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Estimation Of The Atomic Radii Of Periodic Elements Using Support Vector Machine

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Abstract
Atomic radii of elements are experimentally obtained from crystallographic data. However, this is not a feasible approach for some elements with limited number of atoms in existence since radii could not beeasily drawn from severaltypes of bound in ionic, covalent and metallic crystals.Hence, this work employs artificial intelligence approach using support vector machine to accurately predict and estimate the atomic radii of elements in the periodic table in order to pave way for predicting atomic radii of elements that could not be easily determined from crystallographicdata. We obtained an accuracy of over 99% on the basis of the correlation between the experimental and our predicted radii. The simplicity and accuracy of this approachdepict an excellent measure of its tendency to predict atomic radii of any element whose atomic number isknown.

Index terms: Atomic number, Atomic radii, Coefficient of Correlation, Number of electron's orbit andSupport vector machine

1. Introduction

It is generally assumed that atom has no fixed radius[1]. The radius of an atom depends greatly on its surrounding atoms. Atomic radius is usually measured by considering the half distance between the nuclei of two touching atoms. Atomic radii are defined as covalent radii when the concerned nuclei are in covalent boundand estimated as metallic radii for two nuclei in metallic crystals. The Van der waal radii come into play when we measure the minimum half distance between two nuclei of atoms of the elements that are not bound to the same molecule.

Atom of every element has electrons which revolve round the nucleus in a particular orbit known as electron shell where the Newtonian mechanics is violated[2] The number of electrons contained in an atom (i.e. atomic number) of an element is a unique property of that element, since no two atoms of different elements in their neutral states can have the same number of electrons. The trend of atomic radius and atomic number in the periodic table is a plausible indication thatthere exist a kind of relationship between them and one could be obtained from the other. This research work predicts atomic radii of elements using atomic number and the number of orbits (which could be deducted from atomic number) through which electrons revolve.This proposed excellent approach possesses optimum assurance of accuracy while applying it to elementsthat have no actual experimental radii.

After the acceptance of the Bohr atomic model[2], scientists began to think of the ways to measure the size of an atom. The first approach was that of Bragg[3], who obtained universal atomic radii of elements using crystallographic data drawn from metallic, ionic and covalent solids. Bragg's atomic radii were later strengthened by J.C Slater [4]by considering over 1200 bounds observable in different sort of crystals and molecules.This approach adopted by Slater,is not liable to be extended to newly discovered elements such as Ununoctiumbecause only few atoms have been successfully produced. Moreover, the reactivity of these atoms is not well known. The new approach of ours caters for this lapse.

For the purpose of complementing the Bragg and slater's radii, clement et al[5] proposed and presented theoretical modelsthat determine atomic radii of some elements using minimal basis-set atomic function for the ground-state atom. This model obtained atomic radii of all noble gases that could not be obtained by slater due to the fact that the atoms of noble gases are usually inert(except few, such as krypton, xenon and radon)[1], even to other atom of the same element.Several theoretical models obtained atomic radii using different approaches. Atomic radii of elements were obtained by considering the presence of interaction between electrons and neglecting the nature of the interaction[6]. Radial density distribution function was also adopted to obtain atomic radii[7]. Free electron density is another approach through which atomic number could be estimated based on hall measurements[8].The uniqueness of our approach is that itattains very high accuracy using approach that is different from thepopularly knownmethods of predicting atomic radii and can be generalized to all elements.

Among setbacks which call for the urgent need of simple and accurate models in predicting atomic radii is the fact

that some newly discovered elements(such as Ununoctium) have limited number of atoms in existence which makes it extremely difficult to experimentally determine their universal atomic radii from crystallographic data of covalent,metallic or ionic bound with other crystals. The approach of this work remains simple and accurate in predicting atomic radii of these kinds of elements.

In the same vein, elements that are classified as noble gases have distinct properties, among which is that they do not usually react with other elements. To crown it all, an atom of noble gas (such as helium)does not come in contact with another atom of the same element. This property makes it difficult to measure their radii experimentally from crystallographic data. Therefore, it is highly necessary to adopt a simple approach through which atomic radii of these elements can be accurately determined.

The uniqueness of this work is that it adopts a method (i.e. artificial intelligence method using support vector regression) that predicts atomic radii of elements above 99% ofaccuracy on the basis of correlation coefficient using properties that is virtually present in all knownelements. Artificial intelligence has performed excellently in prediction and has been used in several field of study for the purpose of prediction and identification.In oil and gas industries, It performs excellently in the prediction of permeability of carbonates reservoirs[9], in predicting the properties of crude oil system[10][11].Artificial intelligence has also been widely deployed in medical field through identification of skin diseases[12] as well as prostate cancers[13],to mention but few.

Therefore, this work proposed and implemented support vector machine to predict atomic radii of the periodic element purposely to create room for predicting atomic radii of elements that are difficult to determine experimentally.

2.0 Proposed Method

This research work adopts support vector regression (SVR) to predict the atomic radii of elements using their atomic number and the number of electron orbit. The approach of this work as well as the accuracy achieved(above 99%) prove a strong correlation between the atomic number of elements as well as its prominence in been adopted as a tool for determining atomic radii. It makes it possible to quickly obtain atomic radius of any element characterized with atomic number.

Support vector Regression achieves generalized performance by minimizing the generalized error bound instead of the observed training error[14] .The goal of SV regression as published by Vapnik[15]is to employ kennel trick in predicting a function f with at most, ε deviation from the actual target y for all training data set $[(x_i, y_i), ...(x_z, y_z)] \subset PxR$ where P represents the space of the input pattern. Let us examine the case of linear function for the sole aim of simplicity. We can represent the linear functions as

$$f(x) = \langle w, x \rangle + a \text{ With } w \in P \text{ and } a \in R \quad \text{..... (1)}$$

The dot product in the space P of the input pattern is represented as $\langle\ \rangle$ and the flatness is achieved by seeking for small w in the equation (1) through minimization of Euclidean norm[16]. If we desire to write the problem at hand as a convex optimization problem that requires minimizing $\frac{1}{2}\|w\|^2$. The minimization is then subjected to

$$\left.\begin{cases} y_i - \langle w, x_i \rangle - a & \leq \varepsilon \\ \langle w, x_i \rangle + a - y_i & \leq \varepsilon \end{cases}\right\} \text{..... (2)}$$

On the basis that the function f which approximate all pairs of input data (x_i, y_i) with precision ε, actually exist, or we even say that the convex optimization problem is feasible. In order to cope with infeasible constraints of the optimization which can likely occur, one can introduce variable ξ_i and ξ_i^* known as slack variables. Therefore, we arrive at the formulationproposed by Vapnik[15].

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

$$\text{Subject to } \left.\begin{cases} y_i - \langle w, x_i \rangle - a & \leq \varepsilon + \xi_i \\ \langle w, x_i \rangle + a - y_i & \leq \varepsilon + \xi_i^* \\ \xi_i \xi_i^* & \geq 0 \end{cases}\right\} \text{.....} \quad (3)$$

The regularization factor$C$ (which is always greater than zero), measures a kind of tradeoff between the flatness of the function f and amount to which the deviations from the target that are larger than ε is tolerated.

The kernel function is responsible for transforming the data set into hyper plane[17][18]. The variables of the kernel must be computed accurately since they determine the structure of high-dimensional feature space which governs the complexity of the final solution. The most commonly used kernel functions in the literature are[18][15]: Polynomial, Linear, Gaussian, and Sigmoid. Typical kernel functions are:

$$K(\overrightarrow{x_i}, \overrightarrow{x_j}) = (\overrightarrow{x_i} \cdot \overrightarrow{x_j} + 1)^d \text{ ..... (6)}$$

$$\overrightarrow{x_i}, \overrightarrow{x_j}) = \exp\left(-\gamma \left\| \overrightarrow{x_i} - \overrightarrow{x_j} \right\|^d\right) \text{ ..... (7)}$$

Equation (6) is the polynomial kernel function of degree d which will revert to the linear function when d = 1. Equation (7) is the Radial Basis Function (RBF) kernel with one parameter γ [18][19][20].

Other kernel functions are:

Linear: $K(x_i, x_j) = x_i^T x_j$ and sigmoid: $K(x_i, x_j) = \tanh(\gamma x_i^T x_j + r)$

Here $\gamma, r, and\ d$ are kernel parameters.

Regularization parameter (C) determines the trade-off cost between minimizing the training error and minimizing the model's complexity.

The tube size of the ε-insensitive loss function (ε) is equivalent to the approximation accuracy placed on the training data.

Regularization parameters (C) and the tube size of the ε-insensitive loss function (ε) are constant parameters whose values are to be set depending on the problem being addressed.

3.0 Empirical Study

3.1 Data Set Description

The data set employed in this research work is a set of atomic radii drawn from over 1200 bounds observable in different kind of crystals and molecules as published by J.C Slater[4]. Seventy-eight of these radii with their atomic numbers and the number of electron's orbits in each atom were randomly selected across the periodic table and presented in Table 3.1.0Withthe aid ofMicrosoft excel sheet, we obtained the statistical parameters of the data such as mean, median,standard deviation and the coefficient ofcorrelation between atomic radii and atomic number. The statistical results are tabulated in table 3.1.1 and 3.1.2

Table 3.1:0 Atomic number (AN), Number of electron orbit (EO), and Atomic radii (AR) of all the data set

Element	EO	AN	AR(Pico meter)
H	1	1	25
Li	1	3	145
B	2	5	85
C	2	6	70
N	2	7	65
O	2	8	60
F	2	9	50
Mg	3	12	150
Al	3	13	125
Si	3	14	110
P	3	15	100
Cl	3	17	100
Ca	4	20	180
Sc	4	21	160
Ti	4	22	140
V	4	23	135
Cr	4	24	140
Mn	4	25	140
Fe	4	26	140
Co	5	27	135
Ni	5	28	135
Cu	5	29	135
Zn	5	30	135
Ga	5	31	130
Ge	5	32	125
As	5	33	115
Zr	6	40	155
W	10	74	135
Re	11	75	135
Os	11	76	130
Ir	11	77	135
Pt	11	78	135
Au	11	79	135
Ti	11	81	190
Pb	11	82	180
Bi	12	83	160
Po	12	84	190
Ra	12	88	215
La	8	57	195
Ce	8	58	185
Nb	6	41	145
Mo	6	42	145
Tc	7	43	135
Ru	7	44	130
Rh	7	45	135
Pd	7	46	140
Ag	7	47	160
Cd	7	48	155
In	7	49	155
Sn	7	50	145
Sb	8	51	145
Te	8	52	140
Cs	8	55	260
Ba	8	56	215
Hf	10	72	155
Ta	10	73	145
Th	12	90	180
Pa	13	91	180
U	13	92	175
Np	13	93	175
Pu	13	94	175
Am	13	95	175

Se	5	34	115
Br	6	35	115
Rb	6	37	235
Sr	6	38	200
Eu	9	63	185
Gd	9	64	180
Tb	9	65	175
Dy	9	66	175
Ho	10	67	175
Er	10	68	175
Tm	10	69	175
Yb	10	70	175
Lu	10	71	175
Pr	9	59	185
Nd	9	60	185
Pm	9	61	185
Sm	9	62	185

Table 3.1:1 Statistical results of the data set

	Mean	STDEV	Median
Atomic radii	150.2	39.61	145
Atomic number	49	26.41	49
Number of Electron Orbit	7.30	3.35	7

Table 3.1:2 Statistical results of the dataset

	Atomic radii and Atomic Number	Atomic radii and number of electron's orbit
Correlation of coefficient	0.618	0.617

3.2.0Description of the experiment

All the programing work in this research work was done using MATLABenvironment. The data were first shuffled randomly before dividing them into training and testing sets in ratio 9 to 1 respectively. They were then normalized to keep them within same range and facilitate efficient computation. The training datasets were then used in training SVM model used in the atomic radii prediction.

3.2.1Working Principle of Support vector regression system as used in this research work

Support vector regression system is a leaning environment where the predictor parameters are related to the desired target output through a function generated by the system. Two kinds of data set are employed in this kind of environment, the training and testing data set. The generated predicted target output is compared with the desired target so as to determine how they are correlated and modify the function until highly correlated results are obtained. Meanwhile, a well-trained system is characterized bypredictions with high correlation coefficient between the actual and predicted values, low root mean square error as well aslow absolute error. The second set of data is used to test the efficiency and the accuracy of the trained system. In this case, the trained system generates output targets with the predictordata (atomic number and number of electron's orbits). The correlation of these results is also computed. High accuracy in both training and testing data indicates high prediction ability of the trained system, although, high accuracy on the testing data set is highly desired.

3.2.2 Optimal parameter search strategy

Parameter search was carried out purposely to determine the support vector regression parameters that give maximum performance of the system. The high accuracy attained in our predicted values is largely dependent on the value of the regularization factor C, the trend of which is depicted in the fig 3.1. From the graph, at a small value of C (keeping lambda, epsilon, kernel option at constant value of 1e-7, 0.2 and 0.3 respectively and using Gaussian as our kernel), the coefficient of correlation between the actual and the predicted radii is small and starts to increase as the value of C increases. The maximum performance for both testing and training occur when the value of C becomes 130 and remain constant therefrom.

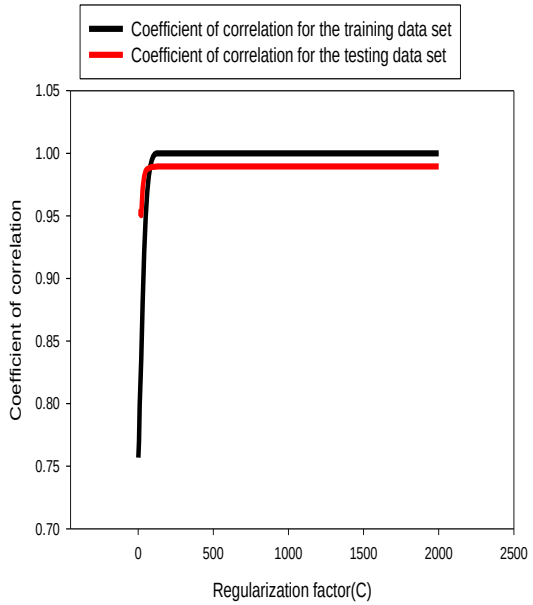

Figure 3.1: The trend of the variation of regularisation factor with the coeficient of correlation while keeping other parameters constant

To ensure accurate utilization of this support vector machine, we vary another parameter (i.e. lambda) at the optimalvalue of C (i.e.130) in order to show the effect of lambda on the Performance of the proposed support vector regression. Our result (as can be seen in the fig 3.2) shows

that the lambda has no influence in increasing or decreasing the performance of the system but rather maintains it at constant value.

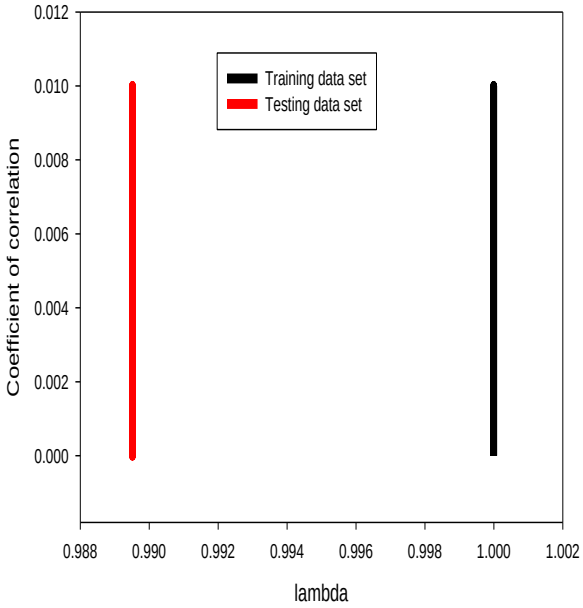

Figure 3.2:The trend of the variation of lambda with the coeficient of correlation while keeping other parameters constant

Another parameter that determines the performance of the proposed system which was also examined is the epsilon. The effect of epsilon, that is, the maximum tolerable deviation from the actual radii, is shown in the fig 3.3. Using the values of C and Lambda (130 and 0.0000001 respectively) at which the highest performance was observed in the previous graphs, while varying the value of epsilon,the coefficient of correlation maintains constant value for both testing and training data set up to a value of 1.4 after which the testing begins to increase and later follows another pattern which shows a decrement. In the case of the coefficients of correlation for the training data set, it decreases after reaching its maximum value. The optimal value that yields excellent performance in our trained system occurs at a value of 1.4.

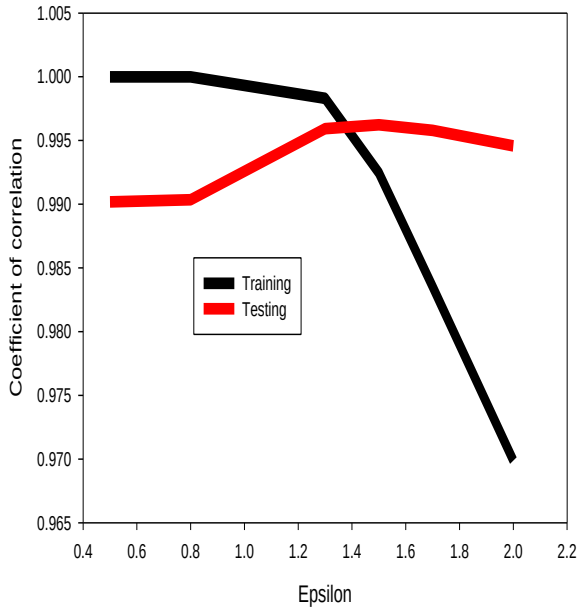

Figure 3.3: The trend of the variation of epsilon with the coefficient of correlation, keeping other parameters constant

By varying any one of the search parameters (using C, lambda, epsilon and kernel option that determine the accuracy of the machine) one after the others, while keeping others constant, the coefficients of correlation between the experimental atomic radii and the predicted atomic radii attain maximum value at the parameters indicated in the table 3.2.

Table3.2: Optimum parameters for SVM

C	130
Lambda	1.00E-07
Epsilon(ε)	0.2
Kernel option	1.4
Kernel	Gaussian

3.3Performance quality measures

The excellent prediction performance of our approach is measured by low absolute error (Ea), low root mean square error (rmse) and high coefficient of correlation between the actual atomic radii and the predicted radii. These prediction performance factors are obtained from the following equations.

$$cc = 1 - \left[\sum_1^n \left\{\frac{R_{exp} - R_{cal}}{R_{exp}^2}\right\}^2\right] \quad \text{..... (3)}$$

$$rmse = \sqrt{\frac{1}{n}\left[\sum_1^n \left\{\frac{R_{exp} - R_{cal}}{R_{exp}^2}\right\}^2\right]} \quad \text{..... (4)}$$

$$Ea = \sum_1^n \left\{\frac{R_{exp} - R_{cal}}{n}\right\}^2 \quad \text{..... (5)}$$

Where $R_{\exp}$, R_{cal} and n represent the experimental atomic radii, the predicted radii and the number of data set respectively.

4.0 Result and Discussion

We compare the actual (experimentally obtained) atomicradii with the predicted radii by the trained support vector regression systemfor the training data set and the result is tabulated in table 4.1. The experimental atomic radii and the atomic radii predicted by our developed systemare so close to the extent that the differences are hardly seen graphically as indicated in the fig 4.1 and the table 4.1

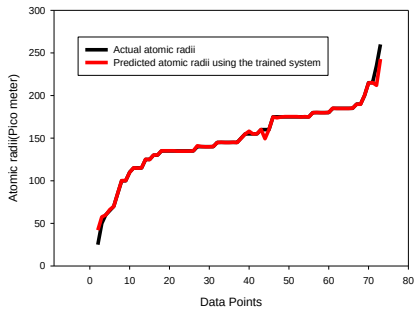

Figure 4.1:A graph of the actual atomic radii and the atomic radii predicted while training our system

Table 4.1: The Actual and predicted atomic radii while training our system (Accuracy of 99.58%)

Element	Experimental atomic radius	Predicted atomic radii
Th	180	179.80
Ti	140	140.20
Li	145	144.80
F	50	50.20
Zr	155	154.80
Sm	185	184.80
Cl	100	100.20
Ag	160	160.20
Ca	180	179.80
Nb	145	145.20
H	25	25.20
Rb	235	234.80
Np	175	174.80
P	100	100.20
Pt	135	135.20
Cr	140	140.20
Mo	145	145.20
U	175	174.80
Al	125	125.20
V	135	135.20
Ce	185	184.80
Os	130	130.20
W	135	135.20
Cs	260	259.80
Tb	175	174.80
Pm	185	184.80
Gd	180	179.80
Pa	180	179.80
Sn	145	144.80
Ra	215	214.80
Dy	175	174.80
Se	115	115.20
Re	135	135.20
Br	115	115.20
Eu	185	184.80
Fe	140	140.20
Hf	155	155.20
Cu	135	135.20
In	155	154.80
Ho	175	174.80
Cd	155	155.20
Ti	190	189.80
Er	175	174.80
C	70	70.20
Tm	175	174.80
O	60	60.20
Nd	185	184.80
B	85	85.20
Sc	160	160.20
Po	190	189.80
Ta	145	144.80
As	115	115.20
Mg	150	149.80
Ge	125	125.20
Ni	135	135.20
Bi	160	159.80
Co	135	135.20
Pb	180	179.80
Yb	175	174.80
Lu	175	174.80
Zn	135	135.20
Sr	200	199.80
Pr	185	184.80
Ir	135	134.80

Ba	215	214.80
Pd	140	140.03
Si	110	110.20
Ga	130	130.20
Mn	140	140.20
Pu	175	174.80
Sb	145	145.20
N	65	65.20

In the same vein, for the testing data set, the actual and the predicted radii were also compared and they are highly connected with close values as can be seen from the fig 4.2 as well as the table 4.2.

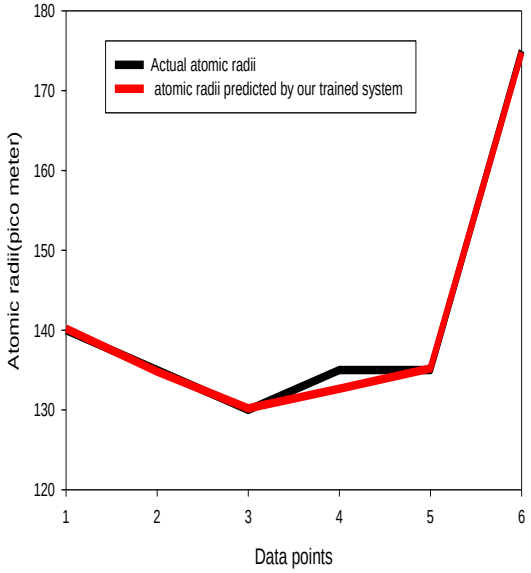

Figure 4.2:A graph of the actual atomic radii and the atomic radii predicted while testing our trained system

Table 4.2: The Actual and predicted atomic radii while testing our trained system (Accuracy of 99.63%).

Element	Experimental Atomic radii(Pico Meter)	Predicted Atomic radii (Pico meter)while testing our system
Te	140	140.2
Rh	135	134.8
Ru	130	130.2
Tc	135	132.652
Au	135	135.2
Am	175	174.8

The accuracy of our results on the basis of the coefficients of correlation between the actual(as atomic radii as obtained experimentally) and the predicted atomic radii using support vector regression is depicted in table 4.3. We also achieved low root mean square and absolute errors for the training and testing data set. These high accuracies in both the training and the testing set give strong indication that the predictor variables (atomic number and the number of electron's orbits) that we employed in predicting the atomic radii are good parameters for the prediction. The chosen predictor parameters facilitate this excellent prediction ability as deducted from its statistical analysis in table1.1.

Table 4.3: Results

	Training data set	Testing data set
Coefficient of correlation	0.996	0.996
Root mean square error	4.255	3.695
Absolute error	1.668	1.940

5.0 Conclusion and recommendation

Our findings in this research work show that the atomic radii elements can be accurately and easily predicted directly from their atomic numbers using support vector machine.Comparison of our predicted atomic radii with actual(experimental obtained) atomic radii shows excellentcorrelation. Thesuccess of this approachconfers confidence in extending and recommending theproposed method to predict atomic radii of elements that are difficult to obtain experimentally.

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