Independent Study

Project

Machine Learning models to Predict Lithium-Ion Cell Power

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Acknowledgement

In successfully completing this project, many people have helped me. I would like to thank all those who are related to this project. First, I would like to express my sincere gratitude to my advisor **Dr Patrick Juola** as he has been an ideal teacher, mentor, and project supervisor, offering advice and encouragement with a perfect blend of insight. Thanks for his support, motivation, patience, and knowledge that helped me to achieve my Master's study. I am really grateful as he was always Flexible, suggesting, and recommending the best. His guidance and experience helped me to complete the project in time. It is an honour to learn from **Dr Patrick Juola**. I extend my heartfelt appreciation to **Dr. Arun Kumar** for his invaluable contributions to this project. His expertise in battery science has been instrumental in shaping the development of my machine learning model. I am grateful for Dr. Arun Kuamr's guidance, insights, and collaborative spirit, which have significantly enriched the interdisciplinary nature of this endeavor.

ABSTRACT

The development of sustainable Li-ion batteries is crucial for the advancement of various industries, including electric vehicles, renewable energy, and consumer electronics. However, the traditional research and development process for battery design can be time-consuming and costly. In this study, I propose to use of a machine learning model to predict and recommend the performance of batteries based on six key variables: power, energy, safety, cost-effectiveness, efficiency, and life. By inputting the desired performance characteristics into the model, Battery Scientists and researchers can quickly determine the optimal values for these variables to achieve a desirable battery(like high power battery, high energy battery, safe battery, cost effective battery, high efficiency battery, long life battery). This approach has the potential to significantly reduce the time and cost associated with battery design while improving the overall performance of the final product.

One of the noteworthy environmental implications of this study lies in the substantial reduction of time required for battery development. Traditional laboratory-based methodologies for battery improvement necessitate extensive hours of experimentation and testing to determine optimal values for key performance variables. This lengthy process, lasting for several years, requires a lot of resources and makes research and development take a long time.

The proposed machine learning model, however, serves as a catalyst for expediting this timeline significantly. By swiftly predicting and recommending optimal values for the six key performance variables—power, energy, safety, cost-effectiveness, efficiency, and life—researchers can curtail the extensive laboratory hours conventionally spent. This reduction in experimentation time not only accelerates the pace of battery innovation but also minimizes the overall environmental footprint associated with prolonged testing processes. The integration of Machine Learning in this context not only enhances efficiency but aligns with sustainable practices by mitigating the environmental impact of extended laboratory work.

This project represents a collaborative effort bridging the realms of machine learning and battery science. Leveraging the expertise of battery scientist Dr. Arun Kumar, who played a pivotal role as a collaborator and provided valuable insights into the intricacies of battery science, the interdisciplinary nature of this study ensures a comprehensive understanding of both the computational and practical aspects.

Contents

1. Introduction

The quest for sustainable energy solutions has become a paramount concern in the face of burgeoning technological advancements and the increasing demand for cleaner and more efficient energy sources. In response to this imperative, the development of advanced batteries stands as a linchpin for progress in electric vehicles, renewable energy systems, and consumer electronics. However, the conventional approaches to battery design are often marred by protracted timelines and exorbitant costs, posing substantial barriers to innovation.

In light of these challenges, this research embarks on a transformative journey at the intersection of machine learning and battery science. The primary objective is to expedite and optimize the intricate process of battery design by harnessing the predictive power of machine learning algorithms. By focusing on six key performance variables—power, energy, safety, cost-effectiveness, efficiency, and life—the study endeavors to streamline the decision-making process for battery scientists and researchers. This approach not only promises to reduce the temporal and financial investments traditionally associated with battery development but also holds the potential to yield batteries tailored to specific performance requirements.

1.1 Battery Science and Laboratory Research

The traditional laboratory-based methodologies involved in battery design include a series of iterative research and experimentation processes. These processes involve the synthesis of new materials, the fabrication of electrodes, and the assembly of cells. The materials are then tested for their electrochemical properties, such as capacity, voltage, and cycle life, to determine their suitability for use in batteries. One of the main challenges associated with these methods is the time it takes to develop new materials and optimize their performance. The process of synthesizing and characterizing new materials can take months or even years, and the optimization of electrode and cell designs can take even longer. Another challenge is the high cost of materials and equipment required for these experiments. To address these challenges, researchers are exploring new approaches to battery design that leverage machine learning (ML) algorithms to accelerate the understanding of new materials, chemistries, and cell designs. ML can be used to characterize battery performance, lifetime, and safety, and to improve battery lifetime predictive modeling and microstructure diagnostics within advanced battery research. In addition, researchers are exploring new materials and chemistries that can improve battery performance and reduce costs.

1.3 Characteristics of a Cell battery

Power is typically measured in watts (W) and represents the amount of energy delivered or consumed per unit of time. It is a dynamic metric that characterizes how quickly a battery can discharge or charge.

Power (P) is calculated using the formula:

Kilowatt-hours (kWh) = Amp-hours (Ah) × Voltage of battery (V) ÷ 1,000

Safety is a critical aspect of battery design, as batteries can be prone to overheating, short-circuiting, and other hazards. Lithium-ion batteries, for example, are known to be susceptible to thermal runaway, which can cause fires or explosions.

The state of charge of a battery describes the difference between a fully charged battery and the same battery in use. It is associated with the remaining quantity of electricity available in the cell.It is defined as the ratio of the remaining charge in the battery, divided by the maximum charge that can be delivered by the battery. It is expressed as a percentage as below.

$SoC/\%=100(Q_0+Q)/Q_{max}=SoC_0/\%+100Q/Q_{max}$

Q_0/mAh= Initial charge of the battery.
Q/mAh=The quantity of electricity delivered by or supplied to, the battery. It follows the convention of the current: it is negative during the discharge and positive during the charge.
Q_{max}/mAh= The maximum charge that can be stored in the battery.

$SoC_0/\%=SoC0/\%=$ The initial state-of-charge $(SoC/\%)(SoC/\%)$ of the battery.

Efficiency is another important factor in battery design, as it determines how much energy is lost during charging and discharging. The efficiency of a battery is determined by its internal resistance, which can be affected by factors such as temperature, state of charge, and age.

Formula

Battery Efficiency = Energy Density of Discharge (EDD)/Energy Density of Charge * 100

For example, if a battery uses 100 units of energy to charge but only provides 80 units of energy when discharging, the efficiency would be:

Efficiency=100/80×100=80%

Cost is also a significant consideration in battery design, as it can impact the adoption of new technologies. The cost of a battery is determined by factors such as the cost of materials, manufacturing, and recycling.

Lifespan is the length of time a battery can be used before it needs to be replaced. The lifespan of a battery is determined by factors such as the number of charge and discharge cycles it can undergo, the rate of capacity fade, and the effects of temperature and aging.

Battery Life can be calculated

Battery Life(in Hours) = Battery Capacity in Ah / Load Current (A)

Energy density is commonly defined as the amount of energy stored per unit volume (Wh/L) or per unit mass (Wh/kg) within a battery cell. It reflects the compactness of energy storage and is a pivotal factor in determining the overall efficiency and practicality of a battery for specific use cases.

Formula for battery energy density

Energy Density = Total Energy(E) / Total Volume(V)

A suboptimal or inefficient battery can be identified by several characteristics, including low power or energy density, poor safety performance, low efficiency, high cost, and short lifespan.

2. Background

Traditionally, the improvement and optimization of battery performance have relied on laborious laboratory experimentation and iterative testing. The complexity of batteries, coupled with the multifaceted nature of performance variables, results in an intricate landscape that demands innovative solutions. Recognizing the limitations of conventional methodologies, this research integrates machine learning algorithms into the battery design process.

Two primary algorithms, Linear Regression and Ensemble Models, take center stage in predicting the power variable—an essential metric in gauging a battery's performance. Linear Regression, a stalwart in predictive modeling, establishes a baseline understanding of the linear relationships between input variables and the target output. Complementing this, Ensemble Models bring a robust and versatile approach by combining the predictive power of multiple algorithms, thereby enhancing the accuracy and generalization capabilities.

Furthermore, in addressing the multi-faceted nature of battery design, a Multi-Output Regressor is employed. This sophisticated algorithm extends the predictive prowess to simultaneously forecast two variables, thereby providing a comprehensive solution to the multifaceted challenges posed by battery optimization.

As we delve into the intricacies of these machine learning models, the overarching goal is to not only revolutionize the battery design paradigm but also to contribute meaningfully to the development of sustainable energy solutions. This research stands as a testament to the synergies achievable through interdisciplinary collaboration and the transformative potential of integrating cutting-edge technologies into traditional domains.

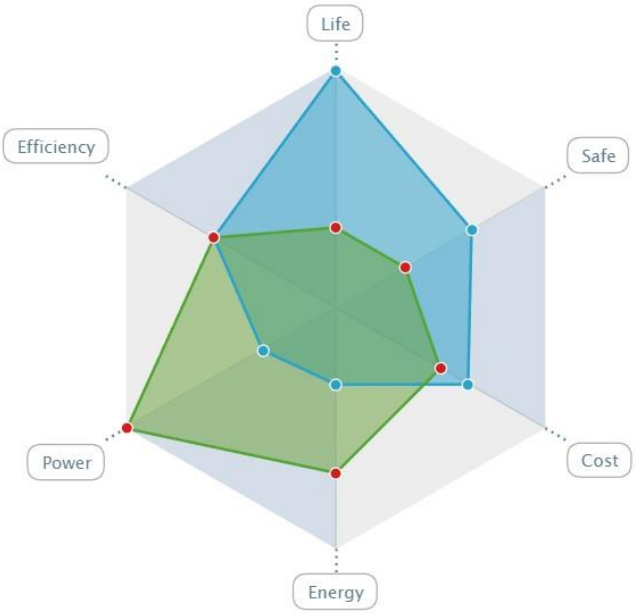

Figure2.1: Hexagonal Representation

3. Data Collection and Preprocessing

In this project, the dataset plays a pivotal role as the foundation for analysis and model development. The dataset, sourced from the Center for Advanced Life Cycle Engineering (CALCE) at the University of Maryland, is a valuable resource that contributes to the

robustness and credibility of the study. CALCE is renowned for its comprehensive and high-quality datasets related to the life cycle and performance of various engineering systems, particularly in the field of advanced energy storage technologies.

The dataset encompasses intricate details and measurements related to the life cycle and performance of batteries, offering a wealth of information on key parameters such as energy density, safety, cost, life expectancy, efficiency, and power. Leveraging this dataset, I applied rigorous methodologies and formulated mathematical models to generate a tailored dataset specifically designed for my project.

The process involved navigating through the complexity of raw data, understanding the relationships between variables, and applying relevant formulas to derive meaningful insights. Addressing the intricacies of battery science and engineering, I employed statistical and machine learning techniques to distill the dataset into actionable information. This process required a deep understanding of battery technologies and a nuanced approach to handle the inherent complexity of the data.

Despite the challenges posed by the complexity of the dataset, the effort invested in understanding and preprocessing the data has been instrumental in achieving the project's objectives. The dataset, enriched with refined variables and tailored features, serves as the basis for training and evaluating machine learning models to predict and recommend optimal battery performance characteristics.

3.1 Raw Data

Incorporating a visual representation of the raw data is a crucial element in conveying the depth and complexity of the dataset. The image provided in the report visually encapsulates the intricacies of the original dataset sourced from the Center for Advanced Life Cycle Engineering (CALCE) at the University of Maryland. This snapshot serves as a visual anchor, offering a glimpse into the diverse array of parameters and measurements related to battery performance. By including this image, the report not only provides transparency regarding the dataset's richness but also highlights the multifaceted nature of the raw data, setting the stage for the subsequent analysis, modeling, and insights derived in the course of the project. The visual representation of the raw data underscores the depth of information and the meticulous approach taken in transforming this wealth of data into actionable insights for advancing battery science and technology.

time_s	Ecell_V	I_mA	EnergyCharge_W_h	QCharge_mA_h	EnergyDischarge_W_h	QDischarge_mA_h	Temperature_C	cycleNumber	Ns
0	3.5387173	1491.3828	0	0	0	0	21.139246	0	0

Figure 3.1.1: Raw Data Variables

- Time_s= Time since beginning of experiment in seconds
- Ecell_V= Cell Voltage
- I_mA = Cell current in milliamperes

- EnergyCharge_W_h= The amount of energy supplied to the cell during charge in watt-hours
- Qcharge_mA_h= The amout of charge supplied to the cell during charge in milliampere-hours
- EnergyDischarge_W_h= The amount of energy extracted from the cell during discharge in watt-hours
- Qdishcarge_mA_h= The amount of charge extracted from the cell during discharge in milliampere-hours
- Temperature_C= Cell surface temperature in degrees celcius
- CycleNumber= Cycle number as recorded by the cell tester
- Ns= Cycle segment (varies, useful for discerning between segments)

In the process of transforming the raw data obtained from the CALCE dataset, battery-related formulas were meticulously applied to derive six key variables crucial to the study: power, energy, life expectancy, cost, efficiency, and safety. These variables represent fundamental aspects of battery performance, each playing a pivotal role in determining the overall effectiveness of the main variable POWER.

Energy Density (Wh/L)	Safety (SOC)	Cost ($)	Life (Hr)	Efficiency (BE)	Power(kWh)
0	-8.300811768	195	#DIV/0!	#DIV/0!	
0.014693225	-8.145514488	505	0	#DIV/0!	

Figure 3.1.2: Main Dataset

- Energy Density (Wh/L) = amount of energy stored per unit volume or mass
- Safety (SOC) = State of Charge
- Cost($) = Average Cell Cost
- Life(Hr) = Battery Capacity in Ah / Load Current (A)
- Efficiency(BE)= Energy Density = Total Energy(E) / Total Volume(V)
- Power (kWh)= Kilowatt-hours (kWh) = Amp-hours (Ah) × Voltage of battery (V) ÷ 1,000

3.2 Preprocessing

In the initial stages of data preprocessing, the project employed a meticulous approach to ensure the quality and reliability of the dataset. A subset of critical columns, encompassing key battery performance parameters such as energy density, safety, cost, life expectancy, efficiency, and power, underwent a transformation using the `pd.to_numeric` function. This conversion not only standardized the data but also addressed any non-numeric entries, enhancing the overall integrity of the dataset.

Furthermore, to mitigate the impact of missing or incomplete data, a judicious decision was made to drop rows where essential parameters such as 'Life (Hr)', 'Efficiency (BE)', and 'Power(kWh)' contained null values. This step was deemed necessary to maintain the robustness of the dataset, ensuring that subsequent analyses and modeling efforts were based on complete and meaningful information.

A critical refinement involved eliminating rows where the 'Energy Density (Wh/L)' value equaled zero. This decision was driven by the recognition that instances with zero energy density could potentially distort the analysis and compromise the accuracy of predictions. The removal of such entries was pivotal for creating a reliable foundation for the subsequent stages of the project.

The final step in this preprocessing phase was the reset of the DataFrame index, ensuring a clean and continuous index structure after dropping rows. This meticulous attention to detail in data preprocessing reflects the project's commitment to data quality and sets the stage for robust machine learning modeling. Finally, after the rigorous cleaning and preprocessing steps, the dataset emerged as a well-curated resource with dimensions of 19,655 rows and 6 columns.

	Energy Density (Wh/L)	Safety (SOC)	Cost ($)	Life (Hr)	Efficiency (BE)	Power(kWh)
0	0.399533	-7.990257	94.0	0.001391	117.083462	0.000005
1	0.414422	-7.990257	195.0	0.002782	58.094492	0.000010
2	0.429318	-7.990257	354.0	0.004173	38.558040	0.000015
3	0.444219	-7.990257	134.0	0.005563	28.815407	0.000021
4	0.459128	-7.958503	233.0	0.006954	22.979489	0.000026
...	...	...	...	...	...	...
19649	11.768819	-8.713908	192.0	-4.328623	73.486003	0.008118
19650	11.768819	-8.699798	437.0	-1.870348	73.493601	0.007463
19651	11.768819	-8.699798	544.0	-1.095794	73.507041	0.006650
19652	11.768819	-8.809319	627.0	-0.950302	73.524342	0.006288
19653	11.768819	-8.841124	113.0	-0.733791	73.541471	0.005648

19654 rows × 6 columns

Figure 3.2.1: After Preprocessing

4. Methodology

In the pursuit of predicting the vital power variable, crucial for evaluating battery performance, two primary algorithms take the lead: Linear Regression and Ensemble Models. The Linear Regression algorithm lays the foundation by unraveling the linear relationships inherent in the dataset, offering a clear interpretative lens. Meanwhile, the Ensemble Models, a powerful amalgamation of algorithms, introduces complexity and depth to the predictive process. Within the ensemble, the synergistic deployment of Linear Regression, known for its interpretability, alongside the dynamic and versatile Random Forest, further refines the prediction of power metrics. This strategic combination harnesses the strengths of both

models, ensuring a more nuanced and accurate understanding of the intricate relationships within the battery dataset.

In acknowledgment of the intricate nature of battery design, a experimental step was taken with the integration of a Multi-Output Regressor into the modeling framework. This sophisticated algorithm not only extends predictive capabilities beyond a single variable but also ventures into the simultaneous forecasting of two critical variables. By addressing the interconnectedness of these variables, the Multi-Output Regressor provides a holistic solution to the intricate challenges posed by battery optimization. This experimental inclusion reflects a commitment to innovation, pushing the boundaries of conventional modeling to offer a more comprehensive understanding of battery behavior.

4.1 Logistic Regression

The implementation of a Linear Regression model for predicting the 'Power(kWh)' variable based on selected features related to energy density, safety, cost, life expectancy, and efficiency. The performance metrics, including Mean Squared Error (MSE) and R-squared value, are indicative of the model's accuracy in capturing the variance in the test dataset.

Here, 80% of the data is utilized for training (X_train and y_train), while the remaining 20% is reserved for testing (X_test and y_test). The random_state parameter ensures reproducibility of the split, providing consistent results across multiple runs.

```
Mean Squared Error: 2.154204009035889e-06
R-squared Value: 0.6149089488094643
Coefficients: [ 1.29422182e-04 -9.87069031e-04  2.60519061e-06  2.67916834e-05
  1.41789872e-03]
Intercept: 0.005626467032007738
```

4.1.1 Figure: MSE & R square

The calculated MSE of 2.154204009035889e-06 indicates the average squared difference between the predicted and actual values, signifying a remarkably low error. The R-squared value of 0.6149089488094643 suggests that approximately 61.5% of the variability in the 'Power(kWh)' variable can be explained by the model. While these results are indicative of a reasonably good fit, it's evident that the model may have limitations in fully capturing the complexities of the dataset.

My decision to explore ensemble models might stem from a desire for enhanced predictive performance. While Linear Regression offers interpretability, ensemble models, which combine the strengths of multiple algorithms, often excel in capturing intricate patterns within the data. The shift to ensemble models represents a strategic move toward improving predictive accuracy and addressing potential limitations observed in the Linear Regression results.

This iterative process of model exploration and refinement demonstrates a thoughtful and dynamic approach to achieving optimal predictive performance. The ensemble model, with its capacity to harness the strengths of diverse algorithms, is poised to offer a more robust and nuanced understanding of the intricate relationships within the battery dataset. This

progression reflects a commitment to continuous improvement and attaining the highest possible accuracy in predicting power metrics for advanced battery technologies.

4.2 Ensemble Model

In pursuit of refining predictive accuracy, the project ventured beyond individual modeling approaches and embraced ensemble modeling—a sophisticated technique combining the strengths of diverse algorithms. Framing a powerful ensemble model using a Voting Regressor, harmonizing the predictive capabilities of a Linear Regression model and a Random Forest Regressor.

Model Training and Evaluation

The dataset undergoes a meticulous division into training and testing sets, a foundational step ensuring the model's capacity to generalize beyond the confines of its training data. Standardization is then applied to maintain consistent scaling across features, a crucial practice for optimal model performance.

Two distinct models, a Linear Regression model and a Random Forest Regressor, are introduced as individual contributors to the ensemble. The ensemble model, orchestrated through the Voting Regressor, seamlessly amalgamates their predictions.

```
Mean Squared Error (Ensemble): 5.616085385449712e-07
R-squared Value: 0.8996054126913193
```

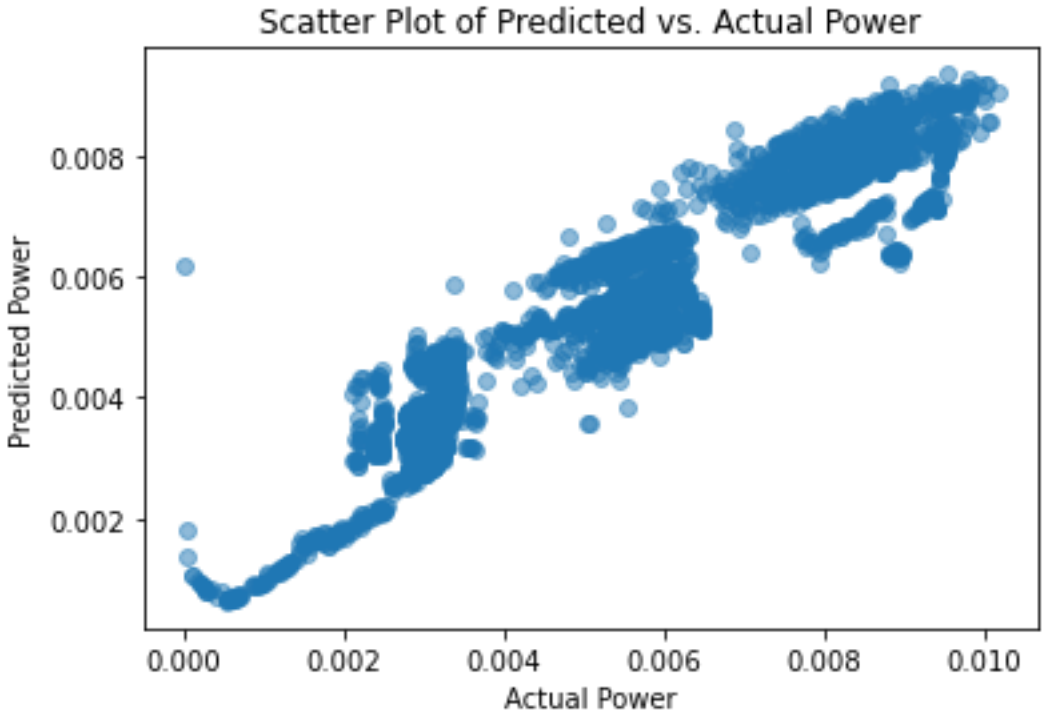

Figure 4.2.1: Scatter Plot

The trained ensemble model demonstrates remarkable predictive prowess, as evidenced by a Mean Squared Error (MSE) of 5.616085385449712e-07 and an R-squared value of 0.8996054126913193. These metrics signify minimal prediction error and a profound ability to explain nearly 90% of the variability in the 'Power(kWh)' variable.

5. Results

Imagine we're peering into the crystal ball of our battery model. We're curious about how much power our battery would produce under certain conditions. So, we feed these conditions like how much energy it can hold, how safe it is, its cost, lifespan, and efficiency into the model.

'Energy Density (Wh/L)': 0.521812,

'Safety (SOC)': -2.192861,

'Cost ($)': 567,

'Life (Hr)': 0.0024281,

'Efficiency (BE)': 55.21289

```
Predicted(Power kWh)Value: 0.048204094366649984
```

figure 5.1: Result

Guess what? The model spits out a number, telling us it thinks our battery would produce about **0.0482** kilowatt-hours of power under these specific conditions.

What Does this Mean?

In simpler terms, this prediction gives us a sneak peek into how well our battery might perform. It's like having a glimpse of the future, helping us make decisions about designing and optimizing batteries.

But, we have to remember, predicting things is tricky. The number we got is like a really good prediction based on the model's smarts, according to research and reports. it helps us imagine and plan for what our battery could do. It's a step forward in understanding and improving sustainable energy solutions.

6. Experimental Learning

I was diving into a bit of an experiment to predict two things at once like 'Power(kWh)' and 'Safety (SOC)' or “Life” and “Energy” vice versa for our battery.

I have data on energy density, cost, life, and efficiency of batteries, and I want to predict both power and safety. So, I split this data into two parts: one to teach our model (training data) and the other to test how well it learned (testing data).

I introduced three actors (models) into my experiment: Linear Regression, Random Forest, and Gradient Boosting. Each has its strengths, and I was curious to see how they perform together.

```
Mean Squared Error (Multi-Output): [1.02304908e-06 1.94574552e-01]
R-squared Value (Multi-Output): [0.81711711 0.6735747 ]
```

The Verdict:

The model doesn't just guess randomly. It's pretty good! The Mean Squared Error (a way to measure how close predictions are to reality) for power is tiny (1.02304908e-06), and for safety, it's a bit larger (0.194574552). The R-squared values (how well the predictions explain the data) are also solid.

```
#     'Energy Density': 0.521812,
#      'Safety': -2.192861,
#      'Cost': 567,
#      'Life': 0.0024281,
#      'Efficiency': 55.21289

Predicted Power: 0.00333280398986765 75
Predicted Safety: -7.381658679332311
```

Figure 6.1: Experiment Result

Importantly, this whole thing was an experiment. I weren't sure if predicting two things at once would work well, but guess what it did! The multi-output model turned out to be a success, showing promise for predicting both power and safety in future Cell battery designs.

But here, there are multiple things that should be taken note of the dataset I generated was completely designed to predict the variable “POWER” so there are some limitations and important measures to be taken in order to predict to variables at same time.

7. Conclusion

In wrapping things up, imagine we've just injected a dose of futuristic tech into how we create Li-ion batteries. We're talking about using smart machines to speed up the whole design process, which is usually slow and expensive. Our fancy model is pretty good at guessing the best values for key battery stuff, making the whole process quicker and cheaper. And you know what's cool? It's not just good for our wallets; it's a win for the planet too.

So, what does this all mean? Well, picture a future where we effortlessly create batteries that are not only super efficient and budget-friendly but also kind to Mother Earth. It's like blending cutting-edge technology with insider knowledge about batteries to make our energy solutions smarter and greener.

In a nutshell, our project isn't just about faster and time efficient batteries; it's about ushering in a whole new era where technology and eco-friendliness team up to give us energy storage solutions that are top-notch and environmentally friendly.

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