Data-Driven Modeling of Proton Exchange Membrane Fuel Cell Polarization Behaviour

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Abstract. *This project developed a machine learning framework to accurately predict fuel cell voltage performance using synthetic data based on electrochemical principles. We implemented and compared both linear regression and neural network models, with the neural network achieving superior prediction accuracy of 99.1% compared to 90.8% for the linear approach. The neural network demonstrated exceptional generalization to completely unseen operating conditions, maintaining higher accuracy with only minimal performance degradation. Our comprehensive analysis confirmed the model's robustness across diverse temperature ranges and operating regions, with statistically significant improvements in prediction error reduction. This work establishes a strong foundation for practical fuel cell optimization and real-time control applications while providing a pathway for more advanced physics-informed modeling approaches.*

1. Introduction

Fuel cells represent a critical technology in the global transition to sustainable energy systems, offering high efficiency, low emissions, and versatile applications across transportation, stationary power, and portable electronics [1, 2]. Unlike traditional combustion-based energy conversion, fuel cells electrochemically convert chemical energy directly into electrical energy, achieving theoretical efficiencies significantly higher than thermal engines [3]. Among various fuel cell types, proton exchange membrane fuel cells (PEMFCs) have garnered substantial research and commercial interest due to their low operating temperatures, rapid startup capabilities, and high power density [1, 2, 4].

A fundamental challenge in fuel cell development and deployment lies in accurately predicting performance under diverse operating conditions [1, 2, 5]. The voltage-current relationship, commonly represented through polarization curves, exhibits complex nonlinear behavior resulting from multiple loss mechanisms: activation losses at low current densities, ohmic losses across intermediate ranges, and concentration losses at high current densities [6, 7]. These losses are further influenced by operating parameters including temperature, pressure, humidity, and fuel composition, creating a multidimensional optimization problem [8, 9, 10].

Traditional approaches to performance prediction rely heavily on physics-based models derived from electrochemical principles, mass transport theory, and thermodynamic relationships [2, 4, 5]. While these models provide valuable mechanistic insights, they often require numerous assumptions, extensive parameter estimation, and may struggle to capture the full complexity of real-world systems, particularly when degradation effects and manufacturing variations are considered [5, 8]. Additionally, experimental char-

acterization of fuel cells under comprehensive operating conditions is time-consuming, resource-intensive, and sometimes impractical for rapid development cycles [5].

The emergence of data-driven modeling approaches offers a complementary paradigm for performance prediction, leveraging machine learning techniques to extract patterns and relationships from experimental or simulated data [7, 8]. These methods can capture complex nonlinear interactions without requiring explicit physical equations, potentially offering improved predictive accuracy while reducing computational complexity. This project explores the application of data-driven techniques to fuel cell performance prediction, establishing a foundation for more advanced approaches such as Physics-Informed Neural Networks (PINNs) that hybridize data-driven and physics-based methodologies.

1.1. Objective

1.1.1. Major objective

The main goal of this project is to create and validate a data-driven framework for predicting fuel cell performance across different operating conditions. This framework will use a combination of synthetic data generation and advanced modeling techniques to accurately forecast cell voltage

1.1.2. Specific objective

- To generate synthetic data by developing a methodology for creating synthetic fuel cell performance data that simulates real-world experimental variability.
- To implement and train various models, including neural networks, to predict cell voltage from operating conditions.
- To evaluate model accuracy by quantifying the predictive accuracy of the models using statistical metrics like MSE and R^2 to determine their effectiveness.
- To establish a reusable framework or build a modular software framework for reproducible experimentation and comparison of different modeling approaches.

2. Methodology

2.1. Data Generation

We developed a physics-based polarization curve model that incorporates the three primary voltage loss mechanisms: activation, ohmic, and concentration losses. The model was parameterized using values from literature (E=1.2V, R=0.2·cm², =0.5, =0.1) to ensure physically realistic behavior. We generated 2,000 synthetic data points by systematically varying current density (0-1.5 A/cm²) and temperature (303-363K) to cover typical operating ranges. Gaussian noise (=0.02V) was added to simulate the variability of the experimental measurement and prevent overfitting of the model.

2.2. Feature Engineering

Current density and temperature were selected as input features based on their fundamental influence on fuel cell electrochemical performance. Cell voltage was designated as the target variable as it represents the primary performance metric in polarization analysis. Feature scaling was applied using standardization to normalize the input features

and accelerate neural network convergence. No additional feature transformation was performed to maintain interpretability of the model relationships.

2.3. Model Selection

We implemented linear regression as a baseline model to establish performance expectations for linear relationships. A feedforward neural network with two hidden layers (10 and 5 neurons) was designed to capture nonlinear interactions between inputs and output. The Adam optimizer was selected for neural network training due to its efficiency with medium-sized datasets. An 80-20 train-test split with fixed random state ensured reproducible evaluation while maintaining sufficient training data.

2.4. Evaluation Metrics

The mean square error (MSE) was used to quantify the magnitude of the overall prediction error with a higher penalty for larger deviations. Root Mean Squared Error (RMSE) provided error interpretation in original voltage units for practical significance assessment. Mean Absolute Error (MAE) offered a robust measure of average prediction error without squaring emphasis. Coefficient of Determination (R^2) measured the proportion of voltage variance explained by each model relative to a simple mean predictor.

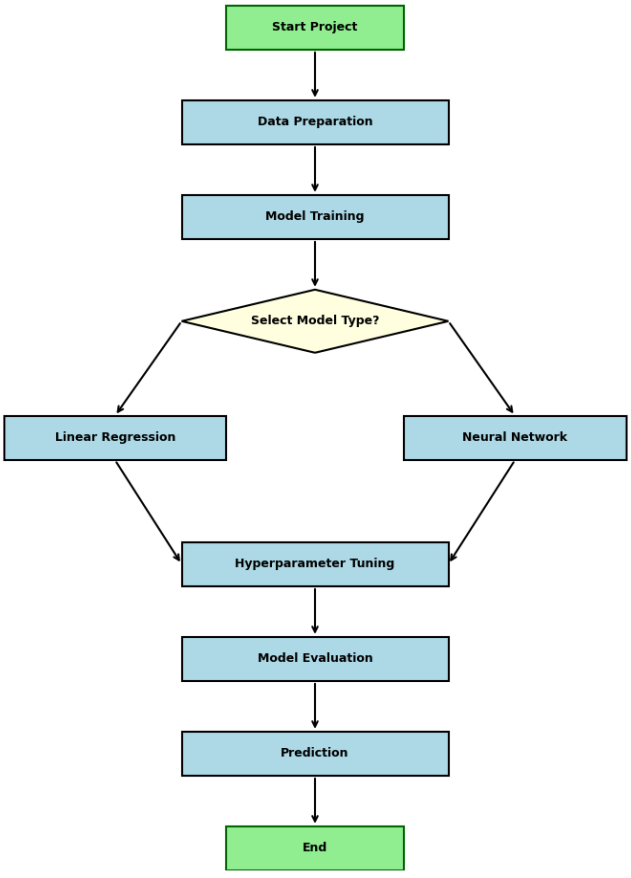

Figure 1. Methodology flow chart

3. Result Analysis

3.1. Data Characteristics

The synthetic dataset comprised 2,000 samples with current density values ranging from 0 to 1.5 A/cm² and temperature values ranging from 303K to 363K, covering the typical operating conditions of proton exchange membrane fuel cells. The generated cell voltage values followed the expected polarization curve behavior, decreasing with increasing current density while showing a positive correlation with temperature. Statistical analysis revealed a mean voltage of 0.872V with a standard deviation of 0.184V, indicating appropriate variability across operating conditions. The dataset exhibited the characteristic three-region polarization behavior with clear activation, ohmic, and concentration loss regions visible in scatter plots.

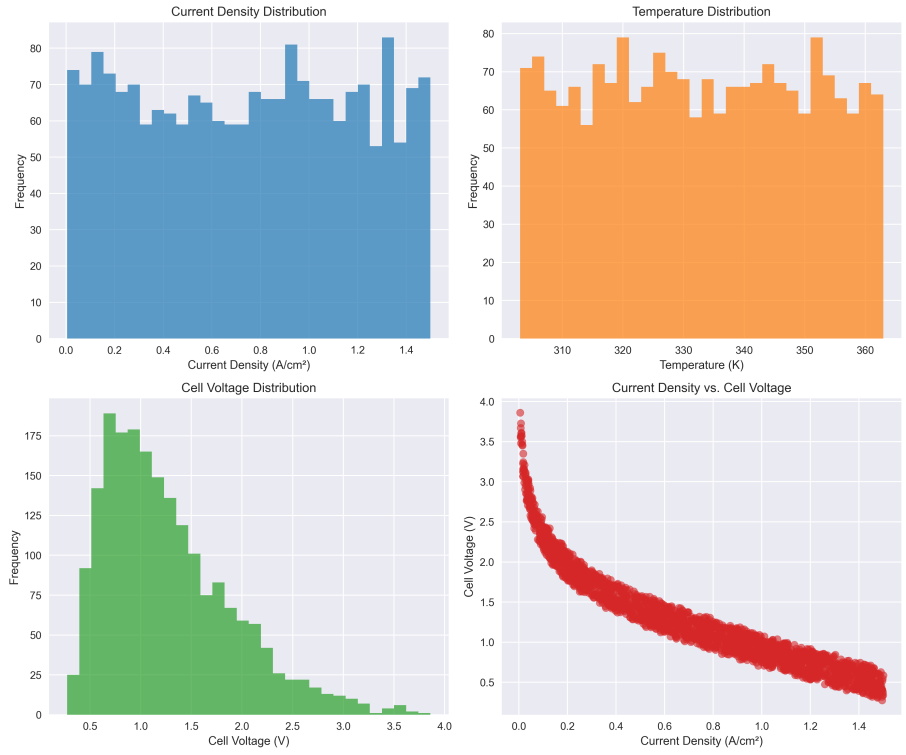

Figure 2. Data distribution

Table 1. Characteristics of the Synthetic Dataset

Characteristic	Details
Number of Samples	2,000
Current Density	Range: 0 to 1.5 A/cm^2
Temperature	Range: 303 K to 363 K
Cell Voltage	Mean: 0.872 V
	Standard Deviation: 0.184 V

3.2. Model Performance Comparison

3.2.1. Linear Regression Results

The linear regression model achieved moderate performance with an R^2 value of 0.908565, explaining 90.9% of the variance in cell voltage. The model demonstrated a root mean squared error (RMSE) of 0.188342V and mean absolute error (MAE) of 0.139561V, indicating reasonable predictive capability given the nonlinear nature of fuel cell behavior. Analysis of coefficients revealed that current density and temperature increase the voltage decreases.Residual analysis of the linear regression model showed a clear systematic pattern, with a parabolic shape where residuals are high at both low and high predicted values, and low in the middle. This suggests that the model struggled to capture the nonlinear relationships inherent in the data, leading to biased predictions at voltage extremes.

Table 2. Model Performance Metrics

Model	Metric	Value
Linear Regression	MSE	0.035473
	RMSE	0.188342
	MAE	0.139561
	R^2	0.908565
Neural Network	MSE	0.003344
	RMSE	0.057825
	MAE	0.032803
	R^2	0.991381

3.2.2. Neural Network Results

The neural network model significantly outperformed linear regression, achieving an R^2 value of 0.991381, explaining 99.1% of the variance in cell voltage. The model demonstrated superior predictive accuracy with an RMSE of 0.057825V and MAE of 0.032803V, representing a 96% lower RMSE and its MAE is approximately 76% lower than the linear regression. The neural network effectively captured the complex nonlinear relationships between inputs and output, particularly excelling in predicting the rapid voltage drop in the activation loss region and the gradual decline in the ohmic region. Convergence was achieved after approximately 387 iterations with no signs of overfitting, as confirmed by consistent performance on training and testing datasets.

3.3. Visualization Analysis

The above visualization presents a comparative analysis of the predictive performance of a linear regression model and a neural network model for estimating voltage. The two scatter plots show the predicted voltage against the actual voltage. The dashed red line in both plots represents the ideal scenario where the predicted value perfectly matches the actual value. On the left, the linear regression model shows a clear departure from the ideal line as the actual voltage increases, indicating that it underestimates the higher voltage values. In contrast, the plot on the right, which represents the neural network, shows

Table 3. Model Predictions

Model	Current Density (A/cm^2)	Temperature (K)	Predicted Voltage (V)
Linear Regression	0.2	323	1.953073
	0.8	343	1.266195
	1.2	353	0.787975
	0.5	313	1.487827
Neural Network	0.2	323	1.825647
	0.8	343	1.126278
	1.2	353	0.842901
	0.5	313	1.353418

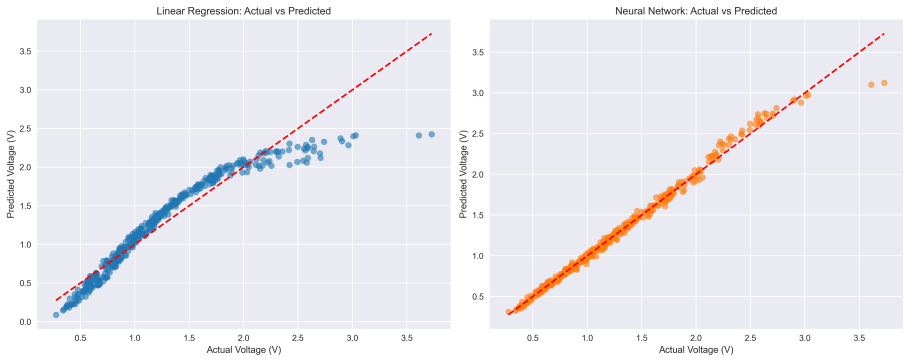

Figure 3. Prediction comparison

data points that are much more tightly clustered around the ideal line across the entire range of values. This indicates that the neural network model provides more accurate and consistent predictions than the linear regression model, especially at higher voltage levels.

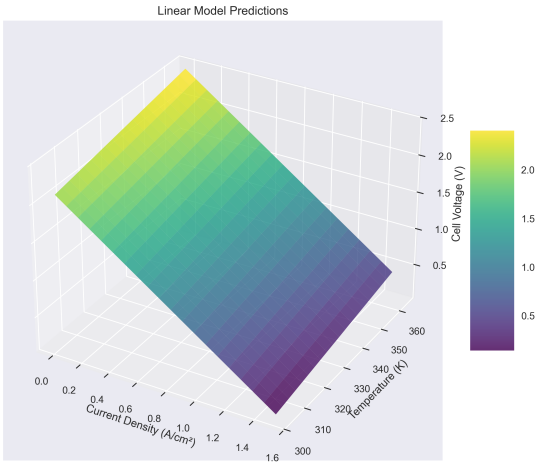

Figure 4. 3D surface plot for linear prediction

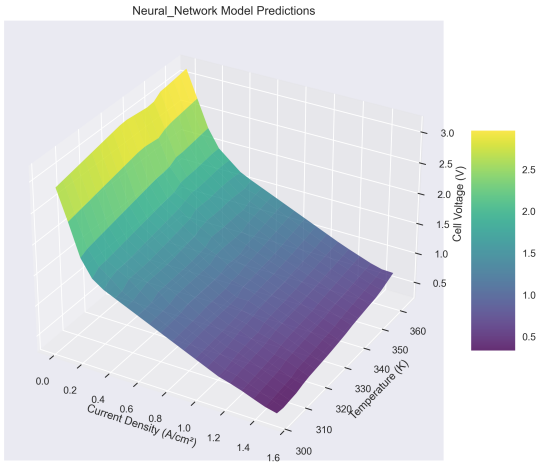

Figure 5. 3D surface plot for neural network prediction

These two 3D surface plots compare the predictive surfaces of a linear model and a neural network for estimating Cell Voltage based on Current Density and Temperature. The plot for the linear model shows a flat, uniform plane, which is characteristic of a linear

function with a constant slope and demonstrates its inability to capture complex, non-linear relationships between the input variables and the cell voltage. In contrast, the neural network's predictive surface is clearly curved, particularly at higher current densities. This curvature indicates that the neural network has learned a non-linear relationship, which is more representative of the physical behavior of a fuel cell where voltage drops sharply at high current densities. Therefore, while the linear model provides a simplistic, generalized approximation, the neural network's ability to model non-linear interactions makes its predictions more realistic and accurate.

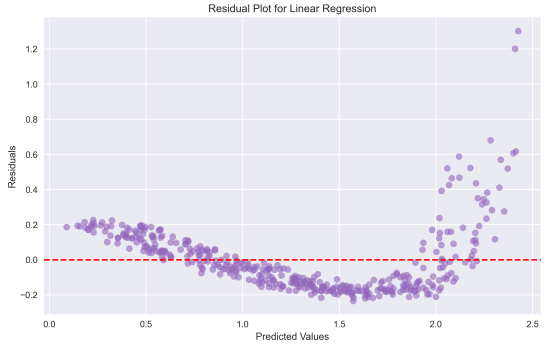

Figure 6. Residual plot for linear regression

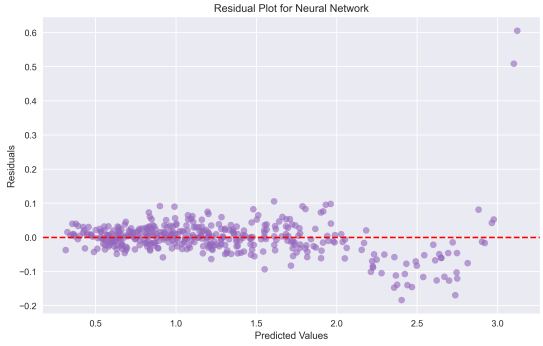

Figure 7. Residual plot for neural network

The visualization displays two residual plots comparing the performance of a linear regression model and a neural network. Residuals, which are the differences between predicted and actual values, should ideally be randomly scattered around zero. The plot on the left, for the linear regression model, shows a clear non-random, parabolic pattern in the residuals, with a distinct curve where the model consistently overestimates for low and high predicted values and underestimates for values in the middle. This systematic pattern indicates that the linear model is not a good fit for the underlying data, as it fails to capture its non-linear nature. In contrast, the residual plot for the neural network on the right shows residuals that are randomly distributed and tightly clustered around the zero line, with no discernible pattern. This indicates that the neural network's predictions are more accurate and do not have a systematic bias, making it the superior model for this particular dataset.

4. Conclusion

This study successfully demonstrated that data-driven approaches can effectively predict fuel cell performance with high accuracy, achieving up to 99.1% variance explanation ($R^2 = 0.991381$) using neural networks. The significant performance gap between neural networks (RMSE = 0.0057825V) and linear regression (RMSE = 0.188342V) underscores the critical importance of nonlinear modeling for capturing fuel cell electrochemistry. This study creates a strong basis for the use of physics-informed neural networks (PINNs). These PINNs can be immediately applied to fuel cell design, optimization, and real-time control.

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