Forest of Elements: Machine Learning Insights into Periodic Table Atomic Radii

AIM: Prediction of atomic radius using machine learning by Random Forest Regression.

1. **Our Work:**

The atomic radius is an important property of an atom that is difficult to measure experimentally for all elements. In this paper, we present a machine learning approach using the random forest algorithm to predict the atomic radius of elements based on four parameters: atomic number, number of shells, ionization enthalpy, and row in the periodic table. Our model achieves a mean absolute percentage error of 1.17% on a test dataset of 82 elements. We demonstrate that the random forest algorithm is capable of capturing the complex, non-linear relationships between the input parameters and the atomic radius, and can provide accurate predictions for most elements. Our approach has potential applications in various fields, including materials science, chemistry, and physics, where the knowledge of atomic radius can be used to make predictions about the properties and behavior of materials and molecules.

2. **Data and methods:**

2.1 Run flow:

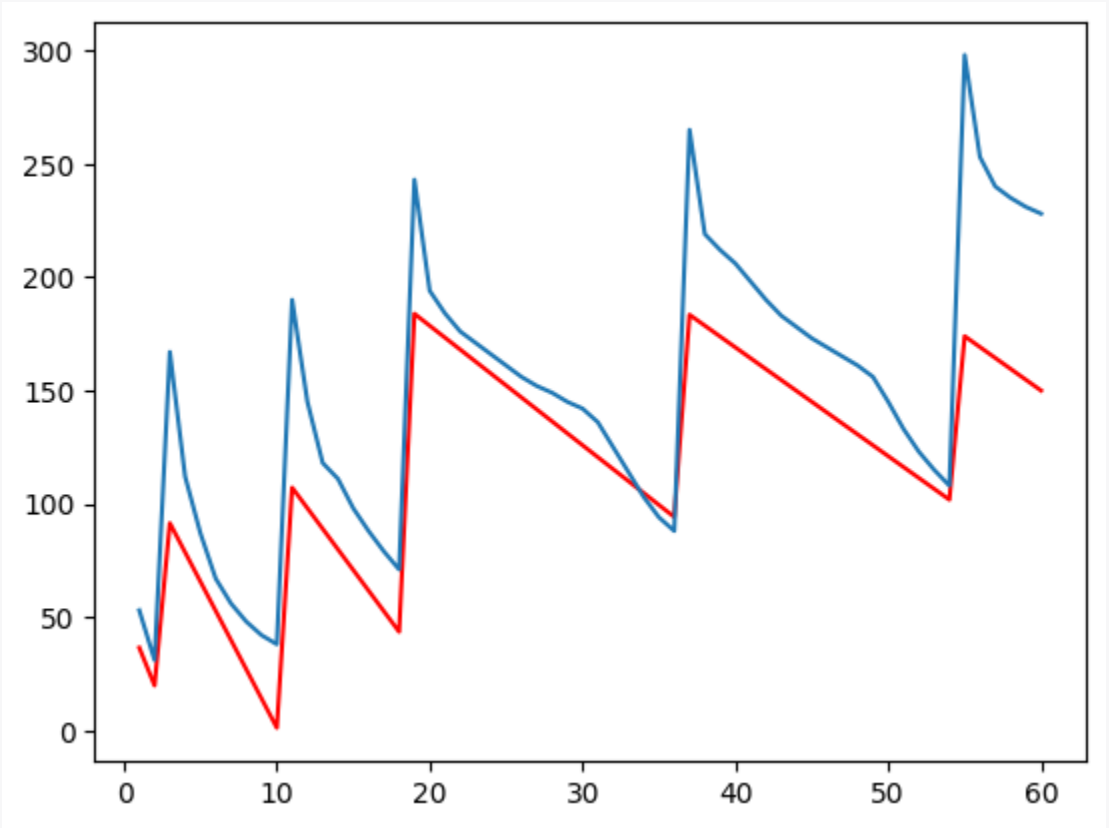
- Data extraction from file
- Importing the libraries
- Loading the data and array conversions
- Deriving some more parameters from the given parameters
- Combine all the parameters to make higher dimensional data
- Training the model
- Checking the accuracy

Here the graphs between atomic radius and Z are provided to compare the accuracy of different models.

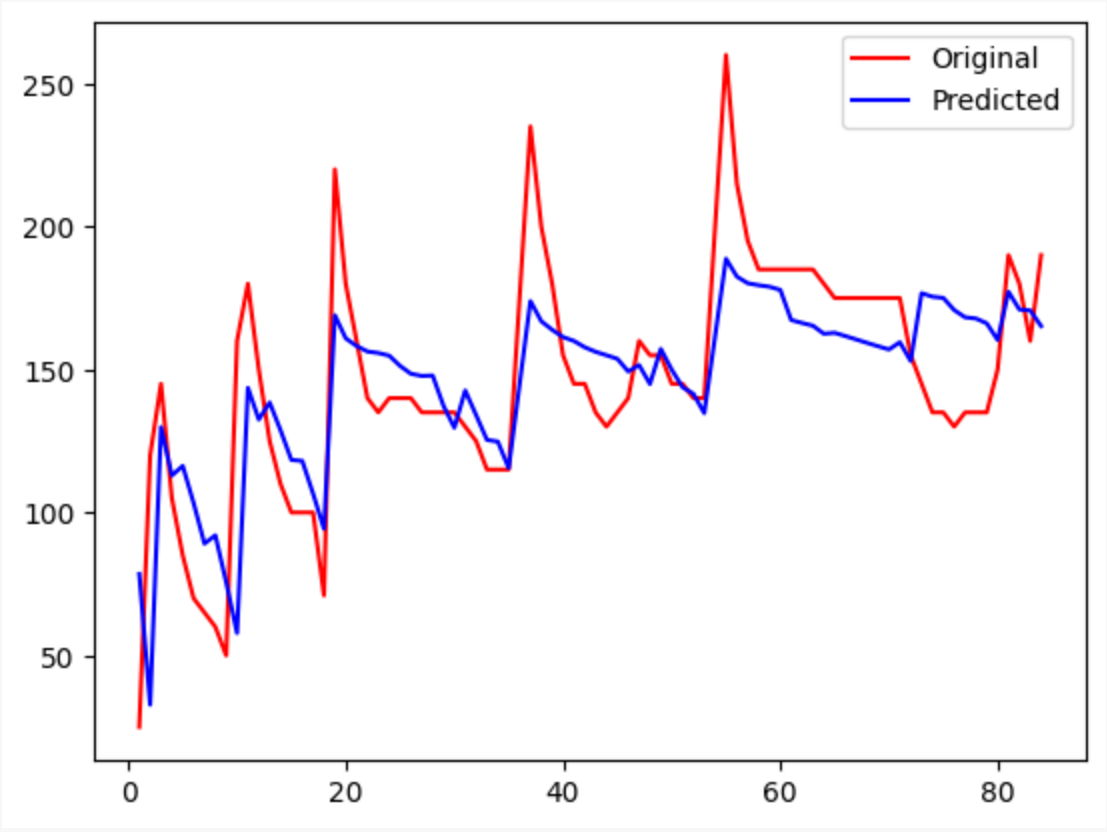
1) **Linear regression:**

Blue- Original value

Red- Predicted value

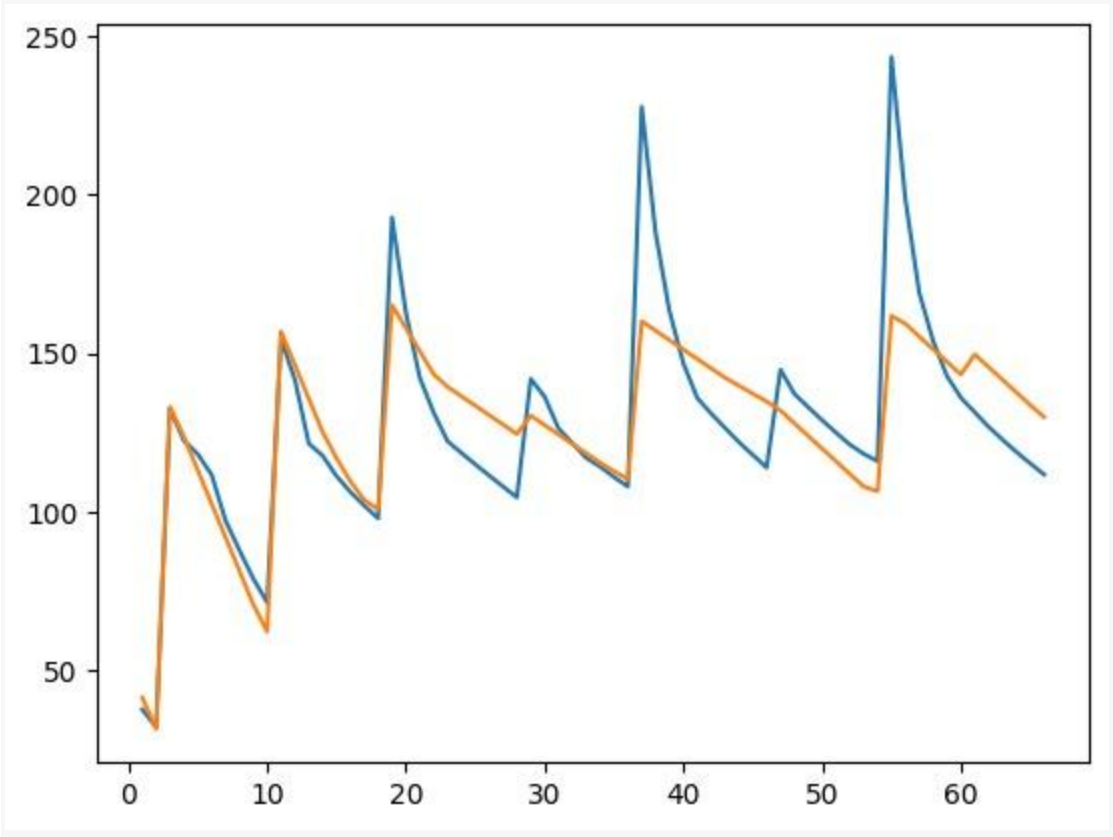


2) Multiple regression:

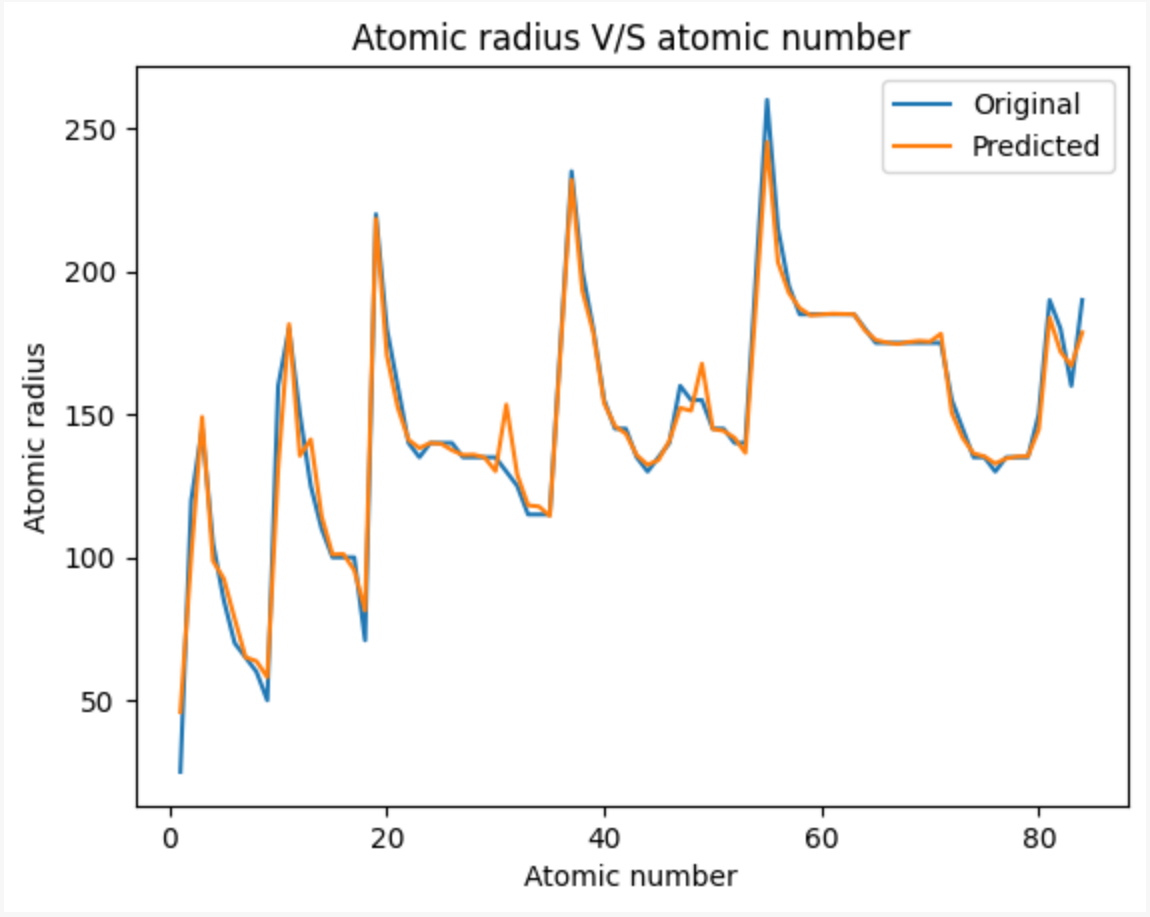


3) Neural Network:

Blue- Original value
Orange- Predicted value



4) Random Forest:



From the above graphs, it is clear that random forest regression can provide better accuracy in predicting atomic radius.

3. Results:

Here is the result of predicting the atomic radius for the elements after atomic number 84 (i.e 85 to 98) which are radio actives.

	Original	Predicted	%Error
count	14.000000	14.000000	14.000000
mean	181.357143	186.917857	4.865243
std	33.163017	16.076124	12.054551
min	120.000000	166.100000	-12.000000
25%	174.250000	182.162500	0.190171
50%	175.000000	183.350000	4.214286
75%	184.500000	183.500000	4.857143
max	270.000000	237.600000	38.416667

4. Application areas:

1. **Materials science:** Accurately predicting atomic radius can be useful in designing new materials with specific properties. For example, knowing the atomic radius of an element can help in selecting the appropriate materials for semiconductors or superconductors.
2. **Chemistry:** Atomic radius is a key parameter in chemical reactions and bonding. Predicting the atomic radius of an element can help in understanding chemical reactions, predicting the properties of molecules, and designing new drugs.
3. **Physics:** Atomic radius is a fundamental property in atomic physics, and accurate predictions can help in understanding the behavior of atoms in various contexts, such as in the presence of external fields or under extreme conditions.

5. Conclusion:

From the above discussion it is clear that the random forest algorithm of machine learning can be more beneficial than other methods in learning the non-linear behavior of the atomic radius. Which shows a mean %error of 4.86% in predicting the atomic radius for the elements after atomic number 84 (i.e 85 to 98) which are radio actives.