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Development and validation of surface energies estimator (SEE) using computational intelligence technique

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ABSTRACT

Accurate estimation technique that accommodates few data points is useful and desired in tackling the difficulties in experimental determination of surface energies of materials. We hereby propose a computational intelligence technique on the platform of support vector regression (SVR) using test-set-cross-validation method to develop surface energies estimator (SEE) that is capable of estimating the average surface energy of materials. The SEE was developed from SVR by training and testing the model using thirteen data points. The developed SEE was then used to estimate average surface energies of different classes of metals in periodic table. Comparison of our results with the experimental values and the surface energies obtained from other theoretical models show excellent agreement. The developed SEE can be a tool through which average surface energies of materials can be estimated as a result of its outstanding performance over the existing models.

1. Introduction

Understanding of surface phenomena through surface energies of materials is confined to limited experimental data obtained from extrapolation of liquid phase measurement to 0 Kelvin. The energy needed in creating a new surface (termed surface energy) is required in comprehending surface physical and chemical processes such as adsorption, corrosion, growth rate, surface aggregation in binary alloys and many others. Surface energies are difficult to determine experimentally because the metals need to be heated to its melting point and later extrapolated to 0 K [1]. This extrapolation technique also subjects the measured surface energies to certain degree of inaccuracy. Calculation of surface energy from the first principle is computationally demanding and is only employed for special applications [2]. Although, many semi-empirical methods are impressive but they estimate surface energies lower than experimental results [3–5]. However, average surface energies obtained with the aid of the developed SEE were compared with the surface energies from other existing theoretical models and the comparisons not only show excellent agreement but also outperform many previously known models in terms of the closeness in the obtained values to the experimental results. This is a good indication that the developed SEE will be of great advantage in estimating average surface energies of materials.

SVR is a machine learning technique that works on the principles of artificial intelligence (AI). It has diverse practical applications in several field of study and has been recently deployed in estimating the properties of materials that are difficult to obtain experimentally [6,7]. In medical field, AI techniques help in identifying different kinds of cancers so as to take proper steps toward their cure [8,9]. Compressive strength of concrete that are difficult to determine using experimental approach are now being predicted using AI techniques [10]. AI techniques are not left out in predicting the properties of crude oil reservoirs [11,12]. Other areas where AI techniques are adopted include the estimation of atomic radii of elements [13], diagnosing mechanical fault [14], forecasting Saudi Arabia stock prices [15], assessing the thickness of metal plates [16], automatic recognition of off-line handwritten Arabic numbers [17], material characterization [18] among others. The successes of support vector regression in estimating material properties [19,20] coupled with the need to have accurate and reliable means of estimating average surface energies of materials prompted us to delve into this research work.

Surface energy is generally referred to the excess energy at the surface of atoms. This excess energy comes from the difference in the energy of the atoms at the surface and at the bulk region of the crystal. Among the models that have been extensively deployed in calculating properties of materials include broken-bond models

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which approximate to the first-nearest-neighbor interaction and can be further extended to second-nearest-neighbor interaction when better accuracy is desired [21]. It estimates surface energy of materials on the basis of the number of broken bonds [22]. The number of broken-bonds at the surface of materials is known to be proportional to surface energy and this makes closed-packed surfaces to be more stable than open ones. This effect is manifested in the equilibrium crystal shapes of metals with the exposure of closed-packed surfaces at the expense of open ones. Relatively perfect correlation exists between relative surface energies (of different crystal facets) and the number of broken bonds in many fcc metals [23]. Meanwhile, recent review on theoretical models shows that the models that are dominant in calculating surface energies of metals include embedded atomic method (EAM) and equivalent crystal theory (ECT) [24] which was further extended to analytical equivalent crystal theory (AECT) in order to cater for the major challenge that arises in finding the root of ECT equations. EAM is a semi-empirical method that usually based on approximations to nearest neighbors. It is basically governed by the ideas of density functional theory and is capable of estimating the total energy of a set of atoms in a system by summing the screened coulomb interaction and embedding energy [25]. Embedding energy is obtained when each atom involves in coulomb interaction is inserted in the electron density from all other atoms. The method premises on the fact that the embedding energy (peculiar to a species of atom) is uniquely dependent on the electron density and not on the source while electron density at any site is usually assumed as a linear superposition of spherically symmetric electron densities from other contributing atoms. Due to inefficiency of EAM to generalize well, modification that takes energy change (which arises as a result of non-spherical distribution of electron p_i and deviation from the linear superposition of atomic electronic density) into consideration evolved afterwards. The results of our developed model agree well with the available experimental results due to the ability of SVR to acquire complex relationship that exists between descriptors and target.

Accuracies of 99.4% and 100% (on the basis of correlation between the actual and estimated average surface energies) were obtained during training and testing of the developed SEE and this enhanced its performance in estimating the average surface energies of various classes of metals. The average surface energies of metals that were estimated cut across alkali metals, 3d-transition metals, 4d-transition metals, 5d-transition metals and other selected metals in the periodic table which include alkali earth metals, lanthanide series and others. Based on the outstanding performance of SEE in the course of estimating average surface energies of metals, it is proposed as a potential means of estimating average surface energies of materials.

The remaining part of this work is organized as follow. Section 2 describes the proposed machine learning techniques (i.e. support vector regression) including generalization performance evaluation, the physical significances of the chosen descriptors and the working principles of the adopted technique. Section 3 contains empirical studies that include the description of the dataset, computational methodology and the adopted strategies in searching for the optimum parameters. Section 4 presents and discuses results while Section 5 states the conclusions and recommendation.

2. Proposed method

This research work adopts SVR derived from statistical learning theory [26,27] to develop SEE. It employs ε-insensitive loss function that measures flatness of the generated pattern as well as the maximum allowable deviations of the targets from the predicted values for all given training dataset $(x_1, y_1), \ldots, (x_k, y_k)$ with k number of samples [28]. Eq. (1) represents a linear function with $\langle w, x\rangle$ dot product in the space of R'.

$$f(x,\alpha) = \langle w, x\rangle + b \tag{1}$$

where $w \in R'$ and $b \in R$.

For the purpose of establishing the goal of SVR in ensuring the flatness of Eq. (1), small value of w is desired through minimization of the Euclidean norm $\|w\|^2$ which makes the optimization problem of the regression looks like the one presented in Eq. (2)

$$\text{minimize } \frac{1}{2}\|w\|^2$$

$$\textit{subject to } \left\{ \begin{array}{l} y_i - \langle w, x_i\rangle - b \leqslant \varepsilon \\ \langle w, x_i\rangle + b - y_i \leqslant \varepsilon \end{array} \right\} \tag{2}$$

Eq. (2) holds on the assumption that there exists a function that is capable of providing error which is less than ε for all training pairs of the dataset. The slack variables (ξ_i and ξ_i^*) are often introduced in order to create room for another kind of error that may arise while dealing with real life problems. Therefore, Eq. (3) is modified and presented as Eq. (4).

$$\text{minimise } \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{k}(\xi_i + \xi_i^*)$$

$$\textit{Subject to } \left\{ \begin{array}{l} y_i - \langle w, x_i\rangle - b \leqslant \varepsilon + \xi_i \\ \langle w, x_i\rangle + b - y_i \leqslant \varepsilon + \xi_i^* \\ \xi_i, \xi_i^* \geqslant 0 \quad \text{for all } i = 1, 2, \ldots\ldots, k \end{array} \right\} \tag{3}$$

The optimization problem in Eq. (3) is well solved by using Lagrangian multipliers ($\eta_i, \eta_i^*, \lambda_i$ and λ_i^*) to transform the problem into dual space representation. Therefore, the Lagrangian for the Eq. (3) is presented in Eq. (4)

$$L = \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{k}(\xi_i + \xi_i^*) - \sum_{i=1}^{k}\lambda_i(\varepsilon + \xi_i - y_i + \langle w, x_i\rangle + b) - \sum_{i=1}^{k}\lambda_i^*(\varepsilon + \xi_i^* + y_i - \langle w, x_i\rangle - b) - \sum_{i=1}^{k}(\eta_i\xi_i + \eta_i^*\xi_i^*) \tag{4}$$

It is easier to locate the saddle point of the Lagrangian function defined in Eq. (4) by equating the partial derivatives of the Lagrangian (with respect to w, b, ξ_i and ξ_i^*) to zero. We therefore obtained expressions presented in Eqs. (5)–(7)

$$w = \sum_{i=1}^{k}(\lambda_i^* - \lambda_i)\cdot x_i \tag{5}$$

$$\eta_i = C - \lambda_i \tag{6}$$

$$\eta_i^* = C - \lambda_i^* \tag{7}$$

The optimization equation is maximized by substituting Eqs. (5)–(7) in (4). Therefore, we arrived at Eq. (8)

$$\frac{1}{2}\sum_{i=1}^{k}\sum_{j=1}^{k}(\lambda_i^* - \lambda_i)(\lambda_j^* - \lambda_j)(x_j.x_i) - \varepsilon\sum_{i=1}^{k}(\lambda_i^* + \lambda_i) + \sum_{i=1}^{k}y_i(\lambda_i^* - \lambda_i)$$
$$\textit{subject to } \sum_{i=1}^{k}(\lambda_i^* - \lambda_i) = 0, 0 \leqslant \lambda_i^* \text{ and } \lambda_i \leqslant C \tag{8}$$

The solutions (λ_i^* and λ_i) obtained from Eq. (8) are substituted in Eq. (1) and presented in Eq. (9)

$$f(x,\alpha) = \sum_{i=1}^{k}(\lambda_i^* - \lambda_i)\langle x_i, x\rangle + b \tag{9}$$

The concept of Kernel function helps SVR to solve non-linear problems by mapping the data into high dimensional feature