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Determination of the Velocity of Detonation of Primary Explosives Using Genetically Optimized Support Vector Regression

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Abstract: Chemical explosives are among the available high energy-dense storage materials with transferable energy to surroundings or adjacent materials during detonation. The effectiveness, ignition energy as well as spark sensitivity of these explosives are governed by the velocity of detonation which needs to be determined before energetic material synthesis purposely to enhance safety and lessen the cost as well as the difficulties associated with material synthesis and evaluation. This present research work proposes hybridization of support vector regression (SVR) and genetic algorithm (GA) for estimation of the velocities of primary explosives for the first time. The performance of the proposed hybrid SVR-GA is compared with the existing Mohammad Jafari et al. model as well as the results of EXPLO5Code's prediction using four parameters for measuring model's performance. The proposed SVR-GA model shows superior performance compared with two existing models in the literature. The performance of the proposed SVR-GA model for explosive velocity estimation strengthens its practical application, circumvents the experimental challenges and minimizes the associated potential risk.

Keywords: Velocity of detonation · support vector regression · genetic algorithm and hybrid model

1 Introduction

Velocity of detonation measures the speed with which the shock wave front or detonation wave propagates along the explosive columns [1]. This parameter simply referred as explosive velocity or detonation velocity, is among the important characteristic features of explosives as it indicates the explosive performance as well as it effectiveness, spark sensitivity and ignition energy [2,3]. Despite these significances, experimental measurement of this parameter is intensive and subjected to series of difficulties [1,4]. In an effort to address this challenge and further open ways through which newly synthesized explosives can be evaluated through determination of their velocity of detonation, many theoretical methods and computer codes have been proposed in the literature[2,3,5–7]. Among the available thermochemical equilibrium codes include FORTRAN BKW, ICT, CHEETAH and EXPLO05 among others [8,9] while computer codes which implement suitable empirical methods for computing detonation velocities include EDPHT[10], LOTUSES[11] among others [12]. Aside from the fact that the available computer codes are cumbersome, assumption of equation of state is also significant to their implementations. This present work elegantly approaches the velocity of detonation determination using hybrid computational intelligence of support vector regression and genetic algorithm. The superiority of the proposed hybrid model is demonstrated by comparing the outcomes of the proposed method with existing models.

Support vector regression (SVR) is a data mining algorithm which handles both non-linear and linear problems. The algorithm implements kernel trick with capacity to transfer input data to high dimensional feature space where modeling and simulation characterized with high degree of precision is carried out. Strong mathematical background of SVR algorithm as well as its non-convergence to local minimum contributes enormously to the uniqueness of the algorithm to maintain its accuracy and precision even while trained with small data-set with few descriptive features [13]. These uniqueness have contributed greatly to the robustness of the algorithm and finds wide applications in condensed matter physics [13–21], circumvention of hazardous effect of explosives [22,23] and other real life applications [24,25]. The significance of proper tuning of SVR parameters to the performance of the algorithm cannot be overemphasized [23]. The hyper-parameters are optimized and tuned in this present work with the aid of genetic algorithm (GA) that operates using biological evolutionary theory [26]. Hybridization of both algorithms enhances the robustness of the model through which the velocities of detonation of primary explosives are estimated with high degree of precision.

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While comparing the outcomes of the proposed SVR-GA model with other two models in the literature using four parameters that measure the performance of the model, the developed hybrid SVR-GA model outperforms both EXPLO5 code prediction (2004) [9] and Mohammad Jafari et al. (2018) [8] model with performance improvement of 69.09 % and 56.24 %, respectively on the basis of root mean square error (RMSE). Similar performance improvement of 67.78 % and 52.15 % are respectively obtained when the developed hybrid SVR-GA model is compared with the aforementioned two models on the basis of mean absolute error (MAE). The developed hybrid model also demonstrates a superior performance using correlation coefficient and mean absolute percentage deviation as performance measuring parameters.

The remaining part of the manuscript is organized as follows: section 2 describes the constituents of the hybrid model which include the mathematical formulation of SVR and genetic optimization algorithms. Section 3 discusses the computational details of the proposed hybrid model including the description of the employed dataset. Section 4 presents the findings of the research work and the superiority of the present model as compared to the existing models in the literature. Section 5 concludes the manuscript and concisely presents the summary of the work.

2 Mathematical Background of the Proposed Hybridization

The mathematical background of SVR chemometric algorithm is presented in this section. The evolutionary description of the implemented genetic optimization algorithm is also presented.

2.1 Formulation of Support Vector Regression Algorithm

Support vector regression (SVR) is a computational intelligence chemometric method with a distinct capacity of patterns acquisition using input features and the desired output [27,28]. The algorithm generates a function $f(x)$ from the training data set $(x_1, y_1), \ldots\ldots..(x_n, y_n) \subset Lx\mathbb{R}$ (where L represents input pattern space) which approximates the desired output with epsilon (ε) maximum allowable deviation. Mapping of input features to space of higher dimensionality through invocation of kernel function remains the backbone of SVR algorithm and enhances its accuracy as well as robustness [29–32]. The general form of SVR linear regression equation is presented in equation (1).

$$f(x) = \langle \omega, x \rangle + b, w \in L, b \in \mathbb{R} \tag{1}$$

where $\langle ., . \rangle$ stands for the dot product for input pattern space represented by L

The objective of the algorithm is to find the value of ω and b such that after inclusion of these values in the main regression equation, the maximum expected deviation does not exceed ε. While determining the vector ω, it is ensured that ω is as small as possible (that is, a flat function is desired) [33]. In order to achieve this, the Euclidean norm $\|w\|^2$is minimized and the resulting optimization problem (which is convex) is contained in equation (2) as described in [19,34].

$$\text{minimize} \frac{\|w\|^2}{2} \quad \text{subjectto} \begin{cases} f_n - \langle w, x_n \rangle - b \leq \varepsilon \\ \langle w, x_n \rangle + b - f_n \leq \varepsilon \end{cases} \tag{2}$$

Equation (2) presumes the existence of a function f_n which directly link the velocity of detonation with the descriptors such that the estimated velocity of detonation does not deviate from the experimentally measured value more than the thresholdε. As a result, the presented convex optimization problem becomes feasible [35,36]. However, inclusion of slack variables caters for any form of constraints that affect the feasibility of the optimization problem and further promotes robustness as well as versatility of the resulting model. The problem is modified as presented in equation (3) after the introduction of non-zero slack variables.

$$\text{minimize} \frac{\|w\|^2}{2} + C \sum_{s=1}^{S} (\xi_s + \xi_s^*) \quad \text{subjectto} \begin{cases} f_s - \langle w, x_s \rangle - b \leq \varepsilon + \xi_s \\ \langle w, x_s \rangle + b - f_s \leq \varepsilon + \xi_s^* \\ \xi_s, \xi_s^* \geq 0 \end{cases} \tag{3}$$

where C represents the penalty factor (also called the regularization factor)

The allowed maximum deviation of the estimated velocity of detonation and the experimentally measured values is traded-off or regularized using the penalty factor (C). In order to adequately solve the optimization problem contained in equation (3), standard dual formalism which allows the implementation of kernel trick as well as data transformation to high dimensional feature space is invoked. The final model through which the velocity of detonation of primary explosives can be estimated is presented in equation (4).

$$f(x) = \sum_{n=1}^{n} (\eta_n - \eta_n^*) K \langle x_n, x \rangle + b \tag{4}$$

Where $\eta_n$and $\eta_n^*$are Lagrange multipliers while $K\langle x_n, x \rangle$ and $b$respectively represents the kernel function and biasing parameter Karush-Kuhn-Tucker theorem (which zeros the product of the dual variables and the constraints at the point of the solution) helps in determining the biasing parameter$b$. Biasing parameter computation is treated extensively elsewhere [37–39]. The kernel function that accurately transfers the data to higher dimensional feature space with least deviation is the Gaussian kernel function presented in equation (5).

$$K\langle x_n, x\rangle = \exp\left(-\frac{\|\mathbf{x}_n - \mathbf{x}\|}{\sigma}\right) \tag{5}$$

where σstands for the kernel option

The choice of SVR hyper-parameters (the penalty factor as contained in equation (3), kernel option of the Gaussian kernel function as contained in equation (5) and epsilon as contained in equation (2) is essential for achieving accurate model [15]. The optimization of these parameters was carried out using genetic algorithm.

2.2 Evolutionary Operational Principle of Genetic Algorithm

Genetic algorithm (GA) is one of the global searching optimization algorithm operated through population generation and navigation using biological evolutionary system [26]. Mechanisms of natural selection and genetics are the fundamental principles upon which the algorithm navigates and locates its global solution. These natural genetic mechanisms include selective reproduction operation, crossover operation and mutation operation. Generation of initial set of solutions which are feasible (these are called the chromosomes) is the initial operational stage of the algorithm. These generated solutions are guided using the upper and lower limit of the population searching space where the possible solutions are highly probable. The characters known as gene are encoded in each of the chromosomes while these characters are replicated as the algorithm navigates [40,41]. The potential as well as the tendency of each of the chromosome to become the desired global solution is assessed using a fitness function which has been predefined. The crossover operator helps in further exploring the search space for the global solution. The operator generates another population set with better strength and enhanced features from the old population. The crossover probability guides and tunes the transference of varying characters of offsprings from proceeding generation to the subsequent generation while elitism mechanism is invoked when retaining the best chromosome from one generation to another. The mechanisms of selective reproduction, crossover as well as mutation proceeds until the stopping criterion is attained.

2.3 Measure of the Predictive Strength of the Developed Hybrid SVR-GA Model

The assessment of the future estimation and predictive strength of the proposed hybrid SVR-GA model was carried out using four parameters which include the root mean square error (RMSE), absolute percentage deviation (APD), mean absolute error (MAE) and correlation coefficient (CC). The mathematical formulations of the parameters are respectively defined in equation (6), equation (7), equation (8) and equation (9).

$$RMSE = \sqrt{\frac{1}{m}\sum_{j=1}^{m} Er_i^2} \tag{6}$$

$$APD = \left|\frac{Er}{V_{\exp}}\right| X100 \tag{7}$$

$$MAE = \frac{1}{m}\sum_{j=1}^{m} \left|Er_j\right| \tag{8}$$

$$CC = \frac{\sum_{j=1}^{m}\left(V_{j(\exp)} - V'_{(\exp)}\right)\left(V_{j(est)} - V'_{(est)}\right)}{\sqrt{\sum_{j=1}^{m}\left(V_{j(\exp)} - V'_{(\exp)}\right)^2 \sum_{j=1}^{m}\left(V_{j(est)} - V'_{(est)}\right)^2}} \tag{9}$$

Where Er_j and m respectively stand for error and the total number of data points. $V_{j(\exp)}$ and $V_{j(est)}$ respectively represent the experimental and the estimated velocity of detonation while $V'_{(\exp)}$ and $V'_{(est)}$ stand for their mean values.

3 Computational Strategy Employed in Algorithms Hybridization

This section presents the computational strategy adopted for hybridizing both algorithms which resulted to the developed SVR-GA model through which the velocity of detonation of primary explosives are estimated. The description as well as the statistical analysis of the employed data set is also presented in this section.

3.1 Dataset Description

The modeling and simulation presented in this research work was carried out using seventy-eight data-points extracted from literature [8,42–44]. The dataset consists of the velocities of detonation of primary explosives as well as the descriptors to the model. The descriptors include the enthalpies of formation, loading density, sum of the moles of gaseous products per gram of explosives, heat of detonation and average molecular weight per gaseous product.

Table 1. Results of the statistical analysis performed on the dataset.

Statistical parameters	Loading densities (g/cm^3)	Enthalpies of formation (kJ/mol)	Sum of the moles of gaseous products per gram of explosive	Average molecular weight per gaseous product (mol/g)	Heat of detonation (kJ/g)
Mean	2.452436	219.4	24.63641	25.34462	2.115897
Maximum	4.93	1130	62.4	35.21	5.33
Minimum	0.38	−836.9	0.61	8.52	0.03
Standard deviation	1.22962	442.8661	18.89942	6.119943	1.222708
Correlation coefficient	−0.00738	0.256123	0.346167	−0.13103	0.64198

The statistical analysis of the dataset was conducted and the results are presented in Table 1. The analysis includes the mean of the dataset which gives the average of data content, the maximum and minimum through which the range of the dataset content can be evaluated, standard deviation which measures the consistency of the dataset and the correlation coefficients which show how the descriptors are linearly correlated with the velocity of detonation. The correlation-cross plots between each of the descriptors and the velocity of detonation are presented in Figure 1. Low values of correlation coefficients between the descriptors and the target show inadequacy of linear modeling technique in handling the velocity of detonation determination; hence the need for the non-linear modeling tool such as the presented hybrid model becomes necessary.

3.2 Computational Details of the Hybridization

Hybrid SVR-GA model that estimates the velocity of detonation of primary explosives was developed using support vector regression (SVR) and genetic algorithm (GA). The function of GA is to optimize SVR hyper-parameters which include the penalty factor, kernel option of the optimum kernel function and epsilon. The modeling and simulation were carried out within MATLAB (2015 version) computing environment. Prior to the commencement of the simulation and modeling, the available data set was randomized to ensure unbiased and efficient computation and separated into training and testing phase in the ratio of 8:2 (sixty-three data points as the training dataset and fifteen data-points as testing dataset). The training dataset helps in generating support vectors whose accuracy and robustness are assessed using testing dataset. The details of the computational procedures go thus:

Step 1: *Initialization and initial population generation:* for a defined search space of each of the parameters to be optimized (that is, hyper-parameters which include the penalty factor, epsilon and kernel option of a kernel function selected from a pool of functions such as *sigmoid, Gaussian, polynomial and hyperbolic tangent*), initial population of feasible solution was generated. The upper and lower limits of the search space for penalty factor were set at 1000 and 1, respectively while that of epsilon were respectively set at 2 and 0.0001. The upper and lower limits of kernel option search space were set at 5 and 0.1. The significance of the empirical number of initial population on the performance of the developed hybrid model was investigated using RMSE as a parameter to measure model performance.

Step II: F*itness evaluation for each of the chromosome*: The fitness (measured by seeking for the minimum root mean square error between the experimentally measured velocity of detonation and the estimated values) of each of the chromosome was computed and evaluated. The details of the computation are itemized below.

a. From a pool of the available kernel functions (*which include sigmoid, Gaussian, polynomial and hyperbolic tangent)*, select one function coupled with each of the initially generated chromosome (that encodes the hyper-parameters of SVR algorithm with a known order of the parameters) to develop SVR based model for each of the chromosome. The value of hyper-parameter that defines the hyper-plane was set at E-7 while the training data set was used for developing SVR model for each of the chromosome.
b. initially generated chromosome were saved as RMSE_training with their respective support vectors. The fitness of each of the chromosomes was ranked (the lower the value, the better the fitness) in accordance to their RMSE value.
c. The saved support vectors in **Step b** were implemented on the testing set of data and the RMSE_testing of each of the model was also ranked. The chromosomes with best fitness, mean fitness and the worst of the population were identified.

Step III: *Selection* of c*hromosome for reproduction purpose*: With the selection probability set at 0.8, some chromosomes with better fitness were allowed to undergo reproduction process. This allows chromosomes of better fitness to be chosen for reproduction.

Step IV: *Implementation of crossover operator and emergence of new population*: Subsequences as well as portions of each of the parents are shared with their offsprings

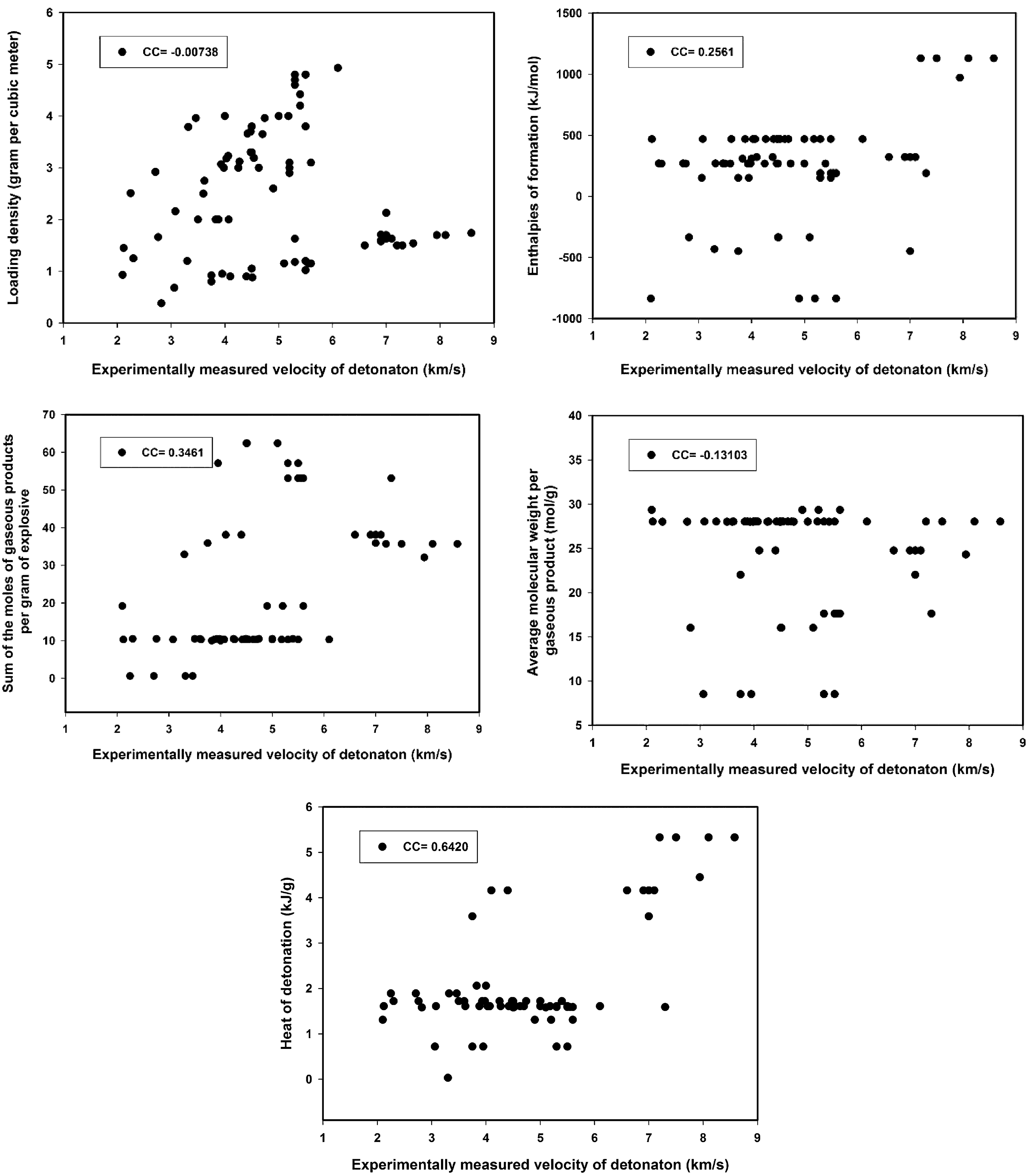

Figure 1. a) Correlation cross-plot between the loading density and experimentally easured velocity of detonation. b) Correlation cross-plot between the enthalpies of formation and experimentally measured velocity of detonation. c) Correlation cross-plot between the sum of the moles of gaseous products per gram of explosive and experimentally measured velocity of detonation. d) a) Correlation cross-plot between the average molecular weight per gaseous product and experimentally measured velocity of detonation. e) Correlation cross-plot between the heat of detonation and experimentally measured velocity of detonation.

through the implementation of crossover operator with crossover probability of 0.65. The significance of this crossover operator implementation is to eliminate the weaker individual chromosome in the population.

Step V: *Application of mutation operator*: this operator helps in changing the random positioning of strings in the chromosomes. The probability was set at 0.009.

Step VI: *Stopping criteria*: the entire process (from **Step I** to **Step V**) was repeated in a continuous manner until fifty consecutive generation returns a constant value of RMSE_testing. The chromosome corresponding to this fitness encodes optimum hyper-parameters of the developed hybrid model.

Step VII: *Final hybrid SVR-GA model*: the saved support vectors corresponding to the chromosome with the global fitness are used for developing the hybrid SVR-GA model through which the velocity of detonation of explosives could be estimated.

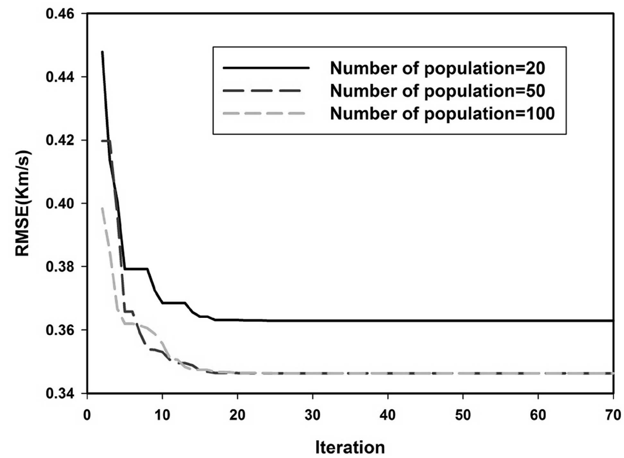

Figure 2. Significance oft the number of population to the global population search.

Table 2. Optimum hyper-parameters for the developed hybrid SVR-GA model.

Hyper parameter	Optimum value
Penalty factor (C)	500
Epsilon	0.1898
Kernel option	0.6034
Kernel function	Gaussian
Lambda	E-7
Number of population	50.

4 Results and Discussions

This section presents the outcomes of the research work. The importance of the initial number of population on the performance of the developed hybrid model is presented. The performance superiority of the developed hybrid model with other two existing models is discussed using four performance measuring parameters which include RMSE, mean absolute error (MAE), correlation coefficient (CC) and absolute percentage deviation (APD).

4.1 Variation of global search Convergence with the Number of Initial Population

The importance of the number of initial population of chromosomes to the performance of the developed hybrid SVR-GA model for velocity of detonation determination is presented in Figure 2. When the initial number of chromosomes was twenty, premature convergence was observed aside from local minimal that appears along the search space. When the initial number of chromosome was increased to fifty, the hybrid model settles at global minimum while further increase in the number of initial chromosome becomes inconsequential to the performance of the model. The contents of the optimum chromosome as well as the initial population number of chromosomes at which the developed model demonstrates its optimum performance are presented in Table 2.

4.2 Correlation cross-plot for the Developed SVR-GA Hybrid Model and other two Existing Models

The correlation cross-plots for the developed hybrid SVR-GA model and other two existing models are presented in Figure 3. The correlation coefficient for the developed model is 98.73 % while that of Mohammad Jafari et al. (2018) [8] and Explo5Code's prediction (2004) [9] are 92.53 % and 87.88 %, respectively. The superiority of the developed hybrid SVR-GA model as compared to other models can be observed from the alignment of its data-points.

4.3 Performance Comparison between the Developed Hybrid Model, Mohammad Jafari et al. (2018) Model and EXPLO5code's Prediction (2004)

The performance of the developed hybrid model is compared with other two existing models using four parameters which include the absolute percentage deviation, root mean square error, correlation coefficient and mean absolute error. Figure 4 presents the comparison on the basis of absolute percentage error.

Fifty-nine out of seventy-eight data-points (over 75 % of the data-points) show absolute percentage deviation less than 4 % for the developed hybrid SVR-GA model while 48 % of the data-points of Mohammad Jafari et al. (2018) [8] model have absolute percentage deviation of 4 %. Similarly, a very small percentage of data-points for Explo5Code's prediction model [9] are having deviation of 4 % while large

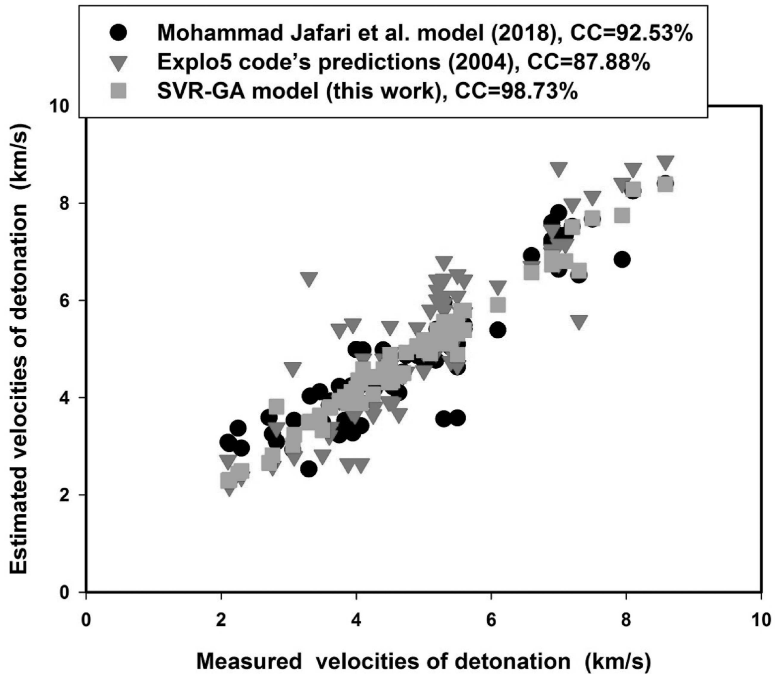

Figure 3. Correlation cross-plot between the measured velocities of detonation and estimated values using different models.

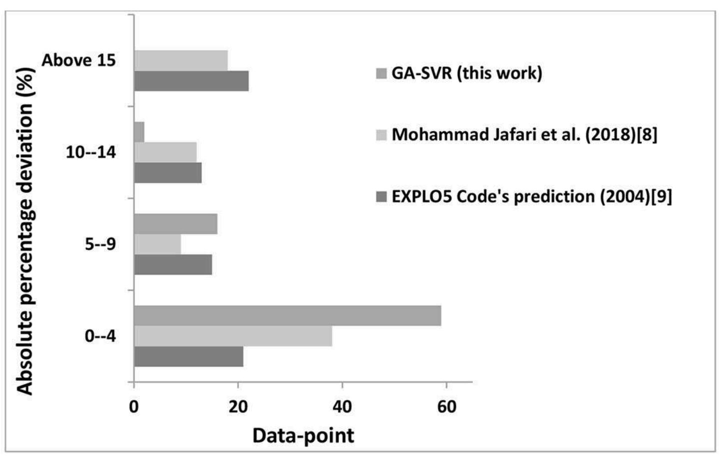

Figure 4. Absolute percentage deviation performance comparison of SVR-GA model, Mohammad Jafari et al. (2018) [8] model and EXPLO5code's prediction (2004) [9].

Table 3. Parameters that measure the performance of the models.

Performance measuring parameters	EXPLO5 Code's prediction (2004) [9]	Mohammad Jafari et al. (2018) [8]	SVR-GA (this work)
CC	0.8788	0.9253	0.9873
RMSE(km/s)	0.7854	0.5548	0.2428
MAE (km/s)	0.6118	0.4119	0.1971

percentage have deviation more than 15 %. On the basis of absolute percentage deviation, the developed hybrid SVR-GA model outperforms other existing models. Figure 5, Figure 6 and Figure 7 respectively compares the performance of the developed hybrid model with other two existing models on the basis of correlation coefficient, root mean square error and mean absolute error. With the correlation coefficient of 87.88 %, 92.53 % and 98.73 % for EXPLO5code's prediction (2004) [9], Mohammad Jafari et al. (2018) [8] and SVR-GA model (this work) respectively, the developed SVR-GA shows superior performance over EXPLO5code's prediction (2004) [9] and Mohammad Jafari et al. (2018) with performance improvement of 12.34 % and 6.70 %, respectively. Table 3 contains the values of the three

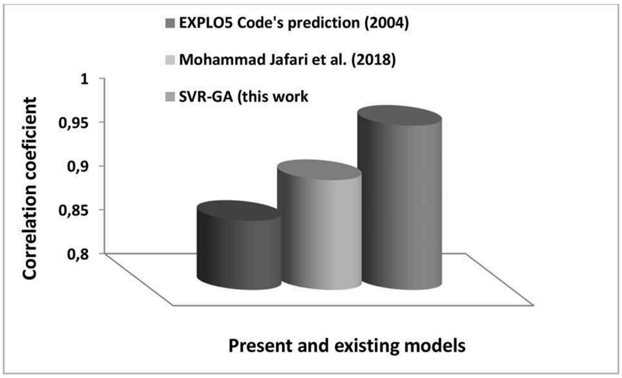

Figure 5. Correlation coefficient performance comparison of SVR-GA, Mohammad Jafari et al. (2018) [8] model and EXPLO5code's prediction (2004) [9].

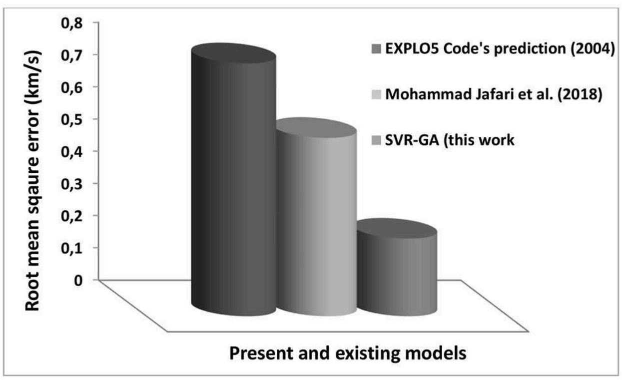

Figure 6. Root mean square error performance comparison of SVR-GA, Mohammad Jafari et al. (2018) [8] model and EXPLO5code's prediction (2004) [9].

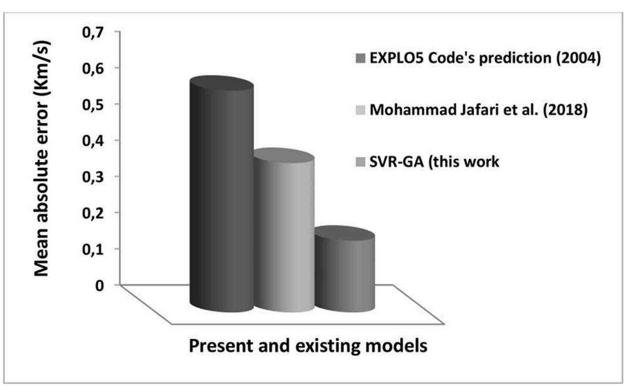

Figure 7. Mean absolute error performance comparison of SVR-GA model, Mohammad Jafari et al. (2018) [8] model and EXPLO5code's prediction (2004) [9].

performance measuring parameters for the present (SVR-GA) and existing {EXPLO5code's prediction (2004) [9] and Mohammad Jafari et al. (2018) [8]} models. Similarly, Table 4 presents the values of these parameters during training and testing phase of the model (hybrid SVR-GA).

Table 4. Performance measuring parameters during training and testing phase of SVR-GA model.

Dataset	CC	RMSE (km/s)	MAE (km/s)
Training dataset	0.9903	0.2107	0.1812
Testing dataset	0.9809	0.3463	0.264

Performance improvement of 69.09 % and 56.24 % were also obtained while comparing the developed hybrid SVR-GA model with EXPLO5code's prediction (2004) [9] and Mohammad Jafari et al. (2018) [8] model on the basis of root mean square error. Comparison on the basis of mean absolute error shows that the hybrid SVR-GA model performs better than other two compared models with performance improvement of 67.78 % and 52.15 %, respectively.

4.4 Comparison of the Outcomes of SVR-GA Model with that of other Existing Models at Different Loading Density

The estimated velocity of detonation of primary explosives and the experimentally measured values at different loading densities are presented in Table 5. The results of the two existing models which include EXPLO5code's prediction (2004) [9] and Mohammad Jafari et al. (2018) model [8] are also presented. From the presented results, the outcomes of the developed SVR-GA model are very close to the measured values followed by the results of Mohammad Jafari et al. (2018) [8] model while the estimates of EXPLO5code's prediction (2004) [9] show the largest deviation.

5 Conclusion

Hybrid SVR-GA model was developed for estimating the velocity of detonation of primary explosives. The significance of the genetic optimization algorithm is to optimize the hyper-parameters of SVR algorithm which strongly affect the accuracy as well as the performance of the algorithm. The performance of the developed hybrid model is measured and assessed using correlation coefficient between the experimentally measured values and estimated values at different loading density, absolute percentage deviation, root mean square error and means absolute error. More than 75 % of the outcomes of the developed hybrid SVR-GA show a deviation of less than 4 % while larger part of the outcomes of other existing models have deviation of more than 15 %. Performance improvements of 69.09 % and 56.24 % are obtained while comparing the developed hybrid SVR-GA model with EXPLO5code's prediction (2004) [9] and Mohammad Jafari et al. (2018) model [8] on the basis of root mean square error. Comparison on the basis of mean absolute error shows that the hybrid SVR-GA model per-

Table 5. Primary explosives and their respective values of velocity of detonation obtained using the present and existing models.

Chemical formula	Loading density (g/cm^3)	Measured Values (km/s)	Mohammad Jafari et al. (2018) (km/s) [8]	EXPLO5 Code's prediction (2004) (km/s) [9]	SVR-GA (this work) (km/s)
$Pb(N_3)_2$	1.45	2.12	3.05	2.17	2.31
	2	3.88	3.42	2.64	3.88
	2	4.07	3.42	2.64	3.88
	2.16	3.08	3.53	2.79	3.24
	2.75	3.62	3.93	3.39	3.81
	3	4.63	4.10	3.67	4.44
	3.12	4.27	4.18	3.81	4.42
	3.18	4.03	4.22	3.88	4.36
	3.19	4.54	4.22	3.89	4.35
	3.23	4.06	4.25	3.94	4.30
	3.65	4.70	4.53	4.46	4.51
	3.66	4.42	4.54	4.48	4.53
	3.7	4.48	4.57	4.53	4.63
	3.8	4.50	4.63	4.66	4.88
	3.8	5.50	4.63	4.66	4.88
	4	5.00	4.77	4.93	5.19
	4	5.18	4.77	4.93	5.19
	4.6	5.30	5.17	5.79	5.11
	4.7	5.30	5.24	5.94	5.31
	4.8	5.30	5.30	6.09	5.56
	4.8	5.50	5.30	6.09	5.56
	4.93	6.10	5.39	6.30	5.91
$C_2N_2O_2Hg$	1.25	2.30	2.96	2.37	2.49
	1.66	2.76	3.25	2.59	2.81
	2	3.50	3.49	2.82	3.33
	2.5	3.60	3.84	3.22	3.79
	3	3.98	4.19	3.65	4.07
	3	4.25	4.19	3.65	4.07
	3.07	3.93	4.24	3.72	4.12
	3.3	4.48	4.40	3.92	4.31
	3.3	4.50	4.40	3.92	4.31
	3.96	4.74	4.87	4.53	4.93
	4	5.00	4.89	4.56	4.96
	4.2	5.40	5.04	4.75	5.12
	4.42	5.40	5.19	4.97	5.21
$C_2H_8N_{10}O$	1.63	5.30	5.96	6.8	5.49
C_3N_{12}	1.02	5.50	5.10	5.25	5.31
	1.15	5.55	5.49	5.75	5.79
	1.15	5.60	5.49	5.75	5.79
	1.5	7.30	6.52	5.59	6.61
$C_4H_2N_{12}$	1.7	7.94	6.84	8.41	7.75
$C_6H_2N_4O_5$	0.9	4.10	4.98	4.80	4.59
	0.9	4.40	4.98	4.80	4.59
	1.5	6.60	6.92	6.7	6.58
	1.58	6.90	7.18	6.98	6.74
	1.6	6.90	7.24	7.05	6.77
	1.63	7.00	7.34	7.16	6.81
	1.63	7.10	7.34	7.16	6.81
	1.71	6.90	7.60	7.45	6.88
$C_6H_3N_3O_9Pb$	0.93	2.10	3.08	2.71	2.29
	2.6	4.90	4.87	5.44	5.06
	2.9	5.20	5.20	6.01	5.33
	3	5.20	5.30	6.21	5.37
	3.1	5.20	5.41	6.42	5.39
	3.1	5.60	5.41	6.42	5.39
$C_6N_{12}O_4$	1.2	3.30	2.53	6.47	3.49
$C_6N_{12}O_6$	1.5	7.20	7.52	7.99	7.51
	1.54	7.50	7.67	8.14	7.69

Table 5. continued

Chemical formula	Loading density (g/cm^3)	Measured Values (km/s)	Mohammad Jafari et al. (2018) (km/s) [8]	EXPLO5 Code's prediction (2004) (km/s) [9]	SVR-GA (this work) (km/s)
	1.7	8.10	8.25	8.72	8.28
	1.74	8.58	8.40	8.87	8.39
$C_6H_{12}N_2O_6$	0.38	2.82	3.09	3.38	3.81
	0.88	4.51	4.41	4.94	4.32
	1.05	4.50	4.85	5.47	4.69
	1.15	5.10	5.12	5.8	4.91
$C_9H_{18}O_6$	0.68	3.06	2.93	4.62	3.02
	0.92	3.75	3.23	5.41	3.94
	0.95	3.95	3.27	5.52	4.08
	1.18	5.30	3.56	6.44	5.22
	1.2	5.50	3.58	6.53	5.31
$Ni[(N_2H_4)_3](NO_3)_2$	0.8	3.75	4.23	3.94	3.94
	1.7	7.00	6.64	6.76	6.81
	2.13	7.00	7.80	8.73	6.81
AgN_3	2.00	3.83	3.53		4.02
	4.00	4.00	4.99		4.19
	2.51	2.25	3.37		2.44
	2.92	2.71	3.59		2.66
	3.79	3.32	4.03		3.51
	3.96	3.46	4.12		3.63

forms better than other two compared models with performance improvement of 67.78% and 52.15%, respectively. Due to the robustness as well as the accuracy of the proposed hybrid model, practical implementation of the developed model would enhance characterization and evaluation of newly synthesized explosives chemicals without experimental stress while potential risk associated with explosive chemicals are circumvented.

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