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Utilizing Machine Learning to Predict the Charge Storage Capability of Lithium-Ion Battery Materials

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ABSTRACT

With the increasing demand for high-performance batteries in applications such as electric vehicles and portable electronics, accurately predicting the charge storage capacity of battery materials is crucial for developing more efficient and reliable energy storage systems. Machine Learning (ML) and data-driven approaches, plays a vital role in enhancing our understanding of Li-ion battery performance, guiding materials design, optimizing system efficiency, and accelerating innovation in energy storage technologies. In this study, an ML-based approach was applied to a dataset of 2345 rechargeable Li-ion battery materials, obtained from the Materials Project online portal, to predict gravimetric charge storage capacity – a key parameter for energy storage capability. To model this relationship, three key independent features were selected: average operating voltage, gravimetric energy density, and charging stability. Given the nonlinear dependencies between these features and the target variable, an ensemble learning algorithm, Gradient Boosting Regression (GBR), was employed. The model exhibited high predictive accuracy, achieving an R^2 value of 0.99 on the test dataset with a Mean Squared Error (MSE) of 20.08 for target feature values. These results confirm the model's effectiveness in capturing complex relationships within the battery materials dataset, demonstrating its reliability in predicting charge storage capacity with minimal error. The feature selection strategy emphasizes practical electrochemical properties, enhancing the model's interpretability and relevance for battery material screening. Its low error metrics indicate strong generalizability, positioning it as a valuable tool for accelerating battery material discovery and optimizing performance. This study distinguishes itself by focusing on gravimetric charge storage capacity prediction using domain-relevant features and an ensemble learning approach, leveraging a large open-source dataset to achieve high predictive accuracy. This is crucial for energy storage capabilities, but it has been less frequently modeled directly in ML-driven battery studies.

1. Introduction

Modern technology relies heavily on batteries to power anything from portable electronics to electric vehicles. Battery technology converts the chemical energy stored in their active materials into the electrical energy. They come in several varieties, each with unique chemistries and uses. Based on the possibility of the reversibility of chemical reaction, they are broadly classified into primary or non-rechargeable and secondary or rechargeable batteries. Some common primary battery includes alkaline batteries and zinc-carbon batteries whereas, lead-acid, li-ion, nickel-metal hydride etc. belongs to rechargeable battery types. Rechargeable battery types are becoming the solution for sustainable energy, especially for different renewable energy sources which can be stored during their peak production and use when in need [1]. Li-ion batteries are widely used in consumer devices and electric cars due to their extended cycle life and high energy density [2-3].

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Because lead-acid batteries are dependable and reasonably priced, they are frequently utilized in backup power systems and automobiles. When robustness and rapid discharge rates are required, nickel-metal hydride (Ni-MH) or nickel cadmium (Ni-Cd) batteries are employed [4]. Battery technology is still developing, with the main goals being to lower the costs, increase energy density, increase charge storage capacity and improve safety [5-8].

Among the major goals of current research in battery technology, this research focus on charge storage capability of the battery materials which is one of the key factors for batteries overall performance using a growing statistical technique integrating with machine learning [9-11]. The performance and efficiency of a battery are largely dependent on the charge storage capabilities of the battery components, which is sometimes measured as capacity. This capacity is reliant on the material's capacity to hold and release ions during charge and discharge cycles: lithium ions in the case of Li-ion batteries [12-13] . The surface area of the active material, the compatibility of the electrolyte with the electrode, and the crystal structure of the material, which impacts ion mobility, are important factors affecting charge storage [14-15]. More ions can be stored in high energy density materials, such as those with layered or spinel structures, resulting in an increase in capacity. Charge storage is also greatly impacted by elements such as the solid-electrolyte interface (SEI) stability, doping or defect presence in the crystal structure, and electrode material particle size [16-18]. The temperature and the frequency of charge/discharge cycles are two more environmental factors that might affect a battery's capacity and lifespan [19-20].

The specific charge storage per unit mass, also called gravimetric capacity (mAh/g) of a battery, is highly dependent on the average operating voltage (V), gravimetric energy density (Wh/kg), and stability during charging and discharging cycles (meV/atom) of the battery material. The quantity of energy that can be provided and stored per unit charge is directly influenced by the average voltage; greater voltages have the potential to produce larger gravimetric capacity, but they may also have negative effects on cycle life and material stability. The gravimetric energy capacity represents energy density per unit mass of the electrode material where a higher value typically representing higher charge storing capacity. The charging stability is another important factor influencing the charge storage capacity of the battery. This characteristic gauge the material's stability across cycles of charging and draining. Higher stability is indicated by a lower stability charge, which implies that the material can withstand more cycles while maintaining its structure and capacity. A high degree of stability guarantees that the material will not degrade significantly over time and can intercalate and deintercalated ions on multiple occasions, maintaining its charge storing capacity.

Several studies [21-25] explore ML applications in lithium-ion battery design, manufacturing, service, and end-of-life management, while also addressing key challenges such as data availability, preprocessing difficulties, limited sample size, computational complexity, model generalization, interpretability, scalability, data bias, and interdisciplinary integration, along with potential mitigation strategies. By selecting average operating voltage, gravimetric energy density, and charging stability, this study focuses on the most influential and directly relevant features for predicting charge storage capacity, ensuring high predictive accuracy while avoiding unnecessary computational complexity. These features align closely with real-world battery optimization strategies, making the ML-model more practical for battery design and materials selection.

This study highlighted the possibility of using machine learning models in materials science by integrating domain-specific knowledge with advance statistical techniques. It provides insight for informed decision-making and tuning the important parameters to achieve the highest possible charge storage capacity in battery materials design and optimization process. By accurately predicting the gravimetric capacity of battery materials considering of intrinsic battery properties such as voltage, energy density and stability, our model contributes to discover and deploy more efficient and sustainable battery solutions.

2. Methodology

This work utilizes the machine learning approach in predicting the charge storage capacity of the lithium-ion batteries taking average operating voltage, gravimetric energy capacity and charging stability as independent factors. ML is a potent technique that uses algorithms to find trends in data and forecast future events. ML can be very helpful in analyzing complex relationships between multiple independent factors and the dependent variable in the context of predicting the charge storage capacity of lithium-ion batteries. In this study, these independent variables as well as charge storage capabilities obtained through experimentation and/or theoretical calculations can be used to train machine learning models.

The study employs a Gradient Boosting Regressor (GBR), to predict the gravimetric charge storage capacity (mAh/g) of Li-ion battery materials based on average operating voltage, gravimetric energy density, and charging stability. The dataset was obtained from Materials Project's (https://next-gen.materialsproject.org/batteries) battery explorer data using Pymatgen v2024.3.23 along with materials project's api key: mp_api, on a personal computer and subsequently transferred to Google Colab, where model training and evaluations were carried out using its cloud-based computing resources. The software environment used was Python 3.10.11 and following Python libraries were used for data processing, machine learning, visualization, and model training: pandas 2.2.0 – for dataset manipulation and preprocessing; numpy 1.26.0 – for numerical computations, scikit-learn 1.3.2 – for train-test splitting, deploying GBR and performance evaluation, matplotlib 3.8.3 & seaborn 0.13.1 – for data visualization and feature importance analysis. By providing detailed information on the computational environment, software, model parameters, and evaluation procedures, this study ensures that the results can be replicated and extended for further research on Li-ion battery material predictions.

Initially the data contain a total of 2440 entries which on preprocessing and cleaning reduced to 2345 entries, shown in Table 1. The data preprocessing and cleaning involved removing 54 entries with missing values in key features of average operating voltage, gravimetric energy density, charging stability and the target variable of gravimetric charge storage capacity, as imputation was avoided to maintain the data integrity. Additionally, 29 outliers were identified and removed using the Interquartile Range (IQR) method, ensuring extreme values did not distort the model's learning process. Lastly, 12 duplicate entries were eliminated to prevent redundancy and bias in model training. These preprocessing steps ensured a cleaner, more reliable dataset for accurate machine learning predictions.

The data was then split into 80% training (1876 entries) and 20% test (469 entries) datasets. Hyperparameter tuning was systematically conducted using grid search to optimize the GBR model. Grid search explored a predefined set of values for key parameters, testing learning rates (0.01, 0.05, 0.1), number of estimators (100, 200, 300), and max depth (3, 6, 9) to identify the best combination based on cross-validation performance. To address model robustness and generalizability, 5-fold cross-validation was employed during the hyperparameter tuning process. This technique was used within the Grid Search to evaluate how well the model performs on different subsets of the data, ensuring that the model does not overfit to any data split. The best configuration – 300 estimators, a learning rate of 0.1, max depth of 3 – was selected based on the highest R^2 score and lowest RMSE during 5-fold cross-validation, ensuring an optimal balance between predictive accuracy and computational efficiency.

The models are trained to identify how changes in voltage, energy density, and stability affect the battery's charge storing capacity by feeding this data into the machine learning algorithms. After being trained, these models use the average voltage, energy density, and stability properties of novel or hypothetical battery materials to predict their charge storage capacity. The benefit of utilizing ML in this study

Table 1. Preview of preprocessed and cleaned dataset for Li-ion battery materials, showcasing key features used in the analysis.

SN	Average voltage (V)	Gravimetric energy (Wh/kg)	Charging stability (meV/atom)	Gravimetric capacity (mAh/g)
1	0.212144	45.687194	0.000000	215.359297
2	1.221144	239.242133	445.086555	195.916336
3	1.462983	14.236724	9.241924	9.731301
4	1.185918	95.560818	40.266981	80.579647
5	0.974059	105.244523	111.004291	108.047398
...	...	...	...	...
2341	3.193511	224.910062	89.547827	70.427199
2342	3.416358	955.025295	56.536830	279.544863
2343	3.390423	938.003662	21.501470	276.662714
2344	4.803133	667.611624	97.221177	138.995614
2345	4.123430	715.250132	38.882774	173.459983

is its capacity to manage sizable datasets and reveal non-linear correlations that could be challenging to identify with conventional statistical techniques. Robust prediction models can be produced via machine learning by processing data from a variety of sources, including simulations and experimental results. The performance of these models may thus be quickly and accurately predicted, negating the need for extensive experimental testing and speeding up the development and optimization of new battery materials. Using machine learning in this research use a data-driven strategy that could lead to faster innovation cycles, more accurate forecasts, and the creation of high-performance lithium-ion batteries with optimal charge storage capabilities.

The model evaluation was conducted using the coefficient of determination (R^2) and Mean Squared Error (MSE) by using Eqs. 1 and 2 to assess prediction accuracy. The R^2 score, which quantifies how well the model explains variance in the target variable, is defined as

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \check{y}_i)^2}{\sum_{i=1}^{n}(y_i - \dot{y}_i)^2} \quad (1)$$

where y_i – represents actual values, $\check{y}_i$ is model-predicted value of the target variable, $\dot{y}$ is the mean of actual values, and n is the total number of samples. An R^2 close to 1 indicates a strong model fit.

The Mean Squared Error (MSE), measuring the average squared deviation between actual and predicted values, is given by

$$\mathrm{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_i - \dot{y}_i)^2 \quad (2)$$

where lower values indicate better predictive accuracy. These metrics were used to evaluate the GBR model, ensuring robust assessment of its performance in predicting gravimetric charge storage capacity.

3. Results and Discussion

The distribution of charge storage capacity (mAh/g) in a dataset of lithium-ion battery materials typically provides insights into the variability and trends of the materials performance. To visualize how charge storage capacity is distributed across the dataset, a histogram or Probability Density Function (PDF) is plotted which shows how often different capacity values occur. The shape of the distribution can provide important insights. To address model robustness and generalizability, 5-fold cross-validation was employed during the hyperparameter tuning process. This technique was used within the Grid Search to evaluate how well the model performs on different subsets of the data, ensuring that the model does not overfit to any data split. Cross-validation helps in assessing the stability of the model's performance and is crucial for confirming its ability to generalize to unseen data. The model's best parameters were selected based on the lowest cross-validation MSE, ensuring that it provides an optimal balance between predictive accuracy and generalization across the data.

Figure 1 illustrates the overall distribution of the target feature, which follows a normal distribution with a slight positive skew, indicating a tendency toward higher charge storage capacity values. The largest frequency occurred between 100 and 150 mAh/g and most data points clustered between 50 and 200 mAh/g. The red curve reflects the probability density function, gives a smooth approximation of the distribution, while the blue bars show the frequency of these values.

Most materials or samples have lower gravimetric capacities, with fewer achieving values above 300 mAh/g which basically represents the values at the outlier regions. Analyzing scatter plots between the target feature and independent features is a crucial step in feature engineering, as it helps identify relationships, trends, and potential nonlinearities in the data. This visualization allows for the detection of correlations, outliers, and feature interactions, guiding the selection and transformation of variables to improve model performance and predictive accuracy.

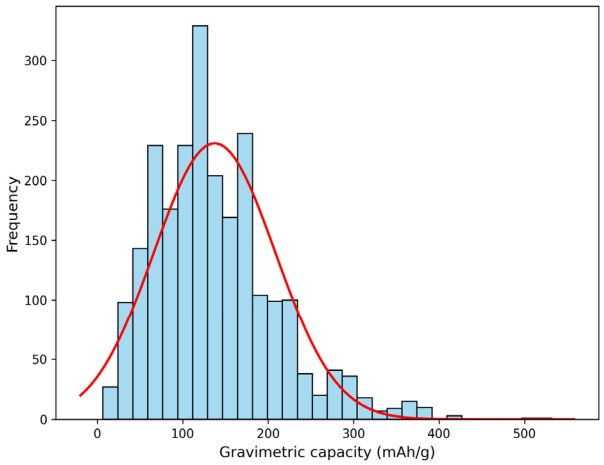

Fig. 1. Distribution of charge storage capacity (mAh/g) showing a normal distribution with slight positive skew for the dataset.

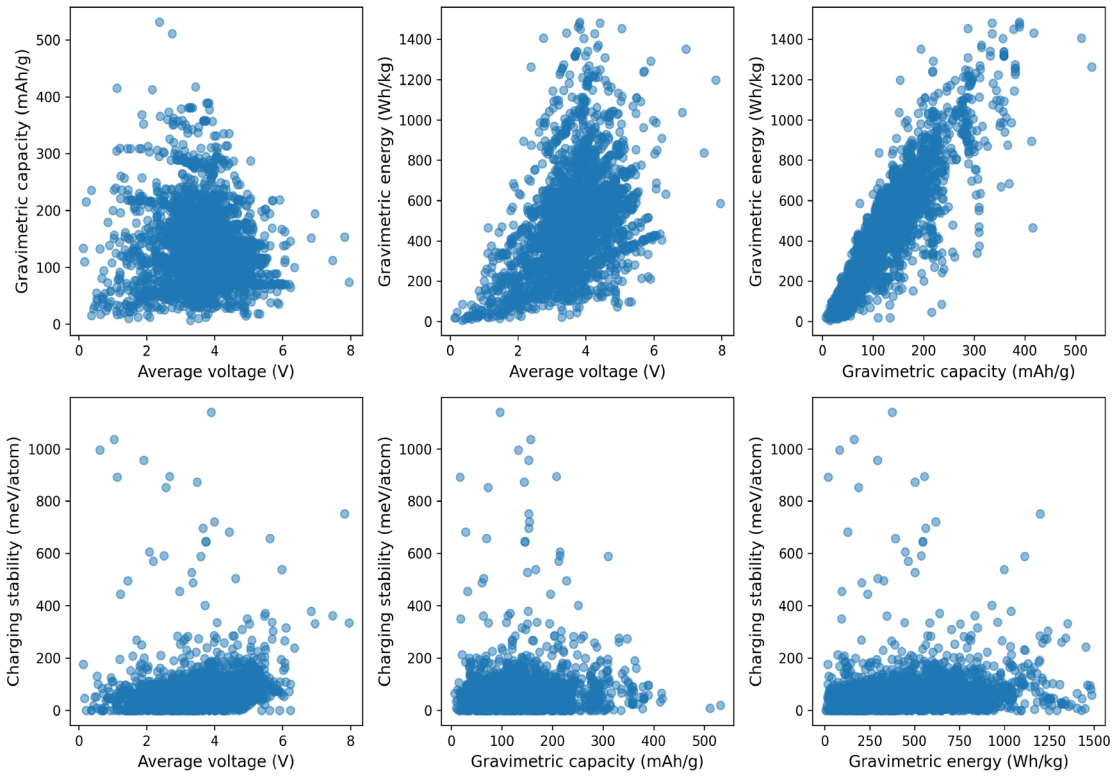

Fig. 2. Scatter plot showing relationships between independent features and the target feature, highlighting a notable correlation between gravimetric energy density and charge storage capacity.

Figure 2 presents scatter plots illustrating the relationships between the target feature and independent features. The analysis reveals weak correlations between most feature pairs, except for a notable correlation between gravimetric energy density and charge storage capacity, indicating their strong interdependence in battery materials. The fact that scatter plots reveal no good correlation between the independent features and the target suggests that the relationship between them is likely non-linear. In many cases, especially with complex systems like battery materials, simple linear relationships between features and outcomes (such as gravimetric charge storage capacity) are insufficient to capture the true underlying dynamics. This makes traditional linear models less effective and highlights the need for more complex models, like Gradient Boosting or other tree-based algorithms, which can capture non-linear interactions.

Given the absence of strong linear correlations, models like GBR are particularly useful. As a tree-based model, GBR partitions the data into regions where localized patterns emerge, allowing it to capture complex, nonlinear relationships that may not be apparent in simple scatter plots. The lack of strong individual correlations doesn't necessarily mean that the features are not useful. It is possible that certain combinations or interactions of features hold valuable predictive power. For example, while average operating voltage or energy density alone may not correlate strongly with the gravimetric capacity, their combined effect (or interaction with other properties like charging stability) could be important. Advanced models, including ensemble methods like Gradient Boosting, are well-suited to capture these interactions without explicitly defining them in the model. Even though scatter plots reveal no obvious correlation, it may be worth exploring transformations of the features to enhance their predictive power. Feature transformations such as logarithms, square roots, or polynomial terms can sometimes reveal hidden relationships that are not immediately apparent in the raw data.

For instance, the relationship between gravimetric energy and the target feature could be non-linear, but a transformation could linearize it. Selecting an appropriate machine learning algorithm is essential to the accomplishment of any prediction model. Algorithms vary depending on the kind of data and complexity of the challenge. Making the correct decision can help ensure that the model reflects the underlying patterns without overfitting or underfitting while striking a balance between accuracy, interpretability, and efficiency.

Since the scatter plot showed no good linear characteristic between the independent feature and target feature, a Gradient Boosting was tested and found effective for predicting gravimetric charge storing capacity. Gradient Boosting combines multiple weak learners, typically decision trees, in a sequential manner, where each tree corrects the errors of the previous one. This method excels in capturing non-linearities of the relationship between the variables.

On the test set, predictions are produced, and the R-squared score, and MSE are used to assess the model's performance. The average squared difference between the predicted and actual values is measured by the MSE, whereas the R-squared score shows the percentage of the target variable's variance that the model can account for. The accuracy measure cannot be solely determined taking R-squared and MSE which may be because of overfitting of the model. However, the model was tested with unseen data as well and made a good prediction.

In materials science, many properties are governed by intricate, multiscale phenomena, and a lack of simple correlations is not surprising. Properties like gravimetric capacity in lithium-ion batteries are influenced by atomic-scale features (chemical structure), mesoscopic properties (e.g., morphology), and macroscopic behaviors (charge/discharge cycles). The machine learning model is likely capturing these complexities, which aren't easily discerned through two-dimensional scatter plots. The lack of direct correlations between features might also necessitate closer scrutiny of the feature importance after training the Gradient Boosting Regressor. Feature importance metrics (such as Gini importance or permutation importance) can help identify which features the model finds most useful, even if they don't show clear individual trends in scatter plots. This can guide future feature selection or engineering efforts.

A residual plot, shown in Fig. 3, was generated to analyze the distribution of prediction errors in the GBR model. The results indicate that residuals are mostly symmetrically distributed around zero, suggesting that the model does not exhibit significant bias in predictions. For lower to mid-range predicted values (<300), residuals remain small, implying strong accuracy in this range. The results showed an excellent measure on R-squared and MSE with values 0.99 and 20.08 respectively for the test set of data. However, a few larger deviations are observed at higher predicted values (>300), which may indicate areas where the model underperforms slightly. The high R^2 value (Training: 0.9991, Test: 0.9958) suggests an excellent model fit, while the cross-validation results (Best MSE: 45.43, across 5 different validation splits during hyperparameter tuning) confirm that the model maintains strong generalizability across different data splits.

Figure 4 presents a comparison between actual and predicted values of the target feature. Most data points align closely with the ideal diagonal line, indicating a strong correlation and high predictive accuracy for charge storage capacity. This suggests that up to about 300 mAh/g, the model predicts values accurately. A few data points above 300 mAh/g show slight deviations from the reference line, indicating that the model slightly underpredicts or overpredicts higher-capacity materials. These minor deviations could be caused by data noise, feature limitations, or inherent variability in battery materials.

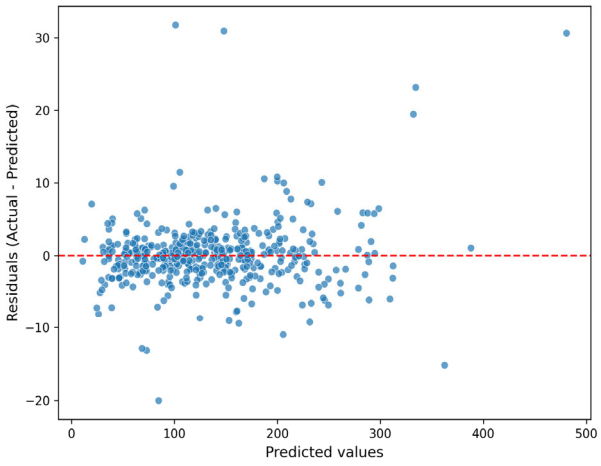

Fig. 3. Residual plot illustrating the performance of the GBR model, highlighting the distribution of prediction errors.

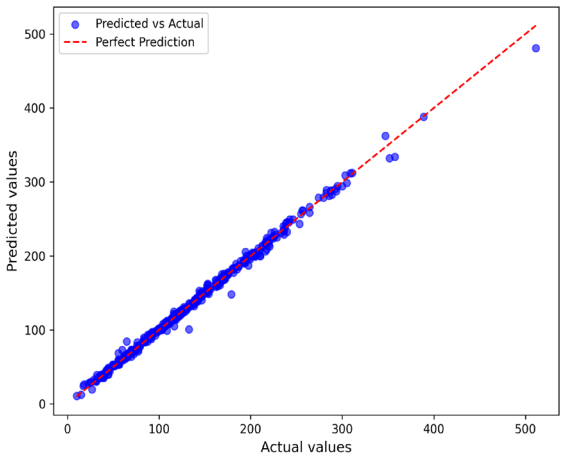

Fig. 4. Comparison of actual versus predicted charge storage capacity for the test dataset, with most data points closely following the ideal diagonal line.

This scatter plot confirms that the model has strong predictive performance, as evidenced by the tight clustering of points along the reference line. Although the model performs well overall, forecasts for greater values might be improved with additional research or improvement. This could suggest room for further refinement in capturing nonlinear relationships at extreme values.

In predicting the target feature, the most influential independent variables were analyzed and are displayed in Fig. 5. The feature importance plot reveals that gravimetric energy density (Wh/kg) is the most significant factor in determining charge storage capacity, with a substantial importance value approaching 0.8, highlighting its dominant role in the prediction model.

This suggests that a key factor in the model's predictions is the gravimetric energy density. On the other hand, stability charge (meV/atom) has little effect and is almost of zero relevance, but average voltage (V) contributes moderately with an importance value of more than 0.2. All things considered, the model mostly depends on energy density as a predictor, with stability and voltage having minimal bearing.

The prior studies have utilized classical regression models (linear regression, support vector machines) or deep learning approaches (neural networks) for battery property predictions [26-30]. This study employs gradient boosting, an ensemble learning method, which is particularly effective for handling non-linear relationships between variables. The exceptionally high R^2 value of 0.99 suggests strong predictive accuracy, which may outperform traditional ML models used in earlier studies. Unlike some ML studies that focus on predicting failure mechanisms or degradation pathways, this study is more aligned with optimizing material selection and energy storage capabilities by providing precise charge capacity predictions, which is directly useful for materials scientists designing next-generation battery materials.

This study improves upon prior works by using a larger, open-source dataset, electrochemically relevant features, and an optimized Gradient Boosting model, achieving higher predictive accuracy while maintaining computational efficiency. The results suggest that ensemble learning approaches like GBR can outperform traditional ML methods and some deep learning previous models for Li-ion battery capacity prediction [26-29].

Using important metrics like R^2 score, MSE, and Root Mean Squared Error (RMSE), the Gradient Boosting Regressor's performance was carefully assessed. The model explains almost all the variation in battery capacity, as evidenced by its high R^2 score of 0.9991 on the training data and 0.9958 on the test data. As is typical of most models, the MSE for the test data was 20.08 and for the training data it was 4.6004, indicating a little decline in performance on the test set. The RMSE values, which offer a more comprehensible measure of the error in the same units as the target variable, were 2.146 for training and 4.487 for testing, to further shed light on the model's performance. As indicated by the slight increase in MSE and RMSE from training to testing, these findings show the model's high predictive skills with little overfitting. These error values are significantly lower than those reported in previous studies using Random Forest (R^2 ~0.92) and Support Vector Regression (R^2 ~0.85) for lithium cell datasets [30].

In addition to these performance indicators, the robustness of the model was evaluated during the GridSearchCV process using 5-fold cross-validation. The dataset was divided into five subgroups, and various combinations of these subsets were used to train and evaluate the model. This procedure yielded the best cross-validation score (MSE = 45.43), demonstrating the model's strong generalization

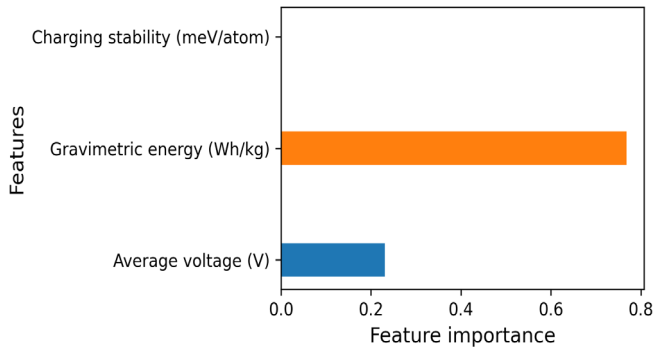

Fig. 5. Feature importance plot illustrating the contribution of each independent variable in predicting the target variable, with gravimetric energy density (Wh/kg) being the most influential factor.

across various data splits and guaranteeing a trustworthy assessment of its performance. The Gradient Boosting Regressor offers accurate and dependable forecasts of battery capacity, according to these quantitative assessments, which also include R^2, MSE, and RMSE. The cross-validation procedure further validates the model's efficacy and reduces the possibility of overfitting.

Future research should focus on validating the model by incorporating real-world experimental measurements to complement the DFT-calculated dataset from the Materials Project. Additionally, exploring deep learning architectures will enable efficient handling of larger datasets (>100,000 samples) while maintaining computational efficiency. Expanding the dataset to include high-capacity materials (>300 mAh/g) and integrating additional features such as lithium diffusivity, redox potential shifts, and phase transformation behavior will enhance predictive accuracy. Furthermore, adapting the model to different battery chemistries, including solid-state, Na-ion, and multivalent batteries, will ensure broader applicability beyond Li-ion systems. Addressing these areas will strengthen the reliability, scalability, and real-world impact of ML-driven battery materials discovery and optimization.

4. Conclusions

This research underscores the transformative potential of machine learning in materials science, particularly in the study of Li-ion battery electrode materials. By focusing on key features such as average operating voltage, gravimetric energy density, and charging stability, we applied the Gradient Boosting algorithm to predict gravimetric charge storage capacity, achieving an impressive R-Squared value of 0.99 and a Mean Squared Error of 20.08. These results demonstrate the efficacy of ML in accelerating materials design and optimization, fostering faster innovation, and supporting the development of sustainable energy solutions. Moving forward, our findings advocate for the continued integration of advanced statistical techniques with ML to significantly enhance battery performance. This approach will expand the ability to predict and optimize the charge storage capacity of lithium-ion battery materials, accelerating the research process and contributing to the development of more efficient, high-performing batteries by accounting for the chemical structures and compositions of electrode materials.

This study's GBR model outperforms traditional ML models (RF, SVM) and even deep learning approaches in terms of R^2 and RMSE, demonstrating an improved balance between accuracy and computational efficiency. The feature selection strategy focuses on practical electrochemical properties, making the model more interpretable and applicable to battery materials screening. The model's low error metrics suggest high generalizability, making it a strong candidate for accelerating battery material discovery and performance optimization.

The findings of this study have significant implications for battery development and industrial applications, particularly in material screening, performance optimization, and accelerating the design of next-generation batteries. By leveraging machine learning (ML) for predictive modeling, this approach can help battery manufacturers, materials scientists, and energy storage companies optimize material selection without relying on costly and time-consuming experimental synthesis and testing. By addressing these challenges and integrating experimental validation and transfer learning, the proposed ML approach can play a crucial role in streamlining battery material innovation, reducing R&D costs, and accelerating commercialization of next-generation energy storage technologies.

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References

[1]. A.G. Olabi, Q. Abbas, P.A. Shinde, M.A. Abdelkareem, Rechargeable batteries: Technological advancement, challenges, current and emerging applications. *Energy* 266 (2023) 126408. DOI: 10.1016/j.energy.2022.126408

[2]. S. Manzetti, F. Mariasiu, Electric vehicle battery technologies: From present state to future systems. *Renew. Sustain. Energy Rev.* 51 (2015) 1004–1012. DOI: 10.1016/j.rser.2015.07.010

[3]. J. Wen, D. Zhao, C. Zhang, An overview of electricity powered vehicles: Lithium-ion battery energy storage density and energy conversion efficiency. *Renew. Energy* 162 (2020) 1629–1648. DOI: 10.1016/j.renene.2020.09.055

[4]. Z. Huang, G. Du, Nickel-based batteries for medium- and large-scale energy storage, in: Advances in Batteries for Medium and Large-Scale Energy Storage, Elsevier, 2015, pp. 73–90. DOI: 10.1016/B978-1-78242-013-2.00004-2

[5]. A. Ulvestad, A brief review of current lithium ion battery technology and potential solid state battery

technologies, arXiv preprint arXiv:1803.04317 (2018).
[6]. S. Sarmah, L. Lakhanlal, B.K. Kakati, D. Deka, Recent advancement in rechargeable battery technologies. *Wiley Interdiscip. Rev.: Energy and Environ.* 12 (2023) e461. DOI: 10.1002/wene.461
[7]. I. Rakhimbek, N. Baikalov, A. Konarov, A. Mentbayeva, Y. Zhang, Z. Mansurov, M. Wakihara, Zh. Bakenov, Efficient Polysulfides Conversion Kinetics Enabled by Ni@CNF Interlayer for Lithium Sulfur Batteries. *Eurasian Chem.-Technol. J.* 25 (2023) 147–156. DOI: 10.18321/ectj1517
[8]. L. Lu, X. Han, J. Li, J. Hua, M. Ouyang, A review on the key issues for lithium-ion battery management in electric vehicles. *J. Power Sources* 226 (2013) 272–288. DOI: 10.1016/j.jpowsour.2012.10.060
[9]. Z. Wei, Q. He, Y. Zhao, Machine learning for battery research. *J. Power Sources* 549 (2022) 232125. DOI: 10.1016/j.jpowsour.2022.232125
[10]. M.F. Ng, Y. Sun, Z.W. Seh, Machine learning-inspired battery material innovation. *Energy Adv.* 2 (2023) 449–464. DOI: 10.1039/D3YA00040K
[11]. M. Aykol, P. Herring, A. Anapolsky, Machine learning for continuous innovation in battery technologies. *Nat. Rev. Mater.* 5 (2020) 725–727. DOI: 10.1038/s41578-020-0216-y
[12]. C. Lv, X. Zhou, L. Zhong, C. Yan, M. Srinivasan, Z.W. Seh, C. Liu, H. Pan, S. Li, Y. Wen, et al., Machine learning: an advanced platform for materials development and state prediction in lithium-ion batteries. *Adv. Mater.* 34 (2022) 2101474. DOI: 10.1002/adma.202101474
[13]. N. Badi, A.R. Erra, F.C. Robles Hernandez, A.O. Okonkwo, M. Hobosyan, K.S. Martirosyan, Low-cost carbon-silicon nanocomposite anodes for lithium ion batteries. *Nanoscale Res. Lett.* 9 (2014) 1–8. DOI: 10.1186/1556-276X-9-360
[14]. K. Sawai, T. Ohzuku, Factors affecting rate capability of graphite electrodes for lithium-ion batteries. *J. Electrochem. Soc*. 150 (2003) A674. DOI: 10.1149/1.1568107
[15]. Q. Pang, X. Liang, A. Shyamsunder, L.F. Nazar, An in vivo formed solid electrolyte surface layer enables stable plating of li metal. *Joule* 1 (2017) 871–886. DOI: 10.1016/j.joule.2017.11.009
[16]. Y.Y. Mamyrbaeva, M.A. Hobosyan, S.E. Kumekov, K.S. Martirosyan, Preparation of lithium cobaltate and electrochemical features for cathode battery materials. *Int. J. SHS* 23 (2014) 1–8. DOI: 10.3103/S1061386214010087
[17]. Y. Zhang, L. Tao, C. Xie, D. Wang, Y. Zou, R. Chen, Y. Wang, C. Jia, S. Wang, Defect engineering on electrode materials for rechargeable batteries. *Adv. Mater*. 32 (2020) 1905923. DOI: 10.1002/adma.201905923
[18]. D.-W. Chung, P.R. Shearing, N.P. Brandon, S.J. Harris, R.E. Garcia, Particle size polydispersity in li-ion batteries. *J. Electrochem. Soc.* 161 (2014) A422. DOI: 10.1149/2.097403jes
[19]. J.M. Bhatt, Effect of Temperature on Battery Life and Performance in Electric Vehicle, *Int. J. Sci. Res.* 2 (10) (2013).
[20]. J. Li, E. Murphy, J. Winnick, P.A. Kohl, Studies on the cycle life of commercial lithium ion batteries during rapid charge–discharge cycling. *J. Power Sources* 102 (2001) 294–301. DOI: 10.1016/S0378-7753(01)00821-7
[21]. A. Valizadeh, M.H. Amirhosseini, Machine Learning in Lithium-Ion Battery: Applications, Challenges, and Future Trends. *SN Comput. Sci.* 5 (2024) 717. DOI: 10.1007/s42979-024-03046-2
[22]. D. Cheng, W. Sha, L. Wang, et al., Solid-state Lithium Battery Cycle Life Prediction using machine learning. *Appl. Sci.* 11 (2021) 4671. DOI: 10.3390/app11104671
[23]. P. Sharma, B.J. Bora, A Review of Modern Machine Learning Techniques in the Prediction of Remaining Useful Life of Lithium-Ion Batteries. *Batteries* 9 (2022) 13. DOI: 10.3390/batteries9010013
[24]. K. Schofer, F. Laufer, J. Stadler, et al., Machine learning-based lifetime prediction of Lithium-Ion cells. *Adv. Sci.* 9 (2022) 2200630. DOI: 10.1002/advs.202200630
[25]. M.K. Tran, S. Panchal, V. Chauhan, N. Brahmbhatt, A. Mevawalla, R. Fraser, M. Fowler, Python-based scikit-learn machine learning models for thermal and electrical performance prediction of high capacity lithium-ion battery. *Int. J. Energy Res*. 46 (2022) 786–794. DOI: 10.1002/er.7202
[26]. P. Fermín-Cueto, E. McTurk, M. Allerhand, et al., Identification and machine learning prediction of knee-point and knee-onset in capacity degradation curves of lithium-ion cells. *Energy and AI 1* (2020) 100006. DOI: 10.1016/j.egyai.2020.100006
[27]. Y. Zhang, Y.-F. Li, Prognostics and health management of lithium-ion battery using deep learning methods: a review. *Renew. Sustain. Energy Rev.* 161 (2022) 112282. DOI: 10.1016/j.rser.2022.112282
[28]. J. Zhao, X. Feng, Q. Pang, J. Wang, Y. Lian, M. Ouyang, A. F. Burke, Battery prognostics and health management from a machine learning perspective. *J. Power Sources* 581 (2023) 233474. DOI: 10.1016/j.jpowsour.2023.233474
[29]. A. Thelen, X. Huan, N. Paulson, S. Onori, Z. Hu, C. Hu, Probabilistic machine learning for battery health diagnostics and prognostics-review and perspectives. *npj Mater. Sustain*. 2 (2024) 14. DOI: 10.1038/s44296-024-00011-1
[30]. S.-A. Amamra, Random Forest-Based Machine Learning Model Design for 21,700/5 Ah Lithium Cell Health Prediction Using Experimental Data, Physchem, 5 (2025) 12. DOI: 10.3390/physchem5010012