Lithium-ion Batteries Performance Prediction using Machine Learning

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Abstract

Lithium-ion batteries have applications in many areas of people's daily life. They are used in cell phones, electric vehicles, and planes. However, their combined finite life span and accidents of fires lead to people hesitant about their usage. We would like to examine how different determinants impact battery performance and which type performs the best.

Introduction

Using data collected from Catenaro and Onori's experiment of experimental data of a lithium-ion battery at different rates and temperatures of Operation, come to a conclusion on different factors. Specifically, we are looking at different battery types, LFP, NCA, and NMC at different temperatures (5, 25, 35 deg C), different charging rates (C/20, 1C, 2C, 3C, and 5C), and different surface temperatures, voltages, and currents for six different trials.

Specific energy is the battery's capacity. It is calculated by
E =(C-rate * Voltage) / battery mass

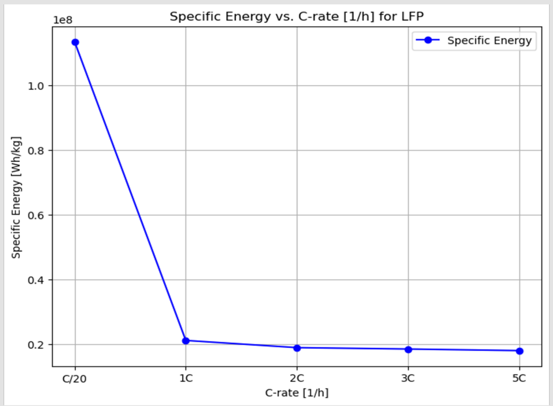
Specific power is the how quickly charge can be delivered. It is calculated by
P = (current * voltage) / batter mass
Charging rate can be defined as how quickly a battery charges. For instance, C/20 means that it takes 20 hours to charge a battery from 'dead' to fully charged. 1C means it takes one hour.

Methodology

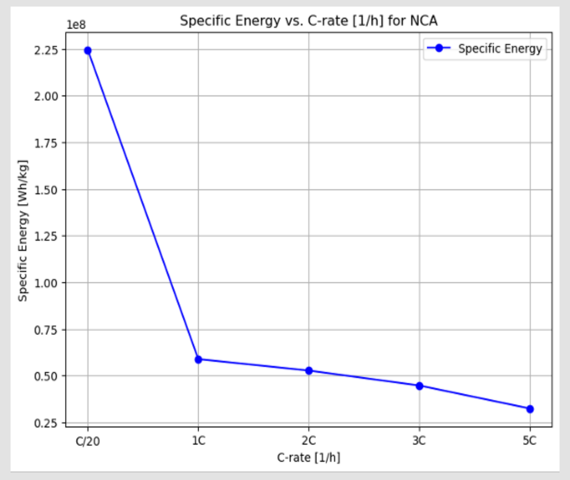
We combined all k trials together and created new columns for C-rate, battery type, at a certain temperature.
We determined the equation for battery capacity, which helps indicate performance.
We also utilized an enhanced Ragone plot to determine which battery type performed the best by calculating based on specific energy and specific power.

Analysis 1: Specific Energy, Charging Rate, and Temperature

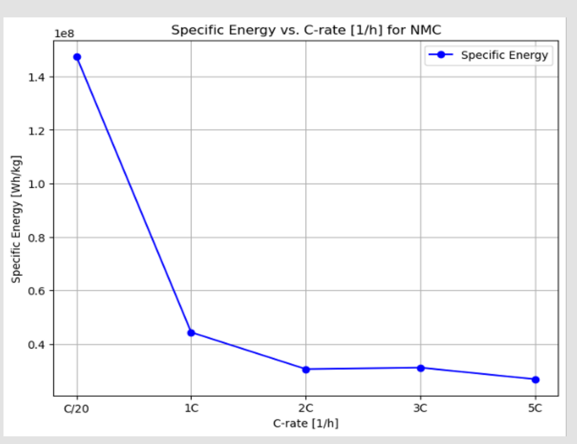
In the research and paper, temperature refers to thermal temperature generated by the battery cell. The relationship between the temperature (thermal energy created by the Li-ion battery) and discharge rates is shown by three plots below. Heat is a product of higher C-rates[1].



From this graph, we can interpret that there is a drastic drop when the charging rate is one-hour. With this increased jump in charging rate, heat will have to be kept in mind as a factor for this drop. The extra heat provided to charge the battery in 20 hours to one hour could alter the difference in performance. The battery gives worse energy as the charging rate increases. However, after charging rate increases past 1C, the energy provided is similar. LFP battery performance in delivering specific energy was the worst at under 0.2 Wh/kg in the 5C condition.



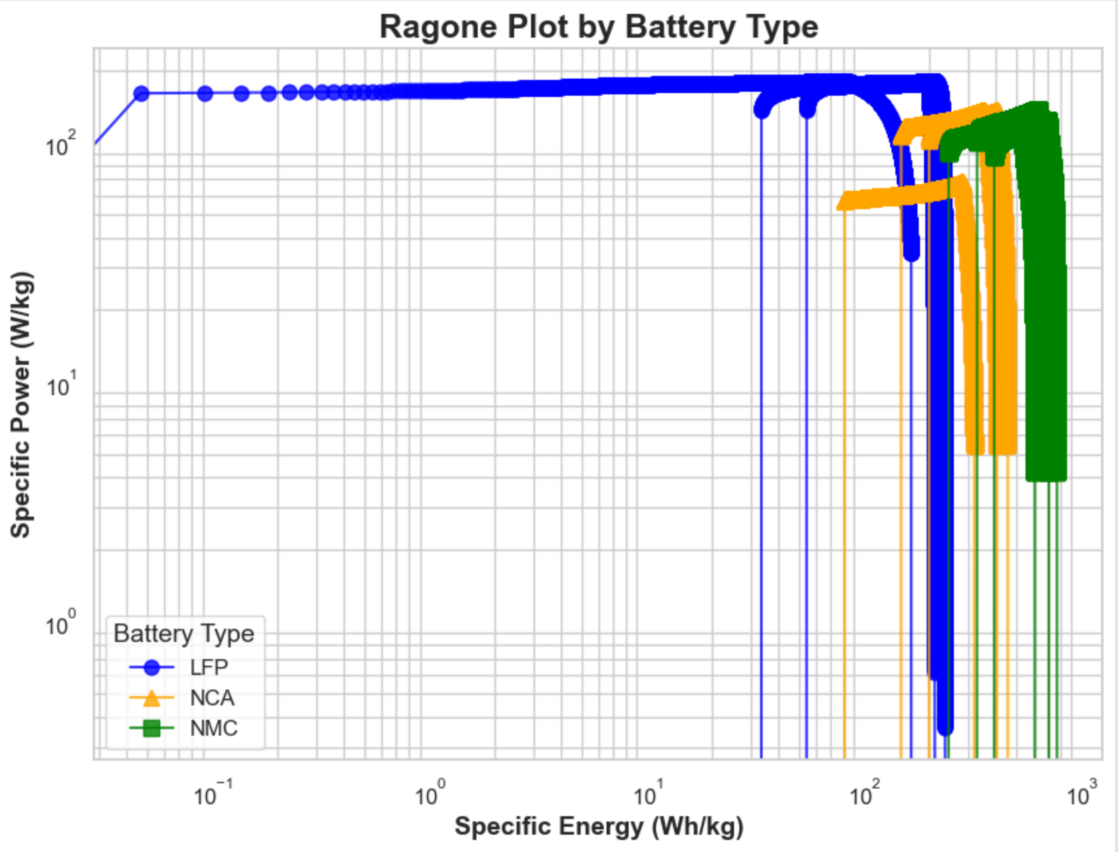
The NCA battery follows the same trend as the LFP battery. There is a drastic change in specific energy to be delivered between charging rate of C/20 and 1C but that tapers as charging rate increases. Compared to the LFP battery, there is more of a change in energy being delivered as C increases. However, there is still an extreme change between C/20 and 1C. At 5C, both batteries end up being around the same energy being delivered. The highest specific energy given at C/20 at 2.25 Wh/kg compared to the other batteries.



NMC follows specific energy decreasing as charging rate increases. NMC follows a similar pattern as NCA and the ending specific energy in relation to 5C. While it is still unclear how temperature is related, it could be a significant factor in decreasing specific energy, or battery capacity, since more heat is generated as charging rate increases.

This indicates that there might be a relationship between specific energy, heat, and C-rate that can be explored further in the polynomial and linear regressions.

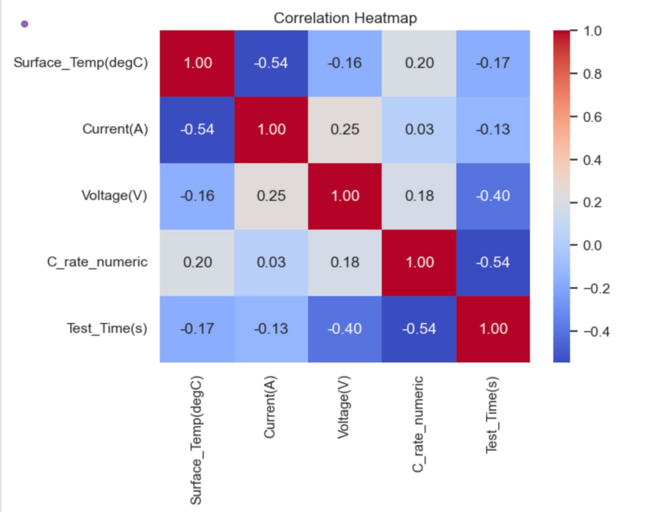
Analysis 2: Enhanced Ragone Plot



This Enhanced Ragone plot demonstrates that the NMC battery had the best performance in specific energy meaning it can last longer than its counterparts. LFP have however, have higher specific power but lower specific energy compared to its counterparts. This means that while LFP's maintain power, they have less capacity for energy storage. There is a wide range of specific energy for LFPs, meaning there is a lot of variability. NCA and NMC are much more stable in terms of specific energy. It offers more specific energy than LFP and less specific power. NCA is in the middle between LFP and NMC. It can deliver moderate specific energy and moderate specific power. NMC has the highest specific energy as it is the furthest right. Its specific power is less than LFP though.

Analysis 3: Linear/Polynomial Regression & L2 Regularization

Our group performed regression analysis using two approaches: linear regression and polynomial regression. In both cases, Surface Temperature (°C) is treated as the response variable, while Current (A), Voltage (V), and C-rate are used as predictors. Based on the correlation heatmap provided in the notebook, Current exhibits the strongest positive correlation with the response variable at 0.54, whereas the other predictors show much weaker correlations, with values of -0.16 and 0.20, respectively. The relationships between the independent variables and the response variable will be further examined through linear and polynomial regression analyses.

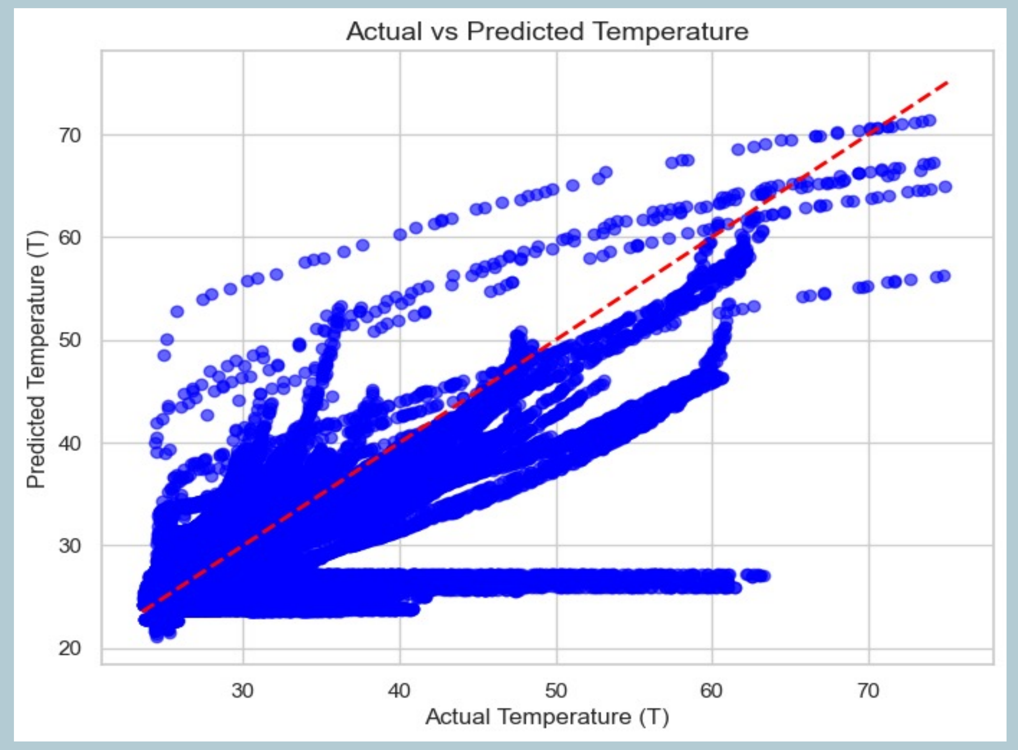


The R-squared value of the linear regression is approximately 0.35, indicating that only 35% of the variation in surface temperature can be explained by changes in current, voltage, and C-rate. Furthermore, the Mean Square Error (MSE) is 4.22, which is relatively low given the surface temperature range of 5 to 75 degrees Celsius. Similarly, polynomial regression was conducted using the same response and independent variables. The R-squared value improved to 0.61, and the Mean Square Error (MSE) decreased to 2.5, indicating that polynomial regression better captures the relationship between the variables than linear regression. To enhance the models, we tested three approaches: Lasso, Ridge, and Recursive Feature Elimination (RFE). The results showed that Ridge regression produced the same R-squared and MSE values as the original polynomial regression, making both the most effective models compared to Lasso and RFE. Consequently, we chose to retain the original polynomial model.

Conclusion

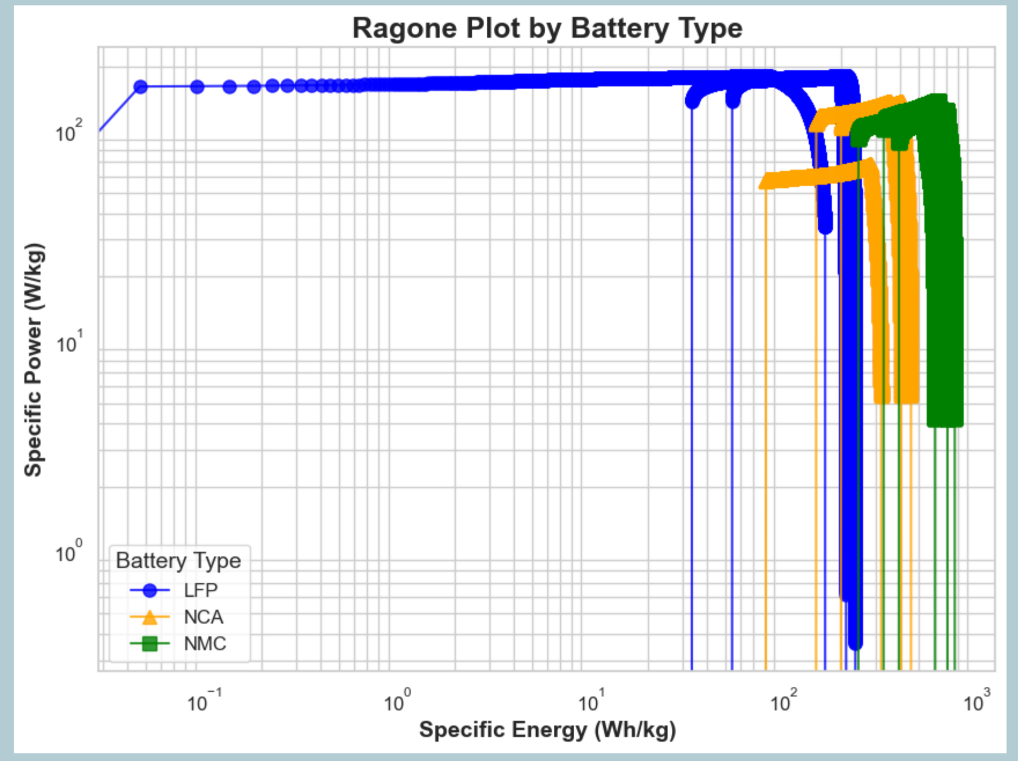
This paper investigates the batteries NCA, NMC, and LFP under various temperatures in specific energy, specific powers, surface temperature, current, and voltage. After evaluating the data with linear regression, the formula turns out to be:

$$\boldsymbol{E = 2.6302\,\{12.796 - 6.1898 * I + 6.5080 * V + 1.4755 * C + 8.55 * 10^{-5} * (test\ time) + 0.0219 * I^2 + 1.6952 * I * V + 0.2643 * I * C - 3.983 * 10^{-5} * I * (test\ time) - 0.8460 * V^2 - 2.862 * 10^{-5} * V * (test\ time) - 0.0841 * C^2 + 3.762 * 10^{-5} * C * (test\ time) - 7.176 * 10^{-11} * (test\ time)^2 + T\}.}$$



Conclusion 1: Temperature of battery directly contribute to *E*, with a linear term, +*T*.

Conclusion 2: Temperautre of battery is additive, and does not affect current and voltage.



Conclusion 3: NMC battery type shows the best efficiency among three Li-ion battery types.

Acknowledgements

Catenaro, E., Rizzo, M.D., & Onori, S. (2021). "Experimental analysis and analytical modeling of Enhanced-Ragone plot". Applied Energy. 291. https://doi.org/10.1016/j.apenergy.2021.116473

Catenaro, E., & Onori, S. (2021). Experimental data of lithium-ion batteries under galvanostatic discharge tests at different rates and temperatures of operation. Data in Brief, 35, 106894. https://doi.org/10.1016/j.dib.2021.106894