for a larger sample size than for a small sample size (with the same level of noise).

– *Selection of ε .* It is well-known that the value of ε should be proportional to the input noise level, that is $\varepsilon \propto \sigma$. Cherkassky and Mulier [13] propose the following (empirical) dependency:

$$\varepsilon = \tau\sigma\sqrt{\frac{\ln n}{n}}$$

Based on the empirical tuning, they propose the constant value $\tau = 3$, which gives good performance for various data set sizes, noise levels and target functions for SVM regression. Here n is the number of the training data samples. They assume that the standard deviation of noise σ is known or can be estimated from the data, which is again a difficult task for a non-expert user.

– The selecting parameter C is equal to the range of the output values [15]. This is a reasonable proposal, but it does not take a possible effect of outliers in the training data into account. Instead, Cherkassky and Mulier [13] propose the use of the following prescription for the regularization parameter:

$$C = \max(|\bar{y} + 3\sigma_y|, |\bar{y} - 3\sigma_y|)$$

where \bar{y} is the mean of the training responses (outputs), and σ_y is the standard deviation of the training response values. They claim that this prescription can effectively handle outliers in the training data. However, the proposed value of the C parameter is derived and applicable for RBF kernels only.

– The use of cross-validation for the parameter choice [13,14]. This is very computation and data-intensive.

– Several recent references present statistical account of SVM regression [17] where the ε parameter is associated with the choice of the loss function (and hence could be optimally tuned to particular noise density) whereas the C parameter is interpreted as a traditional regularization parameter in formulation that can be estimated by cross-validation for example [17].

– Selecting a particular kernel type and kernel function parameters is usually based on the application-domain knowledge and also should reflect the distribution of input (x) values of the training data. Very few works in literature(s) are available to throw light on this.

As evident from the above, there is no shortage of (conflicting) opinions on optimal setting of SVM regression parameters. The existing software imple-

mentations of the SVM regression usually treat SVM meta-parameters as user-defined inputs. For a non-expert user it is very difficult task to choose these parameters as he has no prior knowledge on these parameters for his data. In such a situation, the user normally relies on a trial-and-error method. Such an approach, apart from consuming the enormous amount of time, may not really obtain the best possible performance. In this paper we present a hybrid SVR-DE approach, which not only relieves the user from choosing these meta-parameters but also finds out the optimum values of these parameters to minimize the generalization error.

DIFFERENTIAL EVOLUTION (DE): AT A GLANCE

Having developed an SVR-based process model, a DE algorithm is used to optimize the N -dimensional input space (x) of the SVR model. The DEs were originally developed as the genetic engineering models mimicking population evolution in natural systems. Specifically, DE like genetic algorithm (GA) enforce the “survival-of-the-fittest” and “genetic propagation of characteristics” principles of biological evolution for searching the solution space of an optimization problem. The principal features possessed by DEs are: (i) they require only scalar values and not the second- and/or first-order derivatives of the objective function, (ii) the capability to handle non-linear and noisy objective functions, (iii) they perform global search and thus are more likely to arrive at or near the global optimum and (iv) DEs do not impose pre-conditions, such as smoothness, differentiability and continuity, on the form of the objective function.

Differential evolution (DE), an improved version of GA, is an exceptionally simple evolution strategy that is significantly faster and robust at numerical optimization and is more likely to find a function’s true global optimum. Unlike simple GA that uses a binary coding for representing problem parameters, DE uses a real coding of floating point numbers. The mutation operator here is the addition instead of bit-wise flipping used in GA. And DE uses non-uniform crossover and tournament selection operators to create new solution strings. Among the DEs advantages are its simple structure, ease to use, its speed and robustness. It can be used for optimizing functions with real variables and many local optima.

This paper demonstrates the successful application of DE to the practical optimization problem. As already stated, DE in principle is similar to GA. So, as in GA, we use a population of points in our search for the optimum. The population size is denoted by NP .

The dimension of each vector is denoted by D . The main operation is the NP number of competitions that are to be carried out to decide the next generation.

To start with, we have a population of NP vectors within the range of the objective function. We select one of these NP vectors as our target vector. We then randomly select two vectors from the population and find the difference between them (vector subtraction). This difference is multiplied by a factor F (specified at the start) and added to the third randomly selected vector. The result is called the noisy random vector. Subsequently, a crossover is performed between the target vector and the noisy random vector to produce the trial vector. Then, a competition between the trial vector and the target vector is performed and the winner is replaced into the population. The same procedure is carried out NP times to decide the next generation of vectors. This sequence is continued until some convergence criterion is met. This summarizes the basic procedure carried out in differential evolution. The details of this procedure are described below.

Steps performed in DE

Assume that the objective function is of D dimensions and that it has to be optimized. The weighting constant F and the crossover constant CR is specified.

Step 1. Generate NP random vectors as the initial population: generate ($NP \times D$) random numbers and linearize the range between 0 and 1 to cover the entire range of the function. From these ($NP \times D$) numbers, generate NP random vectors, each of dimension D , by mapping the random numbers over the range of the function.

Step 2. Choose a target vector from the population of size NP : first generate a random number between 0 and 1. From the value of the random number decide which population member is to be selected as the target vector (X_i) (a linear mapping rule can be used).

Step 3. Choose two vectors from the population at random and find the weighted difference: Generate two random numbers. Decide which two population members are to be selected (X_a, X_b). Find the vector difference between the two vectors ($X_a - X_b$). Multiply this difference by F to obtain the weighted difference.

$$\text{Weighted difference} = F(X_a - X_b)$$

Step 4. Find the noisy random vector: generate a random number. Choose the third random vector from the population (X_c). Add this vector to the weighted difference to obtain the noisy random vector ($X'c$).

Step 5. Perform crossover between X_i and $X'c$ to find X'_i , the trial vector: Generate D random numbers. For each of the D dimensions, if the random number is greater than CR , copy from X_i into the trial vector; if the random number is less than CR , copy the value from $X'c$ into the trial vector.

Step 6. Calculate the cost of the trial vector and the target vector: for a minimization problem, calculate the function value directly and this is the cost. For a maximization problem, transform the objective function $f(x)$ using the rule $F(x) = 1/(1+f(x))$ and calculate the value of the cost. Alternatively, directly calculate the value of $f(x)$ and this yields the profit. In case the cost is calculated, the vector that yields the lesser cost replaces the population member in the initial population. In case the profit is calculated, the vector with the greater profit replaces the population member in the initial population.

Steps 1-6 are continued until some stopping criterion is met. This may be of two kinds. One may be some convergence criterion that states that the error in the minimum or maximum between two previous generations should be less than some specified value. The other may be an upper bound on the number of generations. The stopping criterion may be a combination of the two. Either way, once the stopping criterion is met, the computations are terminated.

Choosing DE key parameters NP , F , and CR is seldom difficult and some general guidelines are available. Normally, NP ought to be about 5 to 10 times the number of parameters in a vector. As for F , it lies in the range 0.4 to 1.0. Initially $F = 0.5$ can be tried then F and/or NP is increased if the population converges prematurely. A good first choice for CR is 0.1, but in general CR should be as large as possible [7].

DE has been already successfully applied for solving several complex problems and is now being identified as a potential source for the accurate and faster optimization.

DE-BASED OPTIMIZATION OF SVR MODELS

There are different measures by which SVM performance is assessed, the validation and leave-one-out error estimates being the most commonly used ones. Here we divide the total available data as the training data (75 % of data) and the test data (25 % data chosen randomly). While SVR algorithm was trained on the training data the SVR performance is estimated on the test data.

The statistical analysis of the SVR prediction is based on the following performance criteria:

1. The average absolute relative error (AARE) on the test data should be minimum:

$$AARE = \frac{1}{N} \sum_1^N \left| \frac{Y_{\text{predicted}} - Y_{\text{experimental}}}{Y_{\text{experimental}}} \right|$$

2. The standard deviation of the error (σ) on the test data should be minimum:

$$\sigma = \sqrt{\sum_1^N \frac{1}{N-1} \left(\left| \frac{Y_{i,\text{predicted}} - Y_{i,\text{experimental}}}{Y_{i,\text{experimental}}} \right| - AARE \right)^2}$$

3. The cross-correlation co-efficient (R) between the input and the output should be around unity.

$$R = \frac{\sum_{i=1}^N (Y_{i,\text{experimental}} - \bar{Y}_{\text{experimental}})(Y_{i,\text{predicted}} - \bar{Y}_{\text{predicted}})}{\sqrt{\sum_{i=1}^N (Y_{i,\text{experimental}} - \bar{Y}_{\text{experimental}})^2} \sqrt{\sum_{i=1}^N (Y_{i,\text{predicted}} - \bar{Y}_{\text{predicted}})^2}}$$

SVM learning is considered to be successful only if the system can perform well on the test data on which the system has not been trained. The above five parameters of SVR are optimized by DE algorithm stated below (refer to Figure 3).

The objective function and the optimal problem of SVR model of the present study are represented as:

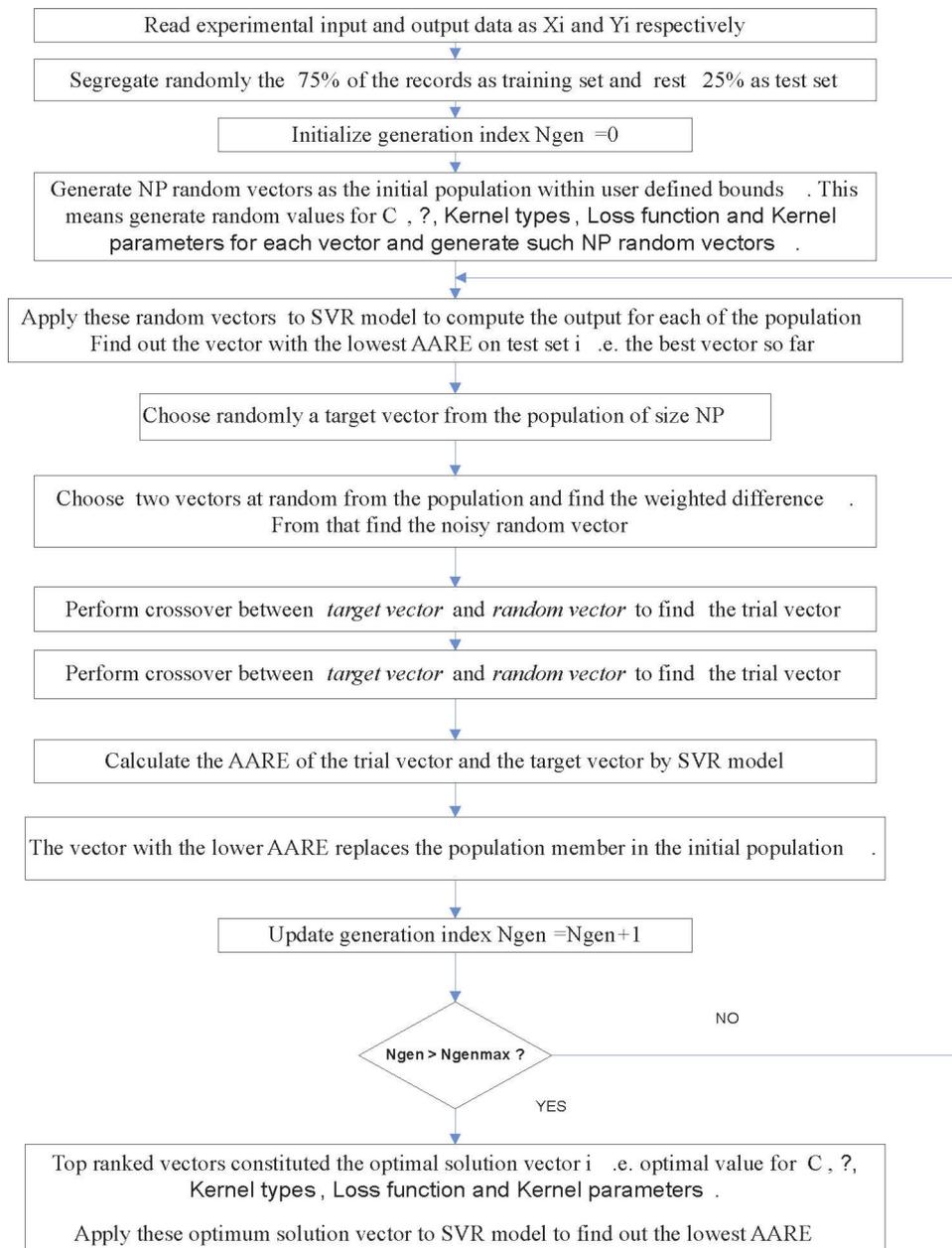


Figure 3. The schematic for SVR-DE algorithm implementation.

Minimize
 AARE(X) on test set
 $X \in \{x_1, x_2, x_3, x_4, x_5\}$
 where
 $x_1 = \{0 \text{ to } 10,000\}$
 $x_2 = \{0 \text{ to } 1\}$
 $x_3 = \{1, 2\}$
 $x_4 = \{1, 2, \dots, 6\}$
 $x_5 = \{1, 2, \dots, 6\}$

The objective function is minimization of the average absolute relative error (AARE) on the test set and X is a solution string representing a design configuration. The design variable x_1 takes any values for C in the range of 0.0 to 10,000. x_2 represents the ε taking any values in the range of 0.0 to 1. x_3 represents the loss function types: e-insensitive loss function and Huber loss function represented by numbers 1 and 2 respectively. x_4 represents the Kernel types: all 6 kernels given in Table 1 represented by numbers 1 to 6 respectively. The variable x_5 takes six values of the kernel parameters (represents the degree of polynomials, etc.) in the range from 1 to 6 (1,2,3,4,5,6) represented by numbers 1 to 6.

Table 1. Different kernel type (u and v - kernel arguments)

Case	Name of Kernel	Equation
Case 1	Linear	$k = uv'$
Case 2	Polynomial	$k = (uv' + 1)^{p1}$ ($p1$ is degree of polynomial)
Case 3	Gaussian radial basis function	$k = \exp(-(u-v)(u-v)/(2p1^2))$ ($p1$ is width of rbfs (sigma))
Case 4	Exponential radial basis function	$k = \exp(-\sqrt{(u-v)(u-v)}/(2p1^2))$ ($p1$ is width of rbfs (sigma))
Case 5	Splines	$z = 1 + u.v + (1/2)u.v.\min(u,v) - (1/6)(\min(u,v)).^3$ $k = \text{prod}(z)$
Case 6	B splines	$z = 0$; for $r = 0: 2(p1+1)$ $z = z + (-1)^r \text{binomial}(2*(p1+1)r) * (\max(0, u-v + p1+1-r)).^(2p1+1)$ end $k = \text{prod}(z)$ ($p1$ is degree of b spline)

The total number of design combinations with these variables is $100 \times 100 \times 2 \times 6 \times 6 = 720000$. This means that if an exhaustive search is to be performed it will take at the maximum 720000 function evaluations before arriving at the global minimum AARE for the test set (assuming 100 trials for each to arrive optimum C and ε). So the strategy which takes few function evaluations is the best one. Considering the minimization of AARE as the objective function, a differential evolution technique is applied to find the optimum design configuration of the SVR model.

CASE STUDY: THE PREDICTION OF CRITICAL VELOCITY IN SOLID LIQUID SLURRY FLOW

The background and the importance of critical velocity

Compared to a mechanical transport of slurries, the use of a pipeline ensures a dust free environment, demands substantially less space, makes the full automation possible and requires a minimum of the operating staff. The power consumption represents a substantial portion of the overall pipeline transport operational costs. For that reason great attention was paid to the reduction of the hydraulic losses. The prediction of critical velocity of slurries and the understanding of rheological behavior makes it possible to optimize the energy and water requirements.

Various investigators [18-20] have tried to show and propose the correlation relating critical velocity with other parameters of the solid-liquid flow, namely solids density, liquid density, particle size, concentration, pipe diameter, viscosity of flowing media, etc. They find that the pressure drop curve passes through minima (point 3 in Figure 2) and the operation at this velocity will ensure the lowest power consumption.

The critical velocity (V_c) is defined as the minimum velocity at which the solids form a bed at the bottom of the pipe demarcating the flow from fully suspended flows. It is also referred to as the minimum carrying or the limiting deposition velocity or the velocity corresponds to the lowest pressure drop and perhaps the most important transition velocity in a slurry transport. The operation velocities below the critical velocity are uneconomical as the critical velocity rises considerably. Apart from its obvious danger of plugging the pipeline, it also produces the excessive erosion in the lower part of the pipe. A system containing particles of the wide granulometric range results in the suspension of smaller particles keeping the larger particles deposited in the pipeline. Thus the long term stability of a heterogeneous flow depends on the reliable prediction of the critical velocity.

The four regimes of the flow can be represented by a plot of the pressure gradient versus the average velocity of the mixture (Figure 2). The critical velocity defined as V_3 velocity at or above which all particles move as an asymmetric suspension and below which the solids start to settle and form a moving bed. For all practical purposes of the slurry transport, the mixture velocity is kept above the V_3 and thus it is very important to know this velocity. From the power consumption point of view, this is the velocity where the pressure drop is minimal, i.e., it corresponds to the lowest power consumption in slurry transport.

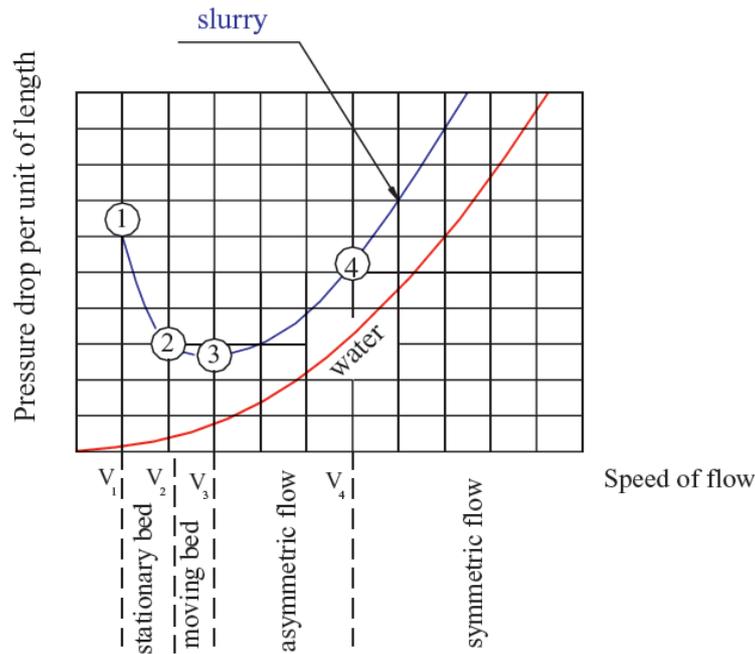


Figure 2. The plot of transitional mixture velocity with the pressure drop.

Despite the large area of application, the available models describing the suspension mechanism do not completely satisfy the engineering needs. To facilitate the design and the scale up of pipelines and slurry pumps, there is a need for a correlation that can predict slurry critical velocity over a wide range of operating conditions, physical properties and particle size distributions. The industry needs quick and easily implementing solutions. The model derived from the first principle is no doubt the best solution. But in the scenario where the basic principles for critical velocity modeling accounting all the interactions for slurry flow is absent, the numerical model may be promising to give some quick, easy solutions for the slurry critical velocity prediction.

This paper presents a systematic approach using robust hybrid SVR-DE techniques to build a critical velocity correlation from the available experimental data. This correlation has been derived from a broad experimental data bank collected from the open literature (800 measurements covering a wide range of pipe dimensions, operating conditions and physical properties).

The development of the support vector regression (SVR) based correlation

The development of the SVR-based correlation was started with the collection of a large databank. The next step was to perform a support vector regression, and to validate it statistically.

Collection of data

As mentioned earlier, over the years researchers have simply quantified the critical velocity of the slurry flow in a pipeline. In this work, about 800 experimental points have been collected from 20 sources of the open literature spanning the years 1950-2002. The data were screened for incompleteness, redundancies and evident inaccuracies. This wide range of database includes the experimental information from different physical systems to develop a unified correlation for critical velocity. Table 2 indicates the wide range of the collected databank for critical velocity.

Table 2. System and parameter studied. Slurry system: coal-water, coal-brine, ash-water, copper ore-water, sand-water, gypsum-water, glass-water, gravel-water, iron-water, iron-kerosene, high density material-water, iron tailings-water, limestone-water, limonite-water, plastic-water, potash-brine, sand-ethylene glycol, nickel shot-water, iron powder-water and ore-water [18,20-30]

Pipe diameter (m)	0.0127-0.80
Particle diameter (m)	$(0.0017-0.868) \times 10^{-2}$
Liquid density (kg/m^3)	770-1350
Solids density (kg/m^3)	1150-8900
Liquid viscosity (kg/m-sec)	0.0008-0.19
Solids concentration (volume fraction)	0.005-0.561
Critical velocity (m/s)	0.18-4.56

Identification of input parameters

After the extensive literature survey all physical parameters that influence the critical velocity are put in a so-called "wish-list".

Out of the number of inputs in a “wish list”, we used the support vector regression to establish the best set of chosen inputs, which describes the critical velocity. The following criteria guide the choice of the set of inputs:

- The inputs should be as few as possible.
- Each input should be highly cross-correlated to the output parameter.
- These inputs should be weakly cross-correlated to each other.
- The selected input set should give the best output prediction, which is checked by using statistical analysis (*e.g.*, average absolute relative error (*AARE*), standard deviation).

While choosing the most expressive inputs, there is a compromise between the number of inputs and the prediction. Based on different combinations of inputs, a trial-and-error method was used to finalize the input set which gives a reasonably low prediction error (*AARE*) when exposed to the support vector regression.

Based on the above analysis, the input variables such as a pipe diameter, a particle diameter, a solid(s) concentration, solid and liquid density and viscosity of the flowing medium have been finalized to predict the critical velocity in a slurry pipeline (Table 2). Table 3 shows some typical data used for the support vector regression.

Table 3. Typical input and output data for SVR training

Particle diameter cm	Solid concentration volume fraction	Solid density g/cm ³	Fluid density g/cm ³	Fluid viscosity Pa s	Pipe diameter cm	Critical velocity cm/s
0.0130	0.0280	1.8340	0.9980	0.0098	7.6200	140.2100
0.0100	0.3000	2.8200	0.9820	0.0130	5.0000	350.0000
0.2200	0.3040	1.6700	1.3250	1.5200	7.6200	90.5000
0.2200	0.3040	1.6700	1.3250	1.5200	10.1600	214.8800
0.8680	0.1650	1.5300	0.9980	0.0098	20.8000	242.7100
0.1830	0.0560	1.5300	0.9980	0.0098	4.0000	55.3200
0.0300	0.1700	3.3600	0.9980	0.0098	10.3000	133.4000
0.0140	0.0220	2.6900	0.9980	0.0098	20.7000	221.7000
0.0090	0.1250	3.0000	0.9980	0.0098	20.7000	321.1000
0.0060	0.0140	3.1000	0.9980	0.0098	14.9000	114.8500
0.1113	0.1920	4.5500	0.9980	0.0098	8.2500	247.9200
0.3346	0.1000	4.5500	0.9980	0.0098	15.0000	300.0000
0.0390	0.4750	1.9840	1.1460	0.0114	5.2200	146.3000
0.0410	0.3220	1.9840	1.1420	0.0120	10.7600	123.4000
0.0410	0.3830	1.9840	1.1420	0.0120	10.7600	123.4000
0.0540	0.3600	2.6500	1.3500	0.0560	5.2450	80.7700
0.0540	0.4200	2.6500	1.3500	0.0560	5.2450	74.6800
0.0500	0.0500	2.6500	1.3500	0.0560	5.2450	54.8600
0.0500	0.1200	2.6500	1.3500	0.0560	5.2450	62.4800
0.0500	0.1800	2.6500	1.3500	0.0560	5.2450	68.5800
0.0500	0.4200	2.6500	1.3500	0.0560	5.2450	76.2000
0.0200	0.1800	2.6500	1.1320	0.3820	5.2450	79.2500
0.0200	0.2400	2.6500	1.1320	0.3820	5.2450	70.1000
0.0490	0.1200	2.6500	1.0950	0.0575	5.2450	115.8200
0.0490	0.1800	2.6500	1.0950	0.0575	5.2450	118.8700
0.0490	0.2400	2.6500	1.0950	0.0575	5.2450	119.4800
0.0250	0.0050	2.6500	0.9980	0.0098	5.1500	72.4200
0.0250	0.0050	2.6500	0.9980	0.0098	5.1500	87.9400
0.2040	0.0250	2.6500	0.9980	0.0098	15.0000	220.7200
0.0850	0.2150	2.6500	0.9980	0.0098	5.0800	147.7100
0.0850	0.2150	2.6500	0.9980	0.0098	5.0800	116.8900
0.0242	0.0080	2.6000	0.9990	0.0100	7.6000	82.4000
0.0242	0.0300	2.6000	1.0000	0.0100	7.6000	122.0000
0.0242	0.0700	2.6000	1.0000	0.0101	7.6000	137.0000

Table 3. Continued

Particle diameter cm	Solid concentration volume fraction	Solid density g/cm ³	Fluid density g/cm ³	Fluid viscosity Pa s	Pipe diameter cm	Critical velocity cm/s
0.0250	0.3000	2.6500	0.9980	0.0098	10.3000	107.5400
0.0250	0.3180	2.6500	0.9980	0.0098	10.3000	103.5200
0.0400	0.0300	2.6500	0.9980	0.0098	10.3000	347.5000
0.0400	0.0620	2.6500	0.9980	0.0098	10.3000	218.5600
0.0400	0.1370	2.6500	0.9980	0.0098	10.3000	230.4500
0.0242	0.0300	2.6000	1.0000	0.0100	7.6000	122.0000
0.0242	0.0700	2.6000	1.0000	0.0101	7.6000	137.0000

RESULTS AND DISCUSSION

As the magnitude of inputs and outputs greatly differ from each other, they are normalized in -1 to +1 scale by the formula:

$$x_{\text{normal}} = \frac{2x - x_{\text{max}} - x_{\text{min}}}{x_{\text{max}} - x_{\text{min}}}$$

75 % of the total dataset was chosen randomly for training and the rest 25 % was selected for validation and testing.

Six parameters were identified as the input (table 2) for SVR and the critical velocity is put as a target. These data were then exposed to hybrid SVR-DE model described above. After the optimization of five SVR parameters described above, the model output was summarized in Table 4. The prediction capability of the hybrid SVR-DE algorithm is plotted in Figure 4. The low *AARE* (6.5 %) may be considered as an excellent prediction performance considering the poor understanding of the slurry flow phenomena and a large databank for training comprising various systems. The optimum value of SVR meta-parameters were summarized in Table 5. From Table 5 it is clear

that there are almost 5 different feasible solutions which lead to same prediction error.

Table 4. The prediction error by a SVR based model

Parameter	Training	Testing
<i>AARE</i>	0.0642	0.0645
σ	0.061	0.0625
<i>R</i>	0.940	0.931

In a separate study, we exposed the same dataset to SVR algorithm only (without the DE algorithm) and tried to optimize different parameters based on the exhaustive search. We found that it was not possible to reach the best solutions starting from arbitrary initial conditions. Specially the optimum choice of *C* and ϵ is very difficult to arrive at after starting with some discrete value. Many times the solutions got stuck up in sub optimal local minima. These experiments justified the use of a hybrid technique for SVR parameter tuning. The best prediction after the exhaustive search along with SVR parameters was summarized in Table 6. From the Table 6 it is clear that even

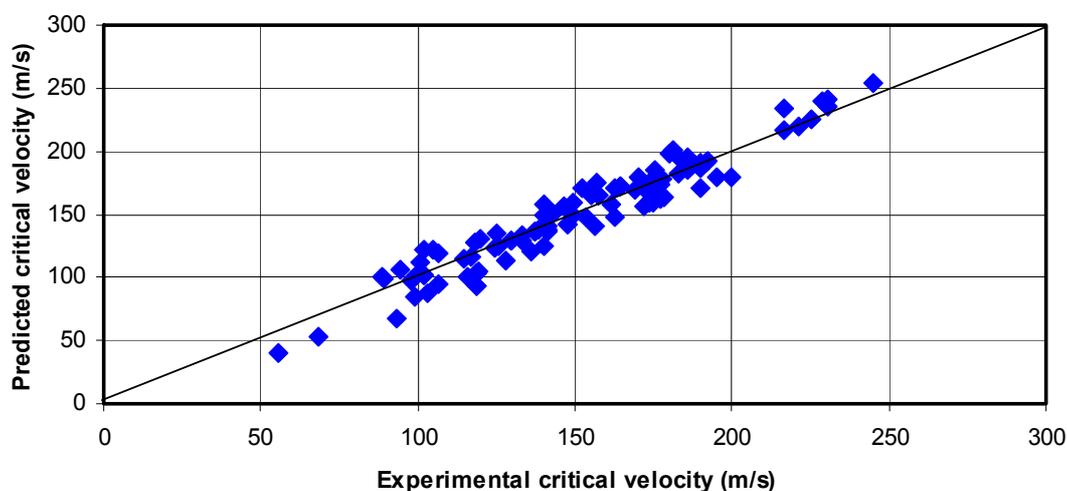


Figure 4. The experimental vs. predicted critical velocity for erbf kernel.

Table 5. Optimum parameters obtained by hybrid SVR-DE algorithm

Serial No.	C	ε	Kernel type	Type of loss function	Kernel parameter	AARE
1	943.82	0.50	erbf	e-Insensitive	2	0.0645
2	2298.16	0.36	erbf	e-Insensitive	3	0.0645
3	3954.35	0.48	erbf	e-Insensitive	4	0.0645
4	6180.98	0.54	erbf	e-Insensitive	5	0.0645

after 720000 runs, the SVR algorithm is unable to locate the global minima and the time of the execution is 4 h in Pentium 4 processor. On the other hand, the hybrid SVR-DE technique is able to locate the global minima with 2000 runs within 1 h. The prediction accuracy is also much better. Moreover, it relieves the non-expert users to choose the different parameters and find the optimum SVR meta parameters with a good accuracy.

Table 6. The comparison of the performance of SVR-DE hybrid model vs. SVR model

Parameter	SVR-DE Testing	SVR Testing
AARE	0.0645	0.0751
σ	0.0625	0.0655
R	0.931	0.901
Execution time, h	1	4

All the 800 experimental data collected from the open literature were also exposed to different formulas and correlations for critical velocity available in the open literature and AARE were calculated for each of them (Table 7). From Table 7, it is evident that the prediction error of the critical velocity has reduced considerably in the present work.

Table 7. The performance of different correlations to predict critical velocity

Reference	AARE / %
18	36.53
20	22.31
21	49.51
22	93.43
23	29.95
24	50.02
25	34.50
26	46.68
27	39.97
28	26.68
29	25.94
30	22.01
Present work	6.45

CONCLUSION

The support vector machines regression methodology with a robust parameter tuning procedure has been described in this work. The method employs a hybrid SVR-DE approach for minimizing the generalization error. Superior prediction performances were obtained for the case study of critical velocity and a comparison with selected correlations in the literature showed that the developed SVR correlation noticeably improved the prediction of critical velocity over a wide range of operating conditions, physical properties, and pipe diameters. The proposed hybrid technique (SVR-DE) also relieved the non-expert users to choose the meta-parameters of SVR algorithm for their case study and find out the optimum value of these meta parameters on their own. The results indicate that the SVR based technique with the DE based parameters tuning approach described in this work can yield excellent generalization and can be advantageously employed for a large class of regression problems encountered in the process engineering.

Nomenclature

- α, α^* : Vectors of Lagrange's multiplier
 ε : Precision parameter
 σ : Width of kernel of radial basis function
 λ : Regularization constant
 ζ, ζ^* : Slack variables

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