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Hybrid chemometric approach for estimating the heat of detonation of aromatic energetic compounds

Hayatullahi B. Adeyemo [a,b], Taoreed O. Owolabi [c,*], Muhammad A. Suleiman [e], Kabiru O. Akande [f], Jamal Alhiyafi [d], Sola Fayose [c], Sunday O. Olatunji [d]

[a] Information and Computer Science Department, King Fahd University of Petroleum and Minerals, Dhahran, 31261, Saudi Arabia
[b] Computer Science Unit, Department of Mathematics, Usmanu Danfodiyo University, P.M.B. 2346, Sokoto, Nigeria
[c] Physics and Electronics Department, Adekunle Ajasin University, Akungba Akoko, Postal code 342111, Ondo State, Nigeria
[d] Department of Computer Science, College of Computer Science and Information Technology, Imam Abdulrahman Bin Faisal University, P.O. Box 1982, Dammam, 31441, Saudi Arabia
[e] Deanship of Graduate Studies, King Fahd University of Petroleum and Minerals, Dhahran, 31261, Saudi Arabia
[f] Institute for Digital Communications, School of Engineering, University of Edinburgh, Edinburgh, Postal code EH8 9AB, United Kingdom

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ABSTRACT

This work presents an elegant technique for estimating the heat of detonation (HD) of thirty organic energetic compounds by combining support vector regression (SVR) and gravitational search algorithm (GSA). The work shows that numbers of nitrogen and oxygen atoms as well as the compound molar mass are sufficient as descriptors. On the basis of three performance measuring parameters, the hybrid GSA-SVR outperforms Mortimer and Kamlet (1968), Mohammad and Hamid (2004) and Mohammad (2006) models with performance improvement of 93.951%, 86.197%, and 47.104%, respectively. The superior performance demonstrated by the proposed method would be of immense significance in containing the potential damage of the explosives through quick estimation of HD of organic energetic compounds without loss of experimental precision.

1. Introduction

The heat of detonation is a quantitative measurement used to assess the detonation performance of explosives and measures the energy content of organic energetic compounds [1, 2]. It indicates the available energy for mechanical activity and further assesses the potential damage to surroundings [3]. The heat of detonation of explosives plays significant roles among the explosives performance measuring parameters (which include detonation pressure and velocity) since other quantities can be determined from it [4]. Hence, precise estimation of the heat of detonation is desired for ensuring optimum performance of the explosives without causing environmental disasters, especially at the early developmental stage. Computational modeling of the heat of detonation of energetic organic compounds and empirical relations are meritorious since they ensure quick estimation of explosives performances apart from being cost effective as it reduces the cost related to synthesis, test and evaluation of such materials, time saving and environmental friendliness are another paramount factors [1]. Although, there are some programs such as CHEETAH in the literature for estimating the heat of detonation, these programs assume equations of state for detonation products and are computationally tedious. In addition, the absence of readily available information on the heat of formation and density significantly limits the implementation of such programs. In comparison, the chemometric approach presented in this work circumvents these issues. To confirm this, the generalization and predictive strength of the proposed GSA – SVR chemometric model is compared with three empirical relations in the literature and the proposed method demonstrates superior performance. This is in addition to the simplicity of its descriptors (which include number of nitrogen, oxygen atoms and molar mass) which are easily available. The uniqueness of the proposed hybrid GSA-SVR model over existing models includes (i) the assumption of a sufficiency of the number of nitrogen and oxygen atoms as well as the compound molar mass as descriptors without the inclusion of the compound specific functional group (ii) ease accessibility of the proposed descriptors and (iii) hybridization of SVR and GSA algorithms.

The SVR chemometric model is a computational intelligence algorithm that acquires linear as well as non-linear pattern by mapping the input variables (i.e. descriptors) to the predictive output (i.e. target) [5].

* Corresponding author.
E-mail address: owolabitaoreedolakunle@gmail.com (T.O. Owolabi).

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The algorithm achieved general minimization error bound by implementing an inductive reasoning structural risk minimization [6, 7]. The structural risk minimization principle aims at converting an empirical risk and Vapnik- Chervonenkis dimension into a convex optimization problem. Coupled with its kernel trick feature, this unique property made SVR to stand out among other machine learning methods [8, 9]. The hyper-parameters of SVR is a crucial factor for optimality of the model in practice, especially with a vague learning patterns from few data-points and descriptive features [10]. Many population based evolutionary optimization algorithms have been applied to various forms of real life problems in the literature [11, 12, 13, 14, 15], however, the fast convergence of gravitational search algorithm (GSA) and the ease of its convergence contributes to its uniqueness [16]. GSA is an optimization technique that operates on the basis of interaction between two or more bodies through gravitational pull [16]. The algorithm has been deployed in a wide range of applications due to its fast convergence to a global solution [17, 18, 19]. This work employs the uniqueness of GSA to develop hybrid model through which the heat of detonation of organic energetic compounds can easily be predicted within the acceptable experimental error.

On the basis of the mean absolute error (MAE) metric as a performance-measuring parameter, the developed GSA-SVR chemometric outperforms Mortimer and Kamlet model, Mohammad and Hamid model as well as Mohammad model with performance improvement of 93.95%, 86.20% and 47.10 %, respectively. The performance gains of the developed model over the existing models are also shown using absolute percentage deviation (APD) and the correlation coefficient (CC) between the experimentally measured and estimated values.

The rest of this work is outlined as follows: Section 2 briefly introduces the mathematical background of the proposed SVR chemometric. The physical principles governing the population-based optimization technique implemented for hyper-parameters selection are also presented in Section 2. Section 3 presents the details of the optimization of SVR with GSA along with the details of the dataset used in this work. Presentation and discussion of the results are contained in Section 4. Finally, Section 5 presents the conclusion.

2. Model

2.1. Computational formulation of the hybridized model

A concise explanation of the mathematical description and theoretical background of the support vector regression model is presented. The section also presents in brief, the principles upon which GSA operates and the description of how optimization is achieved by the algorithm.

2.1.1. A brief description of support vector regression chemometric model

Support vector regression (SVR) chemometric model is a computational intelligence algorithm that acquires pattern and relation that directly link the descriptors with the desired target using structural risk minimization principle [6, 20]. In an effort to make minimal the vapnik-Chervonenkis's dimension and empirical risk which translates to convex ε-insensitive loss function minimization, flattest tubes that encompass most of the training instances are implemented. The general form of SVR algorithm model is represented mathematically in Eq. (1) for input-output dataset $(x_1,y_1),(x_2,y_2)\ldots,(x_s,y_s)\subset QX\Re$

$$F(x,\omega)=\langle\omega,x\rangle+b,\omega\subset Q,b\in\Re \tag{1}$$

where Q, $\langle,\rangle$and b are input pattern space, dot product and biasing factor, respectively.

The convex optimization problem of the algorithm is expressed in Eq. (2) while the constraints are presented in Eq. (3)

$$Min_{\omega}\frac{1}{2}\left|\left|\omega\right|\right|^2 \tag{2}$$

Subject to:

$$\begin{cases} y_i-\langle w,x_i\rangle-b\ \leq\varepsilon \\ \langle w,x_i\rangle+b\ -y_i\leq\varepsilon \end{cases} \tag{3}$$

where ε is the user defined maximum deviation of the training data-points from the desired outputs.

To prevent outliers, some slack variables ξ,ξ^+ are added resulting in obtaining a soft-margin which is similar to the one used in the initially developed classification-based support vector machines [6]. The slack variables define the number of points that can be allowed out of the boundary of the tube while the dimension of the tube is controlled by epsilon (ε). Due to this inclusion, the objective function of the optimization problem is further formulated as presented in Eq. (4) while Eq. (5) presents the new constraints

$$Min\frac{1}{2}\left|\left|\omega\right|\right|^2+C\sum_{i=1}^{N}\left(\xi_i^-+\xi_i^+\right) \tag{4}$$

Subject to

$$\begin{cases} y_i-\langle w,x_i\rangle-b\leq\varepsilon+\xi^-\ \ i=1\ldots N \\ \langle w,x_i\rangle-y_i+b\leq\varepsilon+\ \xi^+\ \ i=1\ldots N \\ \qquad\xi_i^-,\xi_i^+\geq 0\ \ i=1\ldots N \end{cases} \tag{5}$$

The final regression function for the developed model is presented in Eq. (6) while the mathematical expression of the implemented Gaussian kernel function is shown in Eq. (7)

$$f(x)=\sum_{i=1}^{I}\left(\lambda_i-\lambda_i^*\right)K(x_i,x)+b \tag{6}$$

Where λ_i *and* λ_i^* are the Lagrange multipliers

$$K(x_i,x)=\exp\left(-\left(\frac{x_i-x_j}{\sigma}\right)\right) \tag{7}$$

where σ represents the kernel option.

Hyper-parameters of the SVR based model play important role on the optimality of the model. Hence, proper selection of these parameters translates to robust model. In order to ensure optimum selection, the GSA optimization technique is employed.

2.1.2. Working principles of the gravitational search algorithm (GSA) optimization technique

The GSA optimization technique is a population search based optimization algorithm proposed recently [16]. The Newtonian principle of motion and gravity inspired the invention of the algorithm. The solutions in the GSA population are known as agents and interact through the force of gravity. The algorithm presents the interactions between the objects (agents) by measuring their performances through their masses. In a population of agents, those agents with lower masses are attracted to the ones with higher masses. Each agent has its mass position, which represents the possible solution to the addressed problem. This makes the agents with heavy masses to be close to the optimum solution and the agent with the heaviest mass symbolizes the optimum solution in the search space. Each agent is not only characterized by passive gravitational mass and active gravitational mass, but also position and inertia mass, making each agent of the population to have four parameters. GSA implementation has a series of steps as described below:

Step One: Agents Initialization:

The entire agents' positions are randomly initialized.

$$X_i=\left(x_i^1,\ldots,x_i^d,\ \ldots,x_i^n\right).for\ i=1,2,3,\ldots.N \tag{8}$$

x_i^dsignifies i^{th} agent's position in the d^{th} dimension, and the dimension of

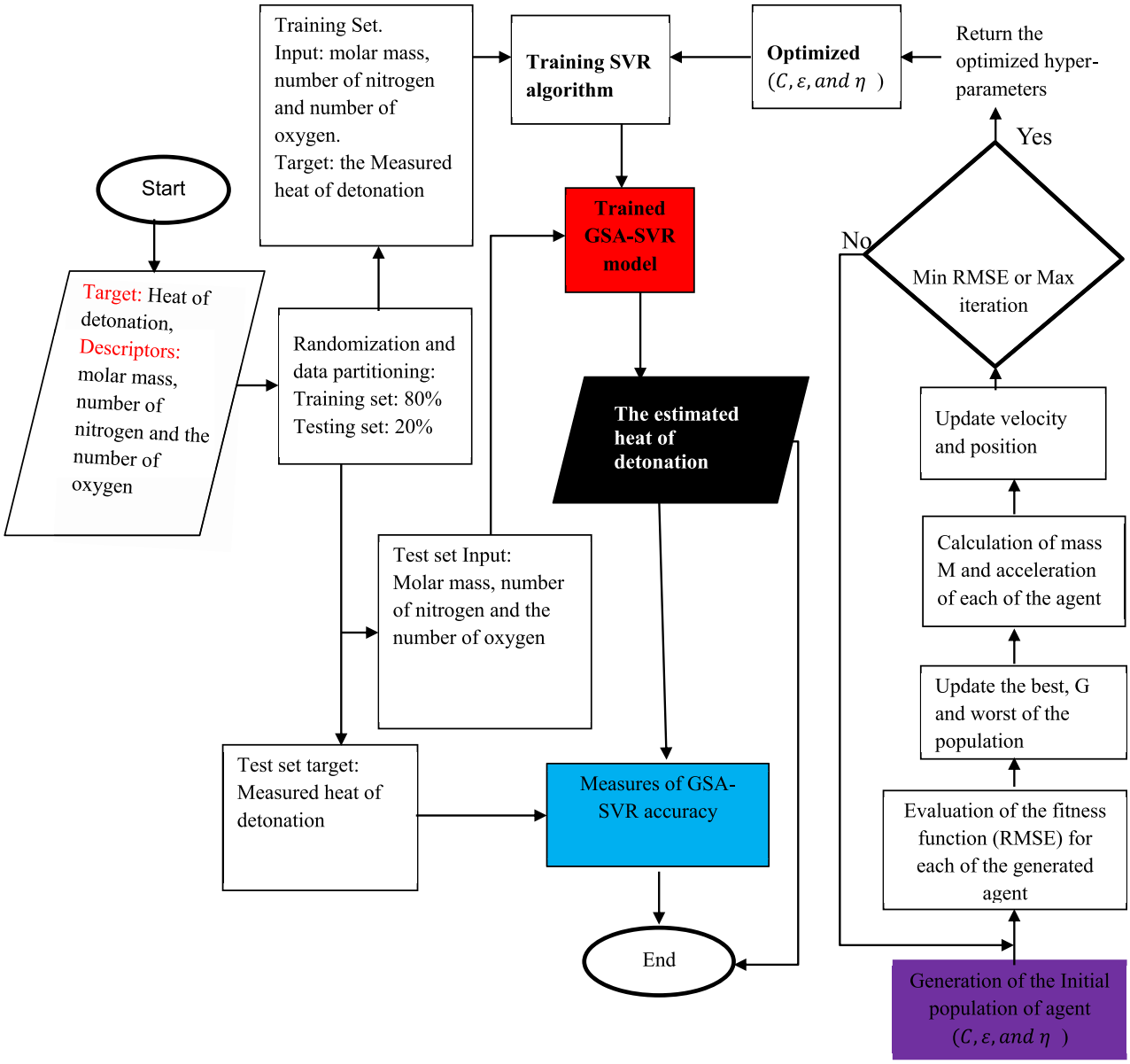

Fig. 1. The Computational flow of the hybrid SVR-GSA model.

the space is denoted by N.

Step Two: Evolution of fitness and computation of the best fitness

The $fit_i(t)$ is computed through the fitness function, where at iteration t, $fit_i(t)$ is each i^{th} agent's fitness value. The worst and the best fitness are used to evaluate the evolution of fitness for all agents during every iteration.

For maximization problem addressed in this work,

$$best(t) = max_{i\in(1\ldots N)} fit_i(t) \tag{9}$$

$$worst(t) = min_{i\in(1\ldots N)} fit_i(t) \tag{10}$$

At iteration t, the worst and best fitness of the agents are denoted by $worst(t)$ and $best(t)$ respectively while the i^{th} agent's fitness value is denoted by $fit_i(t)$.

Step Three: Calculation of gravitational constant

At iteration t, the computation of G - the gravitational constant - is as follows:

$$G(t) = G_0 e^{-\alpha t/T} \tag{11}$$

where the values of G_0 and α are initialized at the beginning of the search and gradually reduced during the search and update the value of $G(t)$. T denotes the total number of iterations.

Step Four: Calculation of the masses of every agent

The inertia mass and the gravitational masses are calculated from the fitness values under the condition that the gravitational and active masses are equal to the inertia mass.

$$M_{ai} = M_{pi} = M_{ii} = M_i \qquad i = 1, 2, 3, \ldots, N \tag{12}$$

$$m_i(t) = \frac{fit_i(t) - worst(t)}{best(t) - worst(t)} \tag{13}$$

$$M_i(t) = \frac{m_i(t)}{\sum_{j=1}^{N} m_j(t)} \tag{14}$$

the terms M_{ai} and M_{pi} are respectively the active and passive gravitational masses, while M_{ii} is the i^{th} agent's inertia mass.

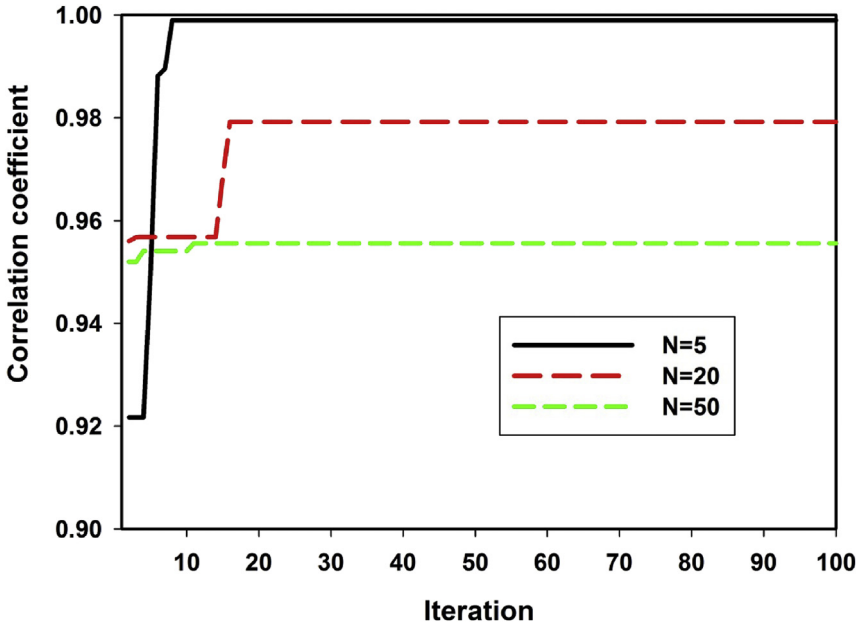

Fig. 2. Dependence of model convergence on the initial population of agent using Gaussian kernel mapping function.

Step Five: Calculation of the agents' accelerations

The next step is the computation of the agents' accelerations, the i^{th} agent acceleration, a_i^d, is calculated at iteration t as follows:

$$a_i^d(t) = \frac{F_i^d(t)}{M_{ii}(t)} \tag{15}$$

where $F_i^d(t)$ is the resultant force exerted on *the* i^{th} agent. It is computed as a randomly weighted sum of d^{th} components of the forces exerted from other agents as follows:

$$F_i^d(t) = \sum_{j \in Kbest.\ \ j=1.\ j \neq i} rand_j F_{ij}^d(t) \tag{16}$$

where the set of top K agents with the heaviest mass and best fitness values is denoted by *Kbest*. Its value decreases linearly with time until the number of agent applying force to others reduce to only one.

$F_{ij}^d(t)$ is also calculated as:

$$F_i^d(t) = \sum_{j \in Kbest.\ \ j=1.\ j \neq i} rand_j F_{ij}^d(t) \tag{17}$$

where $F_{ij}^d(t)$ denotes the force exerted by agent j on agent i at i^{th} iteration and dimension d, while ε represents a small constant and $R_{ij}(t)$ is the Euclidean distance between agent j and agent i during i^{th} iteration. $G(t)$ is the value of the gravitational constant computed above.

$$R_{ij}(t) = \left|\left|X_i(t).\ X_j(t)\right|\right|_2 \tag{18}$$

Step Six: Refreshing the new velocity and positions of agents:

The agent's next velocity (i.e. at iteration (t plus 1)) is calculated by adding its acceleration to its current velocity. Also, its next position is computed by totaling the next velocity to the current position as denoted in the following equations below:

$$v_i^d(t+1) = rand_i \times v_i^d(t) + a_i^d(t) \tag{19}$$

$$x_i^d(t+1) = x_i^d(t) + v_i^d(t+1) \tag{20}$$

Step Seven: Repeating steps two through six

The above-mentioned steps 2 to 6 are repeated until the maximum number of iteration is reached. At the last iteration, the value of the best fitness is calculated and represented the global fitness while the corresponding agent's position is calculated as the global solution of the problem under study.

3. Methodology

3.1. Computational details of the proposed hybrid models

The computational implementation of the proposed hybrid chemometric and the discussion of the employed dataset are presented in this section.

3.1.1. Description of the dataset

A total number of thirty organic energetic compounds with three descriptors were employed in this study. The dataset includes the number of nitrogen (N), the number of oxygen (O) as well as the molar mass (M) of the compound as descriptors while the experimentally measured heat of detonation values were used as targets and extracted from the literature [21, 22, 23]. The three descriptors were assumed to be sufficient without the inclusion of the compound specific functional group.

3.1.2. Computational methodology

In this research work, a hybrid approach that combines SVR with GSA algorithms is developed and implemented within MATLAB computing environment. The dataset used was randomly divided into training and testing sets to enhance data-points distribution. Thereafter, the randomized dataset was partitioned into training and testing subsets in a ratio of 4:1, respectively. That is, 80% of the randomized dataset was used to train the model while the remaining 20% of the randomized dataset was used to test the SVR-GSA model in a cross-validation method. The implemented cross-validation method as described in [9, 24, 25, 26] allows regression to be performed on the training dataset while estimation and generalization accuracy of the developed model is evaluated using the testing phase. The generalization and predictive strength of the developed hybrid chemometric was evaluated and assessed using CC, RMSE, MAE and APD. Fig. 1 is the computational flowchart for the developed hybrid chemometric.

3.1.3. Optimum hyper parameters search strategy

In the research work, GSA was used to search for optimal hyper pa-

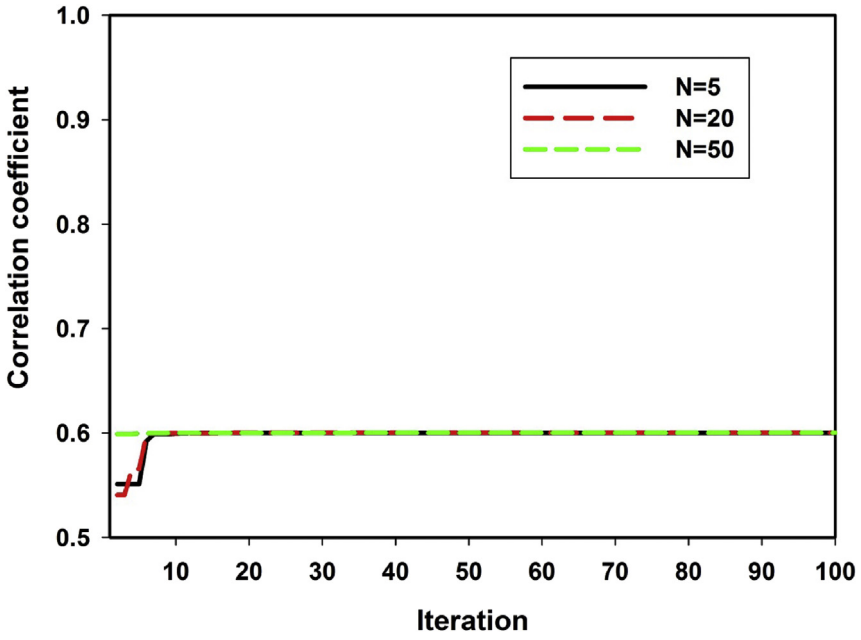

Fig. 3. Dependence of model convergence on the initial population of agent using polynomial kernel mapping function.

rameters for SVR which include the kernel function, regularization or penalty factor (C) and epsilon (ε). In Fig. 1 the process of searching for optimal hyper parameters begins with initialization of agents in GSA, this involves populating a search space with N number of agents and each agent encodes SVR hyper parameters. The fitness of each agent is computed through training SVR algorithm and computing the RMSE for N number of agents. Eq. (14) is used to calculate the mass of each agent, while Eqs. (16) and (17) provide the computation of total gravitational force of each agent and its corresponding acceleration as presented in Eq. (15). Finally, using Eqs. (19) and (20) to compute agent's velocity and position which are updated each time until maximum iteration is reached. Optimal hyper parameter obtained from an agent with maximum fitness value at the maximum iteration is used to finally train the SVR-GSA model. The performance accuracy of the developed SVR-GSA model is measured using the test set where test set input is used to estimate the heat of detonation of the compound. This estimated heat of detonation is compared with the available experimental values using CC, RMSE, MAE and APD as error metrics.

4. Results and discussion

This section presents and discusses the outcomes of the developed hybrid chemometric. Performance measuring parameters and the significance of the initial population of the agent on the effectiveness and convergence of the developed hybrid chemometric are also presented. This section further compares the results of the presented model with the existing theoretical models.

4.1. Dependence of model performance on the initial population of agents in GSA

The significance of the initial population of the agent to the effectiveness and convergence of the developed hybrid chemometric was studied and presented in Figs. 2 and 3 for Gaussian and polynomial kernel function, respectively. A balance should be maintained between the exploration and exploitation strength of the optimization algorithm for enhancing the attainment of a global solution. In the case of optimization problem addressed in this work which centers on optimizing the correlation coefficient between the experimentally measured heat of detonation and the estimated values, five number of initial agents optimize the developed hybrid chemometric for Gaussian kernel function. Exceeding this value worsens the exploitation ability of the model since many agents are searching for a global solution which consequently increases the complexity around the global solution.

In the case of the polynomial kernel option, the number of agents does not significantly influence the performance of the model. More so, the hybrid model developed using a polynomial kernel function as can be deduced from Fig. 3 demonstrates lower performance as measured using the correlation coefficient. Therefore, the final hybrid chemometric was developed using a Gaussian kernel function as can be seen in Fig. 2 that the highest correlation was achieved when N = 5, while the obtained hyper-parameters during the optimization processes are presented in Table 1 with their optimum values.

Table 1
Hyper-parameters and their optimum values.

SVR hyper-parameters	Values of the parameter
Epsilon	0.1002
Regularization factor	228.6169
Kernel option	0.9408
Kernel function	Gaussian
Hyper-parameter lambda	E-7
The initial population of GSA agent	5

Table 2
Measures of model reliability.

Dataset	Correlation coefficient	Root mean square error (KJ/g)	Mean absolute error (KJ/g)
Training	0.999	0.057	0.049
Testing	0.999	0.482	0.419

4.2. Measures of generalization and predictive capacity of the developed hybrid chemometric

The predictive and generalization strengths, as well as the reliability of the developed hybrid chemometric, are measured and assessed using CC, RMSE and MAE. The accuracy of 99.9% was obtained during the training and testing phase of the developed model while root mean

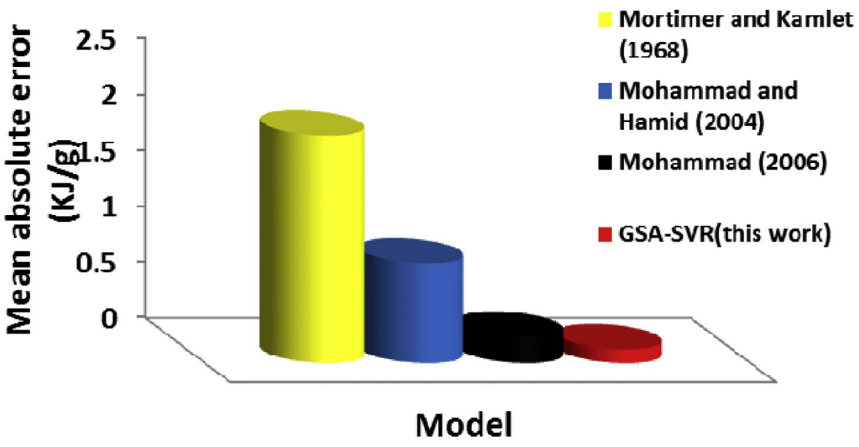

Fig. 4. Comparison of the mean absolute error of the developed GSA-SVR model with the previously developed models.

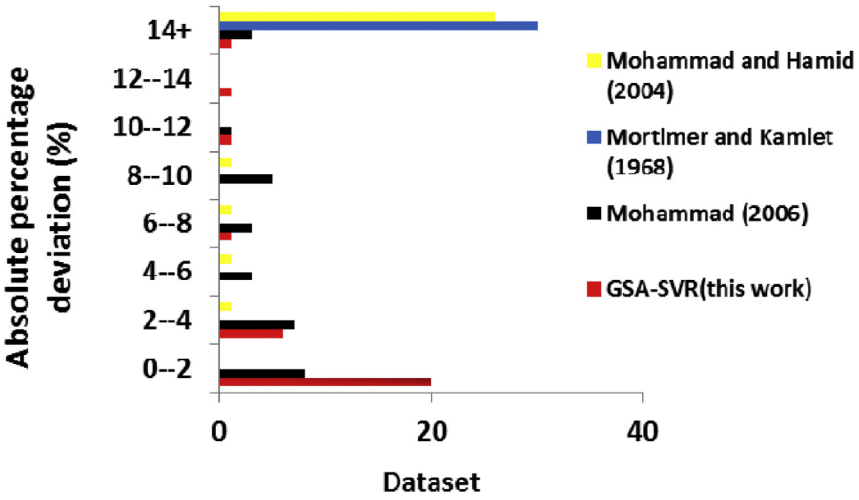

Fig. 5. A Comparison between the models using absolute percentage deviation.

square error of 0.057 kJ/g and 0.482 kJ/g were respectively obtained for the training and testing set of data. Table 2 presents the values of the parameters that determine the reliability of the developed chemometric. The excellent performance obtained from the proposed model can be deduced from the values of the parameters presented in Table 2 which has high CC and low RMSE and MAE.

4.3. Comparison of the measures of the model reliability of the developed hybrid chemometric with the existing models

The generalization and predictive capacity of the proposed hybrid chemometric are compared with the models existing in the literature using MAE, APD and CC as performance measuring parameters. Fig. 4

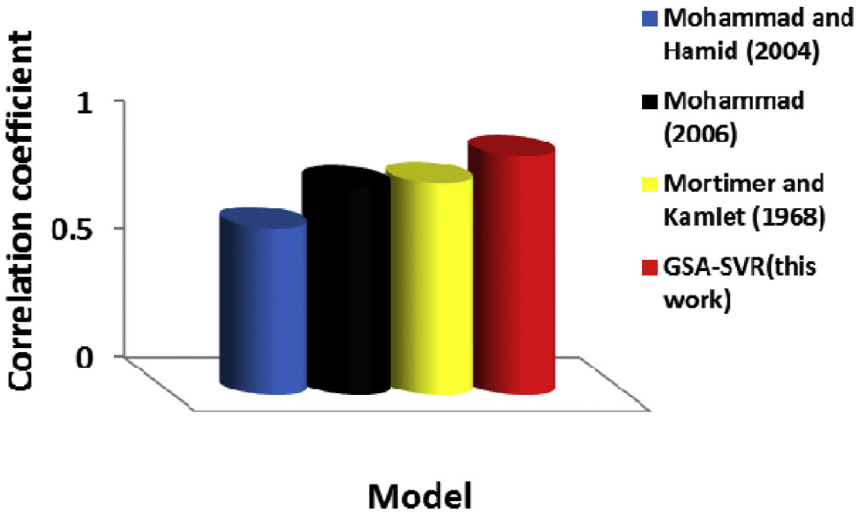

Fig. 6. Comparison of the correlation coefficient of each of the models.

Table 3
Performance comparison between the developed GSA-SVR model and the existing models.

	MAE (KJ/g)	Improvement (%) by GSA-SVR	APD (%)	Improvement (%) by GSA-SVR	CC
Mortimer and Kamlet (1968)	2.029	93.951	58.885	94.586	0.830
Mohammad and Hamid (2004)	0.889	86.197	25.035	87.266	0.654
Mohammad (2006)	0.232	47.104	6.319	49.552	0.814
GSA-SVR (this work)	0.123		3.188		0.936

presents and compares the models using mean absolute error metrics. The developed hybrid chemometric outperforms the model of Mortimer and Kamlet with percentage improvement of 93.951% while percentage improvement of 86.197% and 47.104% were obtained when respectively compared with the models of Mohammad and Hamid (2004) and Mohammad (2006).

Using the absolute percentage deviation as a measure of model performance, the developed hybrid GSA-SVR chemometric outperforms other compared existing models with a maximum number of data-points having less than 2% percentage deviation as shown in Fig. 5. From the figure, Mortimer and Kamlet model has a maximum number of data-points with deviation above 14% followed by Mohammad and Hamid model and later by Mohammad (2006) model.

Using CC between the estimated and experimentally measured heat of detonation of the investigated organic compounds, the developed hybrid chemometric outperforms other compared models existing in the literature as shown in Fig. 6. Table 3 presents the performance comparison between the developed hybrid chemometric and the existing models as well as the percentage improvement in the present GSA-SVR model as compared to other models.

4.4. Comparison of the outcomes of the present hybrid model with other models for each of the investigated aromatic energetic compound

Table 4 presents the comparison of the heat of detonation for each of the investigated aromatic energetic compounds as obtained from the developed hybrid chemometric and other existing models. The results of the developed hybrid chemometric show persistent closeness to the experimentally measured values as compared to the results of other existing models.

5. Conclusion

Heats of detonation of thirty organic energetic compounds are estimated using hybrid support vector regression chemometric and gravitational search algorithm. The influence of the number of initial population of agent assessing the search space for optimum solution search on the effectiveness and convergence of the model is investigated for both Gaussian and polynomial kernel functions. The Gaussian function shows superior performance with CC of 99.9% compared to 60% obtained by the Polynomial function. Comparison of the outcomes of the present hybrid chemometric with other models shows that the developed GSA-SVR chemometric outperforms Mortimer and Kamlet (1968), Mohammad and Hamid (2004) and Mohammad (2006) models with performance improvement of 93.951%, 86.197%, and 47.104%, respectively. On the basis of absolute percentage deviation as a measure of generalization strength of the model, the developed hybrid GSA-SVR chemometric outperforms Mortimer and Kamlet (1968), Mohammad and Hamid (2004) and Mohammad (2006) models with performance improvement of 94.586%, 87.266%, and 49.552%, respectively. The

Table 4
Comparison between the results of the developed GSA-SVR model with experimentally measured values as well as other existing models.

	Aromatic energetic compound	Experimental value	GSA-SVR (this work)	Mohammad (2006) [21]	Mortimer and Kamlet (1968) [22]	Mohammad and Hamid (2004) [23]
EC1	Ammonium picrate (Dunnite)	2.871	2.9263	3.033	5.115	2.288
EC2	Dinitronaphtalene (1,8)	3.064	3.0791	3.075	5.011	2.201
EC3	Dinitronaphtalene (1,5)	3.031	3.0791	3.075	4.978	2.168
EC4	Dinitroorthocresol	3.027	3.0755	3.301	5.31	1.782
EC5	Dinitrotoluene(2,4)	3.192	3.2719	3.225	5.42	2.055
EC6	Dinitrotoluene(2,6)	3.325	3.2719	3.225	5.554	2.188
EC7	Ethyl picrate	3.515	3.519	3.588	5.792	2.23
EC8	Ethyl tetryl	4.058	4.0089	4.033	6.207	2.879
EC9	2,4,6,2′,4′,6′-Hexanitrodiphenylamine	4.075	3.5391	4.316	5.98	3.117
EC10	Hexanitrostilbene	4.088	4.0362	4.027	6.015	3.123
EC11	Metadinitrobenzene	2.666	2.7473	3.228	5.585	2.47
EC12	Picramic acid	2.674	2.7543	2.587	4.816	1.531
EC13	Styphnic acid	2.952	2.9977	2.923	4.835	2.901
EC14	1,3,5-Triamino-2,4,6-trinitrobenzene	3.062	3.1073	3.267	5.071	2.03
EC15	Picric acid	3.437	3.4421	3.751	5.513	3.059
EC16	Trinitroaniline	3.589	3.6151	3.822	5.592	2.54
EC17	1,2-Diamino-2,4,6-trinitrobenzene	4.100	4.0471	4.027	5.369	2.324
EC18	Tetranitroaniline	4.378	4.2998	4.245	6.076	4.341
EC19	2,4,6-Trinitrotoluene	4.564	4.4616	3.546	5.888	2.628
EC20	Tetryl	4.773	4.6588	4.0118	6.331	3.764
EC21	Trinitrobenzoic acid	3.008	3.0582	2.757	5.076	2.556
EC22	2,4,6-Trinitrocresol	3.37	3.3847	3.651	5.547	2.147
EC23	Trinitronaphtalene	3.521	3.5245	3.321	5.547	2.732
EC24	Trinitropyridine-N-oxide	3.533	3.2866	4.11	5.95	4.479
EC25	2,4,6-Trinitroxylene	3.533	3.5316	3.505	5.768	2.327
EC26	Trinitroanisol	3.777	3.3847	3.651	5.955	2.555
EC27	1,3,5-Trinitrobenzene	3.964	3.9235	3.617	5.966	2.911
EC28	Trinitrophenoxethylnitrate	3.911	3.8753	4.03	6.156	3.708
EC29	Tacot	4.1	3.5301	4.217	5.714	3.476
EC30	Trinitropyridine	4.418	3.6633	3.943	6.302	4.286

demonstrated outstanding performance of the developed hybrid chemometric as compared to the existing models will be of immense significance for practical applications such as in determining the heat of detonation of organic aromatic energetic compounds while experimental stress is circumvented without loss of precision. The developed hybrid model is limited to organic energetic compounds. More data-points might be included in order to generalize the models for any class of energetic compounds.

Declarations

Author contribution statement

Hayatullahi B. Adeyemo: Conceived and designed the experiments.
Taoreed O. Owolabi: Performed the experiments; Wrote the paper.
Muhammad A. Suleiman, Kabiru O. Akande: Performed the experiments; Contributed reagents, materials, analysis tools or data.
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References

[1] M.H. Keshavarz, Simple procedure for determining heats of detonation, Thermochim. Acta 428 (1–2) (2005) 95–99.
[2] M.H. Keshavarz, Predicting heats of detonation of explosives via specified detonation products and elemental composition, Indian J. Eng. Mater. Sci. 14 (4) (2007) 324–330.
[3] M.H. Keshavarz, Estimating heats of detonation and detonation velocities of aromatic energetic compounds, Propellants, Explos. Pyrotech. 33 (6) (2008) 448–453.
[4] M.H. Keshavarz, Determining heats of detonation of non-aromatic energetic compounds without considering their heats of formation, J. Hazard Mater. 142 (1–2) (2007) 54–57.
[5] T.O. Owolabi, K.O. Akande, S.O. Olatunji, Development and validation of surface energies estimator (SEE) using computational intelligence technique, Comput. Mater. Sci. 101 (2015).
[6] V.N. Vapnik, The Nature of Statistical Learning Theory, vol. 70–92, Springer-Verlag New York, Inc, Jun. 1995.
[7] H. Drucker, C.J.C. Burges, L. Kaufman, A.J. Smola, V.N. Vapnik, Support vector regression machines, Adv. Neural Inf. Process. Syst. 9 (1996).
[8] T.O. Owolabi, K.O. Akande, S.O. Olatunji, A. Alqahtani, N. Aldhafferi, Incorporation of GSA in SBLLM-based neural network for enhanced estimation of magnetic ordering temperature of manganite, J. Intell. Fuzzy Syst. 33 (2) (2017).
[9] T.O. Owolabi, M.A. Gondal, A hybrid intelligent scheme for estimating band gap of doped titanium dioxide semiconductor using crystal lattice distortion, Comput. Mater. Sci. 137 (2017).
[10] S.O. Olatunji, Extreme learning machines and support vector machines models for email spam detection, 2017, pp. 1007–1012.
[11] A. Garg, K.S. Dazhi, J.V. Vijayaraghavan, An evolutionary framework in modelling of multi-output characteristics of the bone drilling process, Neural Comput. Appl. 29 (11) (2018) 1233–1241.
[12] A. Garg, X. Peng, M. Loan, P. Le, K. Pareek, C.M.M. Chin, Design and analysis of capacity models for Lithium-ion battery, Measurement 120 (2018) 114–120. September 2017.
[13] L. Shui, F. Chen, A. Garg, X. Peng, N. Bao, J. Zhang, Design Optimization of Battery Pack Enclosure for Electric Vehicle, 2018, pp. 331–347.
[14] T.O. Owolabi, Development of a particle swarm optimization based support vector regression model for titanium dioxide band gap characterization, J. Semicond. 40 (2) (2019).
[15] T.O. Owolabi, Modeling the magnetocaloric effect of manganite using hybrid genetic and support vector regression algorithms, Phys. Lett. 383 (15) (2019) 1782–1790.
[16] E. Rashedi, H. Nezamabadi-pour, S. Saryazdi, GSA: A gravitational search algorithm, Inf. Sci. 179 (13) (2009) 2232–2248.
[17] S.D. Beigvand, H. Abdi, M. La Scala, Combined heat and power economic dispatch problem using gravitational search algorithm, Electr. Power Syst. Res. 133 (2016) (2016) 160–172.
[18] H. L, A.R. Y, Betul Sultan Yildiz*, Structural design of vehicle components using gravitational search and charged system search algorithms, Mater. Test. 58 (1) (2016) 79–81.
[19] N.M. Sabri, M. Puteh, M.R. Mahmood, A review of gravitational search algorithm, Int. J. Adv. Soft Comput. Its Appl. 5 (3) (2013).
[20] Cortes, V. Vapnik, Support vector networks, Mach. Learn. 20 (1995) 273–297.
[21] M.H. Keshavarz, Quick estimation of heats of detonation of aromatic energetic compounds from structural parameters, J. Hazard Mater. 143 (1–2) (2007) 549–554.
[22] S.J. J, M.J. Kamlet, "Chemistry of detonations. I. A simple method for calculating detonation properties of C–H–N–O explosives, J. Chem. Phys. 23 (48) (1968) 387–393.
[23] M.H. Keshavarz, H.R. Pouretedal, An empirical method for predicting detonation pressure of CHNOFCl explosives, Thermochim. Acta 414 (2) (2004) 203–208.
[24] T.O. Owolabi, M.A. Gondal, Development of hybrid extreme learning machine based chemo-metrics for precise quantitative analysis of LIBS spectra using internal reference pre-processing method, Anal. Chim. Acta (2018).
[25] T.O. Owolabi, K.O. Akande, S.O. Olatunji, Estimation of superconducting transition temperature TC for superconductors of the doped MgB2 system from the crystal lattice parameters using support vector regression, J. Supercond. Nov. Magnetism 28 (1) (2014).
[26] T.O. Owolabi, K.O. Akande, S.O. Olatunji, Computational intelligence method of estimating solid-liquid interfacial energy of materials at their melting temperatures, J. Intell. Fuzzy Syst. 31 (2016) 519–527.