

Predicting Magnetic Susceptibilities of Rare Earth Ions Using Machine Learning Algorithms

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The accurate prediction of magnetic susceptibility in rare earth (RE) compounds presents a significant challenge due to their intricate electronic structures and strong magnetic interactions. This study leverages machine learning (ML) techniques as powerful tools to model and predict the magnetic susceptibilities of RE compounds, focusing on their magnetic properties. By employing ML algorithms such as linear regression, decision trees, random forests, XGBoost, and neural networks, we aim to address the computational challenges associated with traditional numerical methods for solving magnetic field problems in materials with partially filled 4f orbitals. Analysing a dataset of RE halides, oxides, sulfates, and sulfides, we demonstrate the robustness of ensemble methods like random forests and XGBoost in delivering accurate predictions even with limited data. The research highlights the potential of integrating ML into the computational analysis of magnetic material properties, offering a streamlined and data-driven alternative to traditional approaches. By improving the efficiency and accuracy of susceptibility predictions, this study contributes to advancements in computational electromagnetics, with implications for the design of materials tailored for specific magnetic applications.

Index Terms— magnetism, machine learning, magnetic susceptibility, rare earth compounds

I. INTRODUCTION

Predicting magnetic properties like susceptibility is essential for material design and electromagnetic applications. For rare earth (RE) compounds, traditional quantum-based models struggle due to complex 4f electron behavior and computational demands. Machine learning (ML) offers a data-driven alternative—unlike traditional methods, it identifies non-linear patterns in empirical data and enables rapid, scalable predictions across diverse compounds. By learning from known examples, ML can generalize to new materials, accelerating discovery without intensive simulations.

Recent studies have demonstrated ML's potential in this domain. For example, Zhang et al. used regression, support vector machines, random forests, and neural networks to predict diamagnetic susceptibility in organic compounds, achieving R^2 values from 0.9831 to 0.9928 [1]. Afantitis et al. developed QSAR models using molecular descriptors to predict diamagnetic behaviour [2]. These findings support the broader application of ML to more complex systems like RE compounds. Our study evaluates regression-based ML models trained on dataset of quantized features of RE compounds such as ionization state, atomic number, molecular attributes, theoretical and experimental susceptibilities. We thereby analyze model performance and discuss its implications for material screening and design.

II. BACKGROUND

A. Magnetic Susceptibility

Magnetic susceptibility, a key property of RE compounds, reflects their response to external magnetic fields and depends on the electronic configuration of partially filled 4f orbitals. Theoretical approaches, including Van Vleck paramagnetic theory, predict susceptibility using quantum numbers, Landé g-factors, and temperature [2].

The molar magnetic susceptibility (χ_{mol}) is expressed as:

$$\chi_{mol} = \frac{N_A \mu_B^2 g^2 J(J+1)}{3k_B T} \quad (1)$$

Where μ_B and k_B are constants, and J , the total angular momentum, depends on the RE ion's electronic structure. However, complexities like crystal field effects and lanthanide contraction limit these theoretical methods, highlighting the need for data-driven approaches.

B. Theoretical Calculations

In this study, theoretical values for molar magnetic susceptibility were computed for various RE ions across halides, oxides, sulfides, and other compounds. The process involved:

1. Determining the electronic configuration of RE ions.
2. Applying Hund's rules to establish quantum states (L, S, J).
3. Calculating Landé g-factors using:
$$g = \frac{3}{2} + \frac{S(S+1) - L(L+1)}{2J(J+1)} \quad (2)$$
4. Using the computed g-factor to calculate susceptibility values at room temperature using (1).

These values augmented the training dataset, improving the model's understanding of theoretical and experimental relationships.

C. Algorithms Employed

This study employs these algorithms: linear regression for modeling relationships between variables, decision trees providing interpretable decision-making rules, random forests to enhance accuracy by combining multiple decision trees, and XGBoost to improve predictive performance with gradient boosting techniques and neural networks for complex pattern recognition and feature learning in large datasets.

III. RESULTS AND DISCUSSION

We conducted an exploratory analysis of the dataset, which includes experimentally measured susceptibilities taken from [3]-[4] and theoretically calculated values for RE compounds.

Attempts to incorporate SMILES-derived fingerprints as given in [1] did not enhance the model, so we focused on chemical features for predicting molar susceptibility.

The dataset was split 70% for training and 30% for testing, with theoretical data always included in the training set. Models were implemented using Python (numpy, sklearn, xgboost, PyTorch) and evaluated with R^2 and Mean Squared Error (MSE).

From values shown in evaluation metrics plots (Figs.1-4) and as listed in TABLE I, the linear regression model provided a baseline with moderate accuracy with some variability due to random variability, the small gap between the curves (Fig.4. (a)) reflects noise and the models simplicity, yet maintaining a testing $R^2 > 0.6$. From Fig.1. the regression tree model offers robust predictions and reveals how increasing tree depth can enhance training performance but risks overfitting when applied to new data. This underscores the importance of selecting an optimal depth for practical applications.

When compared to the Fig.1., the random forest algorithm (Fig.2.) yielded significantly better results. While a single decision tree can overfit the data, random forests mitigate this by aggregating multiple trees trained on different random subsets, improving robustness and generalization. Overall, XGBoost model as shown in (Fig.3.) outperforms other models, delivering results that are nearly as good as the previous models but with greater stability. The combination of ensemble learning (boosting), hyperparameter tuning, and efficient regularization in XGBoost makes it a powerful tool for complex prediction tasks with reduced risk of overfitting. Risk of overfitting is associated with the limited dataset we have, which will be addressed with stronger attribute generalization.

Although the Neural Network model exhibited strong training performance (Fig. 4(b)), capturing non-linear patterns effectively, it did so less efficiently due to the limited size of the dataset, which hindered its ability to generalize.

Hyperparameters like tree depth, number of estimators, ReLU activation, and Adam optimizer were crucial in optimizing model performance, improving prediction accuracy and generalization.

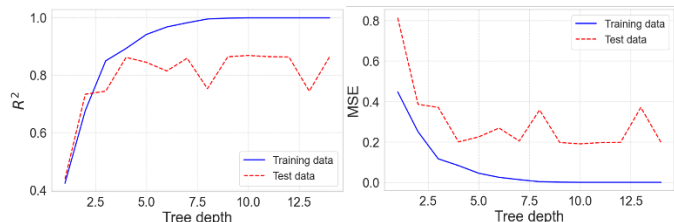


Fig. 1. Model Performance vs. Tree Depth: R^2 and MSE for Regression Tree

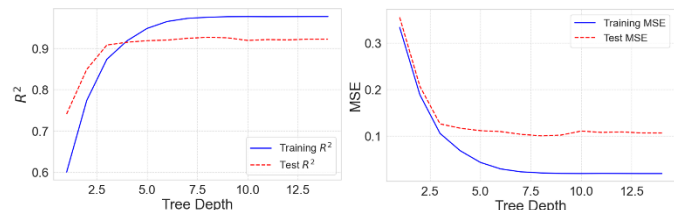


Fig. 2. Model Performance vs. Tree Depth: R^2 and MSE for Random Forest

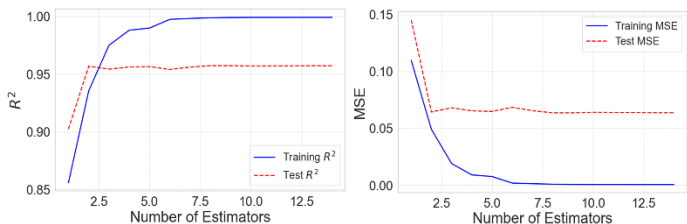


Fig. 3. Model Performance vs. Number of Estimators: R^2 and MSE of XGBoost

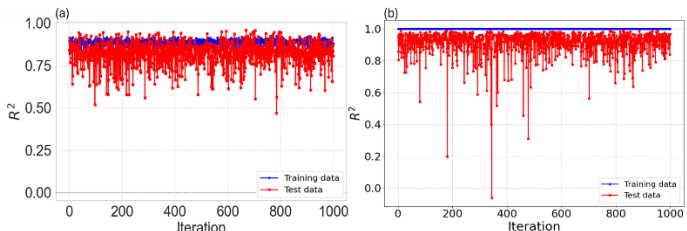


Fig. 4. R^2 variation across iterations (a) linear regression (b) neural network

TABLE I
COMPARATIVE PERFORMANCE METRICS OF ML MODELS

Model	Training R^2	Testing R^2	Training MSE	Testing MSE
Linear Regression	0.8796	0.8163	0.0987	0.2404
Decision Tree	0.9991	0.8684	0.0007	0.1905
Random Forest	0.9776	0.9271	0.0187	0.1000
XGBoost	0.9991	0.9572	0.0007	0.0637
Neural Network	0.9995	0.9087	0.0036	0.9503

IV. CONCLUSION

This study demonstrates that machine learning models, trained on both experimental and theoretical data, can predict the magnetic susceptibility of rare earth compounds with high accuracy. Among the models evaluated, Random Forest and XGBoost showed exceptional performance, achieving R^2 values of 0.927 and 0.957, respectively. These results highlight the robustness of ensemble methods in capturing complex, non-linear relationships that traditional models often overlook. By leveraging quantized descriptors like ionization state and atomic number, this work highlights data-driven framework that accelerates material screening and enables the discovery of new materials with tailored magnetic properties. Unlike traditional quantum simulations, which are computationally intensive, our ML-based approach offers a scalable, efficient alternative, advancing material design.

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