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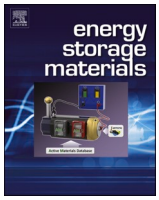

Reevaluating feature selection in phase field models for battery performance: A call for robust statistical approaches

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ABSTRACT

Han and Lin's phase field model for lithium-ion batteries utilizes LASSO regression to analyze battery performance during galvanostatic cycling, aiming to simplify the relationship between parameters and Coulombic efficiency. Despite demonstrating accuracy, this paper critiques the reliance on LASSO for feature selection, highlighting its potential inadequacy in capturing nonlinear interactions within chemical properties. Traditional performance metrics, such as MAE, RMSE, and R^2, provide limited insights regarding individual feature contributions and the nuanced relationships present in the data. This paper advocates for adopting nonparametric statistical methods, such as Spearman's correlation and Kendall's tau, which can better elucidate complex variable associations and validate feature importance. Incorporating these methods will enhance the robustness of findings, promoting a clearer understanding of battery performance dynamics.

Han and Lin developed a phase field (PF) model for a full-cell battery undergoing galvanostatic cycling, employing the least absolute shrinkage and selection operator (LASSO) regression to analyze and predict the battery's performance evolution throughout the cycling process [1]. Their objective was to derive a straightforward and interpretable expression for Coulombic efficiency as a function of the battery's parameters, leveraging LASSO's effective feature selection capabilities. To evaluate the model's performance, the authors utilized metrics such as mean absolute error (MAE), root mean square error (RMSE), and the coefficient of determination (R^2) [1].

While Han and Lin have highlighted the impressive accuracy of PF models, this paper raises critical concerns regarding the reliance on LASSO for feature selection and validation through standard performance metrics such as MAE, RMSE and R^2. The inherent linearity of LASSO may be inadequate for capturing the complexities of chemical properties, which frequently exhibit nonlinear and nonparametric behaviors. This limitation can result in the omission of significant interactions and relationships within the data, potentially skewing the model's predictive capabilities.

Moreover, interpreting feature importances derived from machine learning models like LASSO can be misleading when using metrics such as MAE, RMSE, and R^2. These metrics primarily evaluate overall model performance rather than the validity of individual feature contributions [2,3]. Consequently, without a robust framework for validating feature importance against ground truth values, the insights gained from these models may lack reliability. It is essential for Han and Lin to differentiate between accuracy in target prediction and accuracy in feature importance. The metrics of MAE, RMSE, and R^2 are indicative of model fitting but do not effectively validate the accuracy of feature importance, raising questions about the robustness of the conclusions drawn from their analysis [2,3].

Metrics such as RAE, RMSE, and R^2 primarily assess model fitting rather than prediction accuracy. To accurately evaluate prediction accuracy, regression models can be converted into classification models using one of two methods: transforming continuous target values into integers or employing a ranking system. In classification models, users can then compute a variety of metrics, including sensitivity, specificity, and overall accuracy, among others. However, it is important to note that high prediction accuracy or strong model fitting does not necessarily ensure the reliability of feature importances due to the absence of ground truth values for validation.

Machine learning models, including LASSO, inherently produce biased feature importances due to their model-specific nature [4,5]. Over 100 peer-reviewed articles addressed non-negligible bias in feature importances from models. In the absence of ground truth values, different models may generate distinct feature importances, further compounding the bias in the results. This variability highlights the necessity for caution when interpreting feature importances derived from these models, as they may not accurately reflect the underlying relationships within the data.

To establish genuine relationships between the target variable and its features, Han and Lin should consider three fundamental components: data distribution, statistical relationships between variables, and statistical validation through p-values. Understanding the data distribution is crucial, as it influences the appropriateness of the modeling techniques employed; neglecting to consider nonlinear relationships—which may arise from various arithmetical operations on the initial physical quantities—can obscure meaningful patterns in the data. Additionally, exploring the statistical interactions between the target and predictor variables is essential, as employing methodologies that can capture these complexities—such as nonparametric approaches—could yield a more accurate representation of the relationships present in the data. Lastly, incorporating statistical validation techniques, such as hypothesis testing and p-value analysis, is necessary to substantiate claims regarding feature importance and ensure that observed relationships are not artifacts of random variation.

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Rather than relying on linear models like LASSO, we recommend utilizing nonlinear models such as random forests to effectively capture the nonlinear patterns present in the data for target prediction. To accurately assess the relationships between the target variable and features, as well as for feature selection, this paper advocates for the application of Spearman's correlation [6,7] and Kendall's tau [8,9], supplemented with p-values for statistical significance. Additionally, it is essential to conduct a Variance Inflation Factor (VIF) analysis prior to applying statistical methods to identify and eliminate features exhibiting collinearity and interaction effects, thereby mitigating feature inflation.

Instead of relying on the linear LASSO model for feature selection, this paper advocates for the use of bias-free, robust statistical methods, such as Spearman's correlation with p-values [6,7] and Kendall's tau with p-values [8,9], both of which are nonlinear and nonparametric approaches. These methods provide valuable insights into the relationships between variables while accounting for the complexity inherent in chemical properties. The paper recommends that Han and Lin reevaluate their analysis by incorporating these robust statistical techniques to ensure more reliable and valid outcomes. By focusing on true associations through these methods, they can enhance the integrity of their findings and provide a deeper understanding of the underlying relationships in their data.

This paper acknowledges that the complexity and variability inherent in different domains and datasets make it challenging to establish a one-size-fits-all standard. However, we believe that creating a framework of best practices and guidelines is not only feasible but also essential. Such a framework can be tailored to accommodate specific industry needs while promoting consistency and reproducibility across studies.

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