**Superconductivity Data Analysis and Machine Learning**

INT 354 – Machine Learning 1

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**Abstract**

Superconductivity prediction is a crucial aspect of material science, with applications ranging from energy transmission to medical imaging. In this research, we utilize data from the UCI Machine Learning Repository to build predictive models for superconductivity. The dataset contains various material properties that influence superconductivity, making it an ideal candidate for machine learning analysis. We employ several regression techniques, including linear regression, polynomial regression, regularized regression (Lasso and Ridge), support vector regression (SVR), and decision tree regression, to predict critical temperature, a key indicator of superconductivity. Our analysis focuses on comparing the performance of these models in terms of training time, accuracy, recall, and F1 score. Through this study, we aim to provide insights into the effectiveness of different regression techniques for superconductivity prediction.

Keywords: Superconductivity, Predictive Modelling, Machine Learning, Regression Analysis, UCI Machine Learning Repository.

**Introduction**

Superconductivity is a phenomenon characterized by zero electrical resistance and the expulsion of magnetic fields from a material when cooled below a critical temperature. Understanding and predicting superconductivity is of great importance in various fields, including energy transmission, magnet technology, and medical imaging. The ability to accurately predict superconducting materials can lead to the development of more efficient devices and technologies.

Machine learning techniques have shown promise in predicting superconductivity based on material properties. By leveraging datasets containing information about the chemical composition and structural characteristics of materials, researchers can build models to predict critical temperatures, a key factor in determining superconductivity.

In this research, we aim to explore the effectiveness of different regression techniques in predicting critical temperatures of superconducting materials. We utilize data from the UCI Machine Learning Repository, which provides a comprehensive dataset of material properties and corresponding critical temperatures. By applying various regression algorithms to this dataset, we seek to identify the most accurate and efficient method for superconductivity prediction.

**Literature** **Review**

Previous studies have explored the use of machine learning techniques for superconductivity prediction, often focusing on regression analysis due to its ability to model continuous target variables. Notable research includes the work of Kam Hamidieh, who employed regression models to predict critical temperatures based on material descriptors such as atomic and crystal properties. Hamidieh's study demonstrated the potential of machine learning in identifying patterns and correlations within complex datasets.

Other researchers have investigated the use of advanced regression techniques, such as support vector regression (SVR) and decision tree regression, in superconductivity prediction. These methods offer advantages in handling non-linear relationships and high-dimensional data, which are common characteristics of material datasets.

Despite the progress made in superconductivity prediction, challenges remain in achieving high accuracy and efficiency in modelling. The choice of features, model complexity, and computational resources all impact the performance of regression algorithms in this context. Therefore, further research is needed to evaluate the effectiveness of different techniques and address these challenges.

**Methodology**

**1. Dataset's Info**

- The dataset used in this research is obtained from the UCI Machine Learning Repository and contains various material properties, including atomic mass, atomic radius, and lattice constants, along with the critical temperature of superconducting materials.

- The dataset comprises X samples and Y features.

**2. Train\_valid\_test\_split**

- The dataset is split into training, validation, and test sets using a standard split ratio (e.g., 70% training, 15% validation, 15% test).

**3. Exploratory Data Analysis (EDA)**

- Exploratory data analysis is conducted to gain insights into the distribution, correlation, and characteristics of the dataset.

- Summary statistics, histograms, correlation matrices, and scatter plots are used to visualize the data.

**4. Feature Selection**

- Feature selection techniques, such as correlation analysis, recursive feature elimination, or domain knowledge-based selection, are applied to identify the most relevant features for superconductivity prediction.

**5. Principal Component Analysis (PCA)**

- PCA is performed to reduce the dimensionality of the dataset while preserving its variance.

- The principal components are used as input features for regression models.

**6. Linear Regression**

- A linear regression model is trained using the selected features to predict the critical temperature of superconducting materials.

**7. Polynomial Regression:**

- Polynomial regression models of different degrees are trained to capture non-linear relationships between features and the target variable.

**8. Regularized Regression (Lasso):**

- Lasso and Ridge regression models are employed to penalize the coefficients of the regression model and prevent overfitting. We only use Lasso as it is sufficient.

**9. Support Vector Regression (SVR):**

- SVR is utilized to model non-linear relationships between features and the critical temperature by mapping the data into a higher-dimensional space.

**10. Decision Tree Regression:**

- Decision tree regression is applied to partition the feature space into subsets and fit a regression model to each subset.

**Results**

The performance of various regression techniques for predicting the critical temperature of superconducting materials varied significantly, as indicated by the results presented in Table 1.

* **Linear Regression**: Demonstrated moderate performance with a training accuracy of 0.57 and a test accuracy of 0.59. The model achieved an R-squared score of 0.59 on the test set.
* **Polynomial Regression**: Outperformed linear regression, with a training accuracy of 0.71 and a test accuracy of 0.73. Utilizing polynomial features of degree two, the model significantly improved its predictive capability, yielding an R-squared score of 0.73 on the test set.
* **Lasso Regression**: Exhibited performance similar to linear regression, with a training accuracy of 0.57 and a test accuracy of 0.58. The model achieved an R-squared score of 0.58 on the test set.
* **Support Vector Regression (SVR)**: Showcased comparable performance to linear regression, with a training accuracy of 0.56 and a test accuracy of 0.58. SVR yielded an R-squared score of 0.57 on the test set.
* **Decision Tree Regression (DTR)**: Demonstrated the highest accuracy among all models, with a training accuracy of 0.73 and a test accuracy of 0.74. The model achieved an impressive R-squared score of 0.74 on the test set.

These results suggest that while traditional linear regression methods provide a baseline for superconductivity prediction, polynomial regression and decision tree regression offer improved accuracy. Lasso regression and SVR, although similar in performance to linear regression, may require further optimization to enhance their predictive capabilities.

**Conclusion**

In conclusion, this research underscores the potential of machine learning techniques in advancing the prediction of superconductivity based on material properties. By applying a range of regression algorithms to the UCI dataset, we have systematically explored various modeling approaches and evaluated their performance in terms of accuracy and efficiency. Our analysis reveals several notable findings:

* **Diverse Performance**: Different regression techniques exhibited varying levels of accuracy and efficiency in predicting critical temperatures of superconducting materials.
* **Optimal Models**: Polynomial regression and decision tree regression emerged as top-performing models, demonstrating superior accuracy compared to other methods.
* **Baseline Performance**: Traditional linear regression methods provided a foundational understanding of superconductivity prediction but were surpassed by more advanced techniques.
* **Further Optimization**: Regularized regression methods, such as Lasso, and support vector regression (SVR) showcased potential for improvement with additional fine-tuning of hyperparameters and feature engineering.

By elucidating these insights, our study contributes to the ongoing efforts to enhance superconductivity prediction through machine learning. The findings underscore the importance of leveraging diverse modelling approaches and optimizing algorithmic parameters to achieve robust and accurate predictions.

**Results Table:**

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
|  | Linear Regression | Polynomial Regression | Lasso | SVR | DTR |
| Train Acc. | 0.57 | 0.71 | 0.57 | 0.56 | 0.73 |
| Test Acc. | 0.59 | 0.73 | 0.58 | 0.58 | 0.74 |
| MSE | 469.52 | 303.55 | 471.68 | 479.22 | 298.40 |
| R2 Score | 0.59 | 0.73 | 0.58 | 0.57 | 0.74 |
| Train F1 | 0.94 | 0.94 | 0.94 | 0.95 | 0.98 |
| Test F1 | 0.94 | 0.93 | 0.94 | 0.95 | 0.99 |

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