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Battery Degradation Modeling for Mining BEVs

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1 **Battery Degradation Overview**

2 Battery Degradation Models

3 Physics-informed Machine Learning

4 Current Challenges and Future Work

Background – What is Battery Degradation

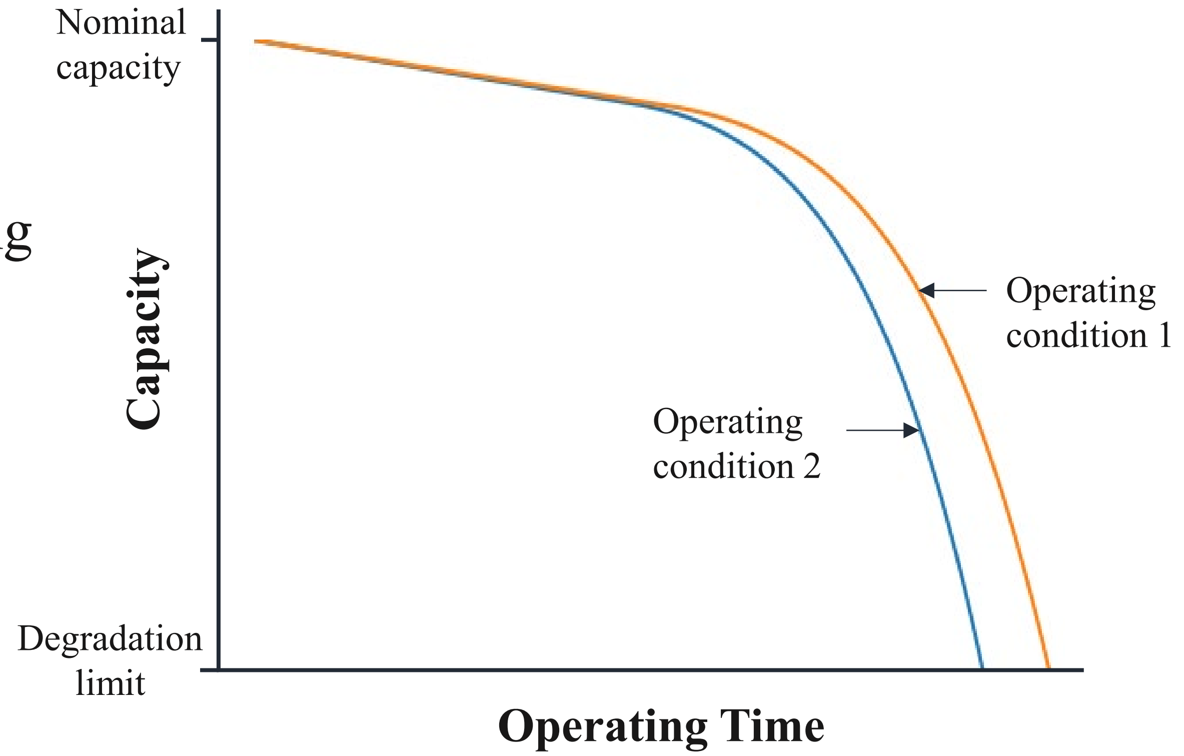
Battery Degradation:
the decline in performance and capacity of the battery over time

Degradation from Calendar Aging:
due to battery's exposure to environmental conditions, independent of its usage

Degradation from Cycling Aging:
due to repeated charge and discharge cycles, directly related to how the battery is used

Motivation

- Current lack of study on battery degradation for mining BEVs
- Study the different patterns of battery degradation in underground and surface mining vehicles
- Forecast battery longevity for mining duty cycles
- Investigate the factors that most significantly influence battery degradation



Battery Degradation Mechanisms

Solid–electrolyte interphase (SEI) growth

- The electrolyte reacts with the anode surface and decomposes, forming a solid layer
- Initial layer thickens during charging and discharging cause **loss of lithium inventory** from electrolyte
- Decreases capacity and increases internal resistance or impedance

Loss of active material

- Active electrode particles become electrically isolated due to cracking, mechanical stress, or binder degradation
- Reduces the amount of material available for lithium intercalation, leading to capacity loss

Lithium plating

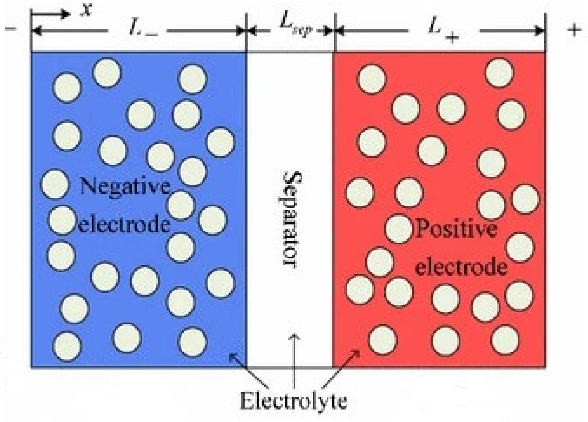
- Li+ ions from the electrolyte form Li metal on the graphite surface
- Plated lithium grows in needle-like, branching structures called **dendrites,** they can potentially create an **internal short circuit** if long enough
- Form extra SEI

Physics Model - Introduction

Doyle-Fuller-Newman Model (DFN)

Detailed 'Pseudo-2D' model that resolves electrochemical processes across two key dimensions:

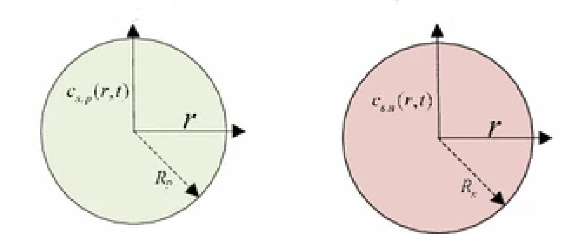
- Across the cell (x-direction): how ion concentration and potential change through the anode, separator, and cathode
- Inside particles (r-direction): lithium diffusion within the active material particles



Single Particle Model (SPM)

Highly simplified version of the DFN that assumes the electrolyte concentration and potential are spatially uniform:

- Across the Cell (x-direction): electrolyte concentration and potential are assumed uniform, and each electrode is reduced to a single representative particle
- Inside Particles (r-direction): lithium diffusion is resolved radially within the average spherical particles of the anode and cathode



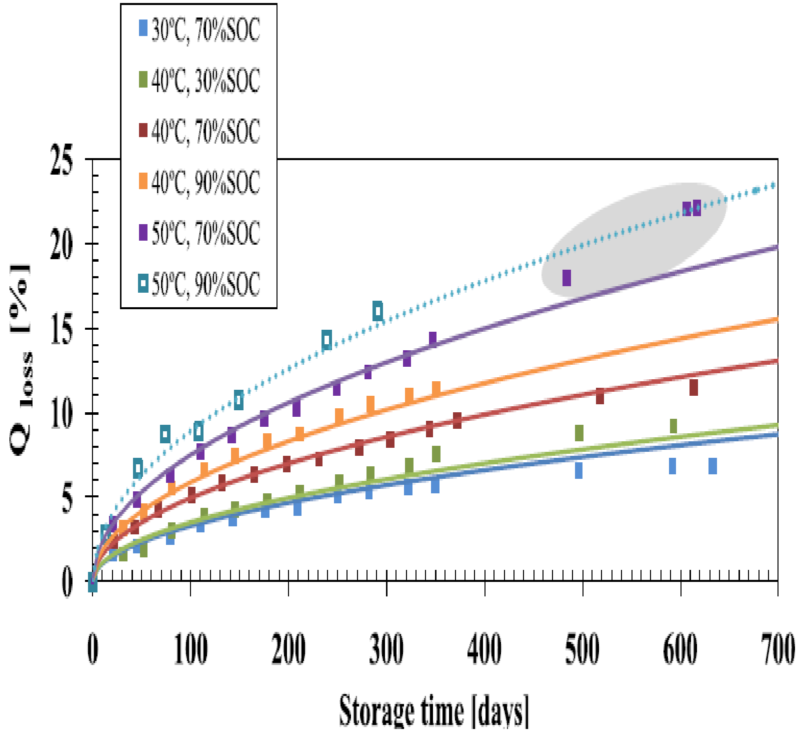
Source: Kofi et al., J. Appl. Electrochem. (2017)

Physics Model – Computational Comparison

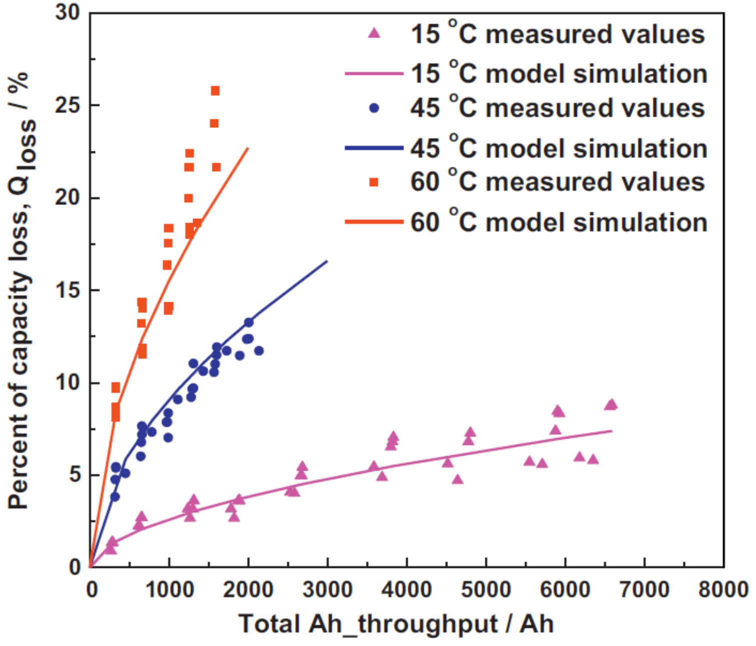
	Doyle-Fuller-Newman Model (DFN)	Single Particle Model (SPM)
Lithium Diffusion in Solid Particles	$\frac{\boxed{\partial c_s(x,r,t)}}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(D_s(c_s,T)\, r^2 \frac{\partial c_s}{\partial r}\right)$	$\frac{\boxed{\partial c_s(r,t)}}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(D_s(c_s,T)\, r^2 \frac{\partial c_s}{\partial r}\right)$
Lithium Transport in Electrolyte	$\frac{\partial(\varepsilon_e c_e)}{\partial t} = \nabla \cdot (D_e^{\text{eff}} \nabla c_e) + \frac{1-t^+}{F} a j_{\text{tot}}(x,t)$	Not included for SPM
SEI growth	$\frac{\partial L_{\text{SEI}}(x,t)}{\partial t} = \frac{M_{\text{SEI}}}{\rho_{\text{SEI}} F} j_{\text{SEI}}(x,t)$	$\frac{dL_{\text{SEI}}(t)}{dt} = \frac{M_{\text{SEI}}}{\rho_{\text{SEI}} F} j_{\text{SEI}}(t)$
⋮	⋮	⋮

- Both DFN and SPM are modeled by solving Partial Differential Equations (PDE). PyBaMM is an open-source Python library specialized in this
- SPM is much easier to solve since it assumes uniform electrolyte concentration and has no *x*-dependence

Empirical Model



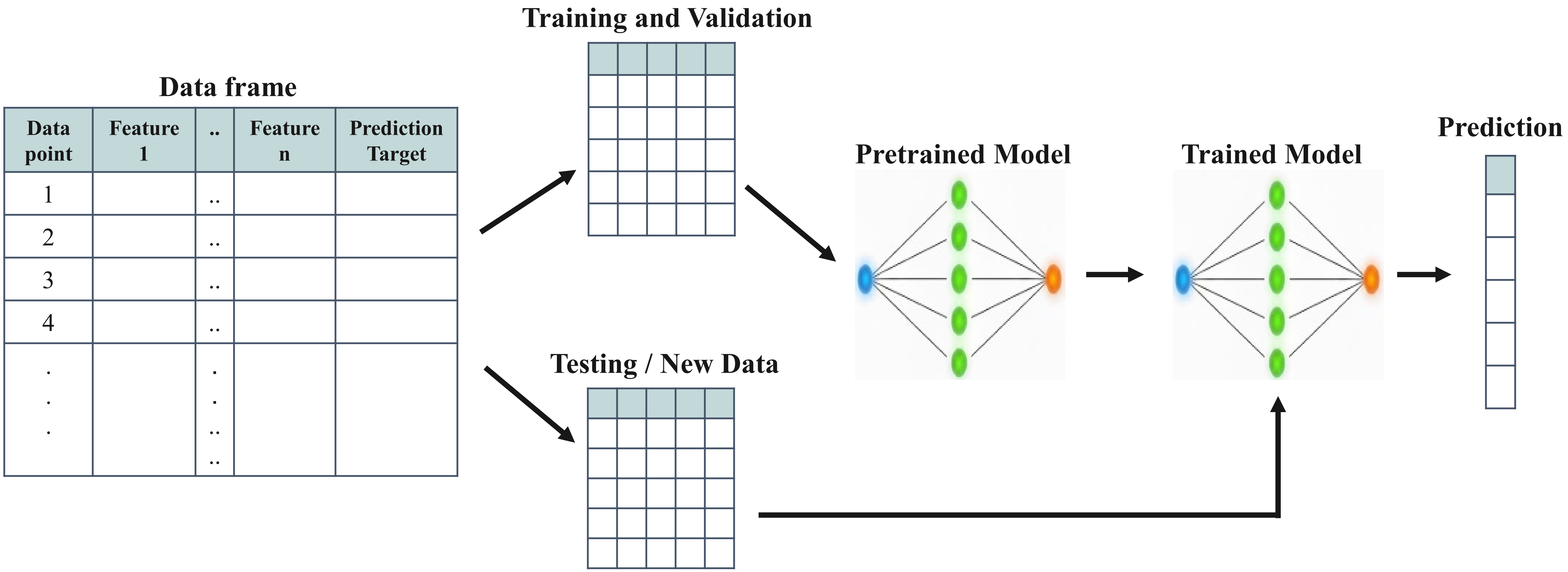
Source: Sarasketa-Zabala et al.(2014)



Source: Wang et al. (2011)

- For empirical models, the goal is to find a function that calculates degradation based on all parameters of interest (temperature, depth of discharge, charge/discharge rate, etc.) with minimum error using empirical data

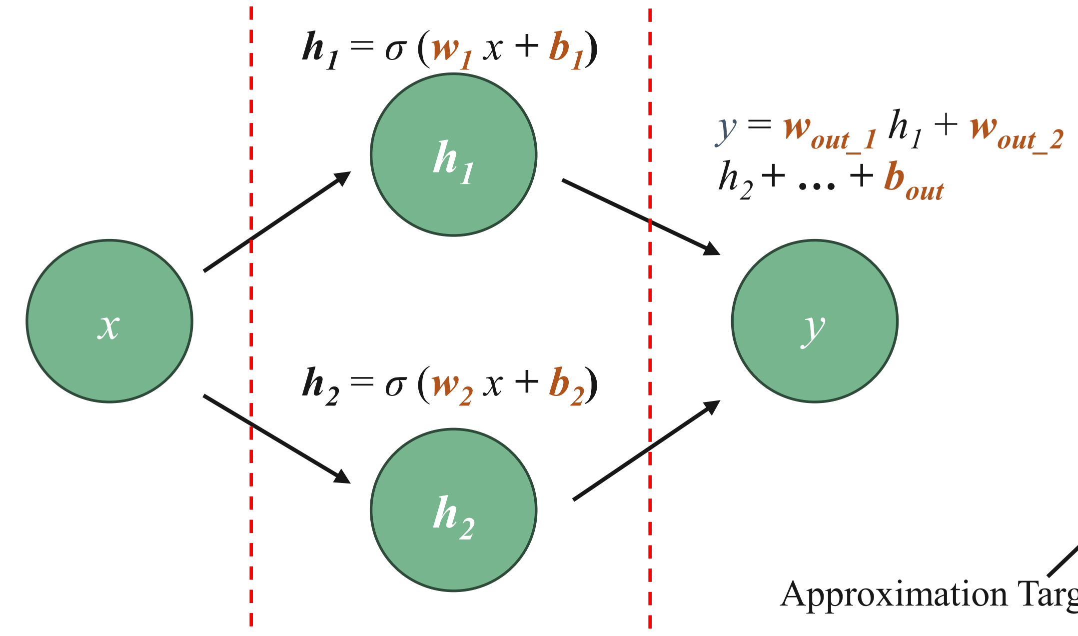
Machine Learning - Introduction



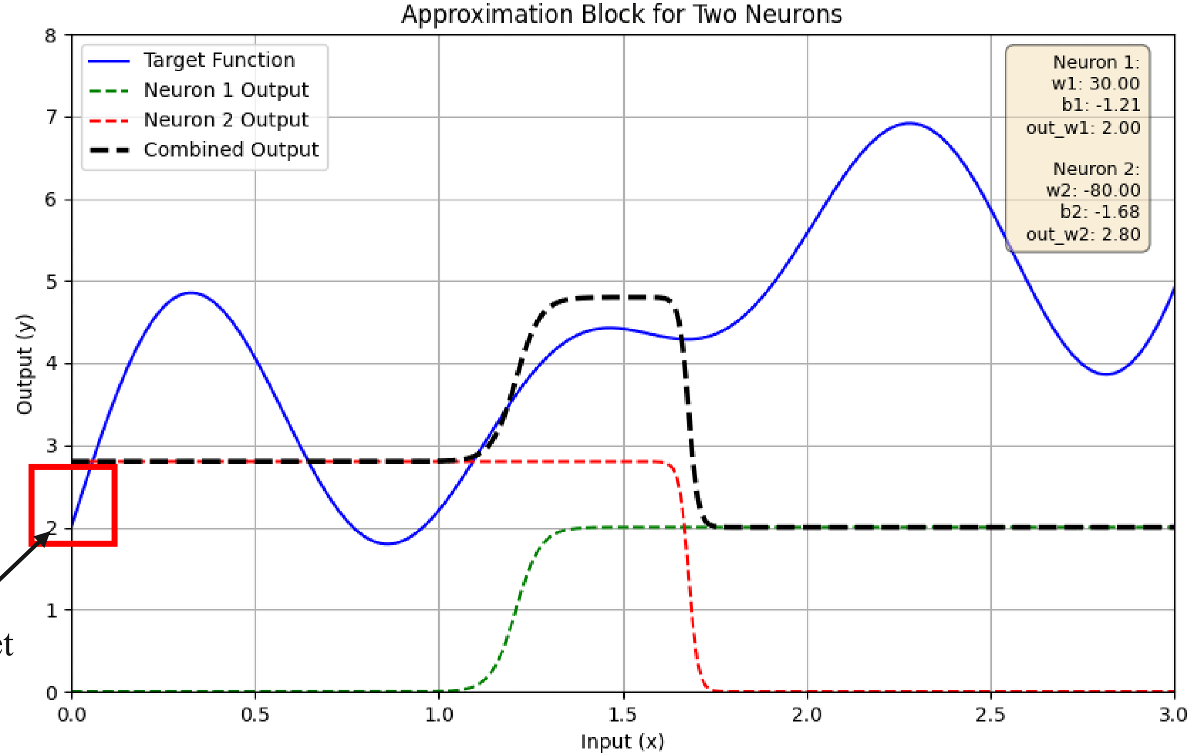
- For machine learning (ML) models, the inputs are called features, which are more flexible compared to those in physics or empirical models. ML models learn the underlying relationships between the features and the prediction target

Machine Learning – Why it works

Input Layer **Hidden Layer** **Output Layer**

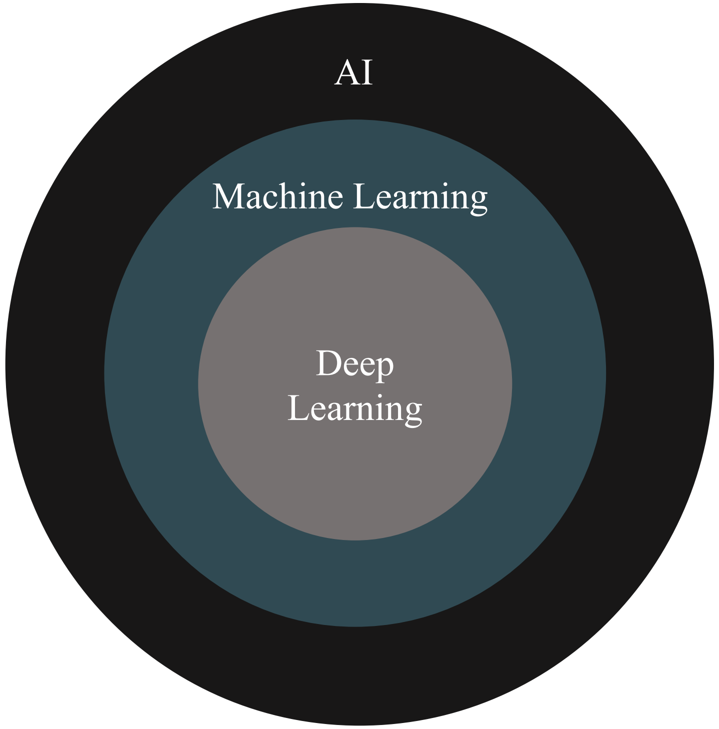


Approximation Target



- **Universal approximation theorem**: one hidden layer, a non-linear activation function, and enough neurons can approximate any continuous function to a certain degree

Machine Learning – AI and Machine Learning



Multilayer Perceptron (MLP)
- basic deep learning model
- number prediction
- label classification

Convolutional Neural Network (CNN)
- image classification
- object identification and detection

ChatGPT Gemini

Generative AI
- content creation

Copilot GitHub Copilot

Agentic AI
- automated project management
- operate independently without constant human input

Agent Builder

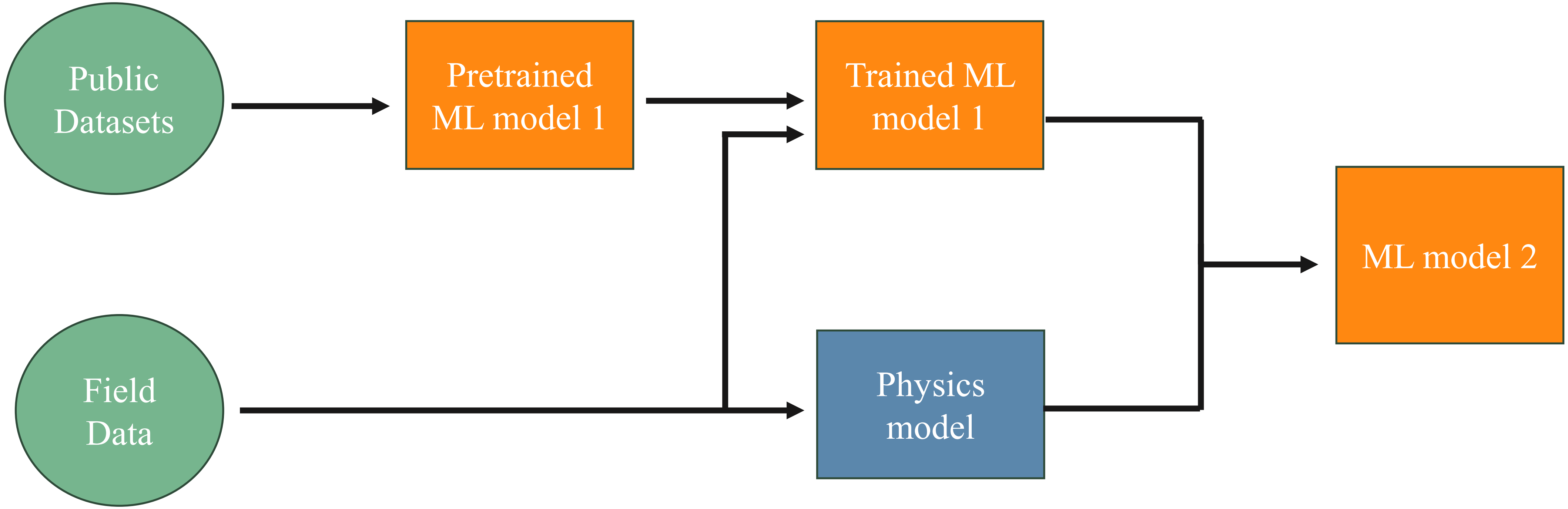
Parameters for Models

Model type	Input parameters	Field obtainable
Physics (SPM)	Electrode capacity	❌
	Average particle radius	❌
	Reaction kinetics (exchange current)	❌
	Solid diffusion coefficients	❌
	SEI growth / side reaction rates	❌
	Operating data (current, voltage, temperature, SoC)	✔
Empirical	Equivalent full cycles (EFC)	✔
	Operating data (current, voltage, temperature, SoC)	✔
	Calendar aging usage (SoC storage, Temperature)	✔
Machine Learning	Flexible, can be field data or electrochemical properties or both	✔

Model Comparison

Model	Pros	Cons
Physics	• Can be used with limited field data • Provides physical interpretability and allows for extrapolation	• Requires electrochemical properties that are unobtainable from field data
Empirical	• Very fast to compute • Good for trend prediction • Interpretable	• Only reliable for the operating conditions and data used for fitting • Little physical insight • Requires full-life data from multiple batteries
Machine Learning	• Very flexible about input features • Can capture hidden relationships between input futures and prediction target • Good at handling complex non-linearity	• Poor extrapolation outside training distribution • Limited interpretability • Requires full-life data from multiple batteries

Physics-informed Machine Learning



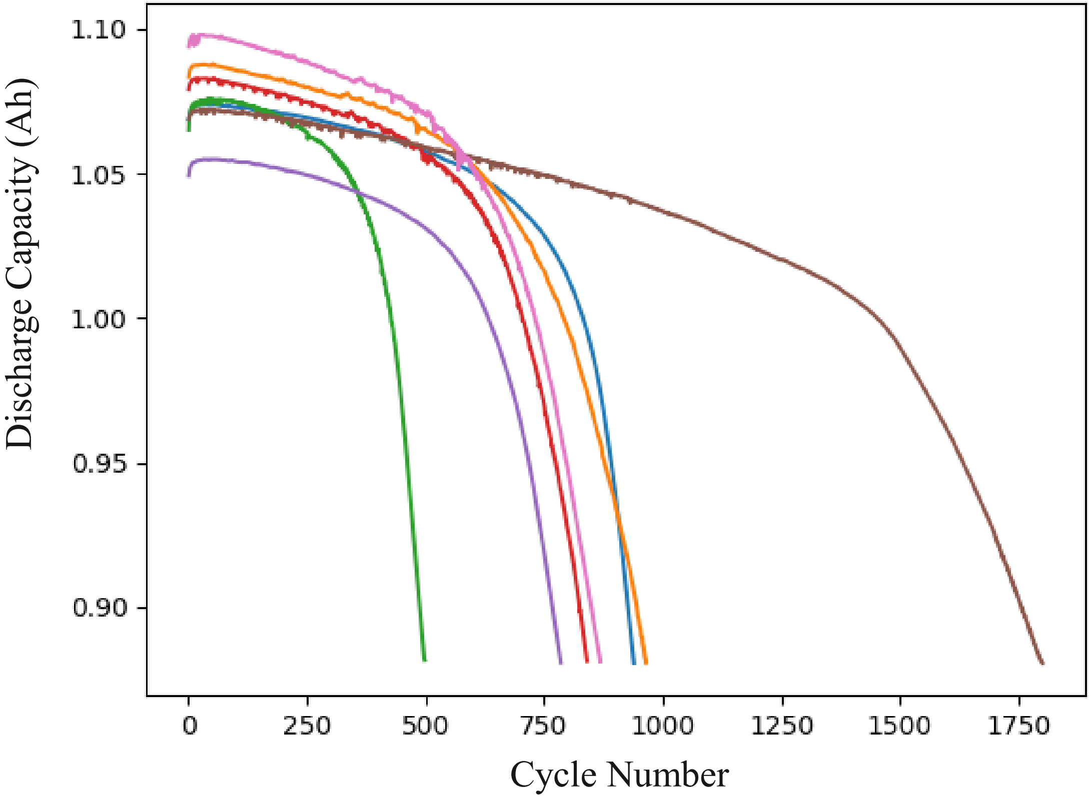
- In the proposed Physics-informed Machine Learning model, public datasets are first used to train a ML model to capture the relationship between cycling data and capacity. Field data are then passed through both the trained ML model and a physics model. The physics states and the residuals between the two models are used as input features to train a final ML model
- It offers greater interpretability than a standalone ML model and mitigates the limited field data challenge for ML

ML Model 1 – Data Overview

	Chemistry	Number of Cells	Nominal Capacity (Ah)	Temperature (°C)
1	LFP	200	1.1	30
2	NMC	55	2	~ 20 (room)
3	NCA	66	3.5	25, 35, 45
4	NMC	55	3.5	25, 35, 45
5	NMC + NCA	9	2.5	25

Datasets: https://data.matr.io/1/projects/5c48dd2bc625d700019f3204
https://zenodo.org/records/10963339
https://zenodo.org/records/6405084

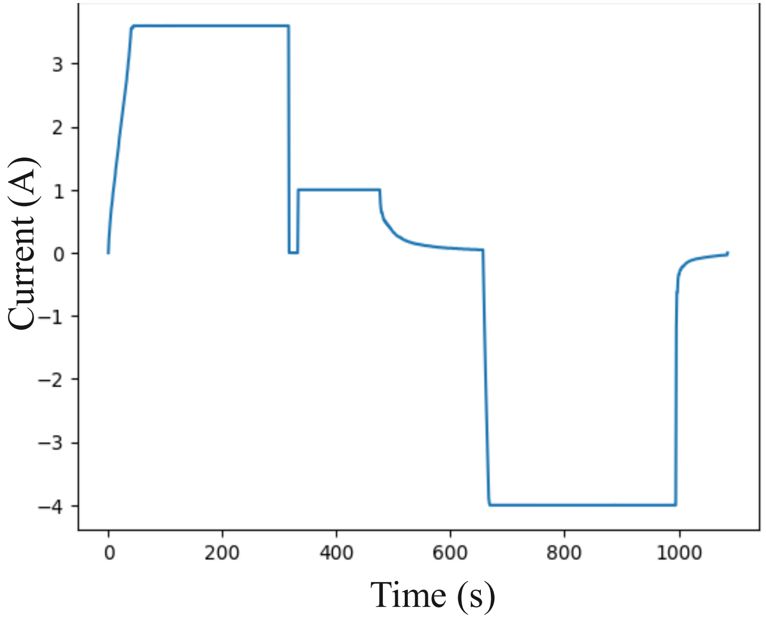
Example: Discharge capacity vs cycle number for 8 cells from the dataset



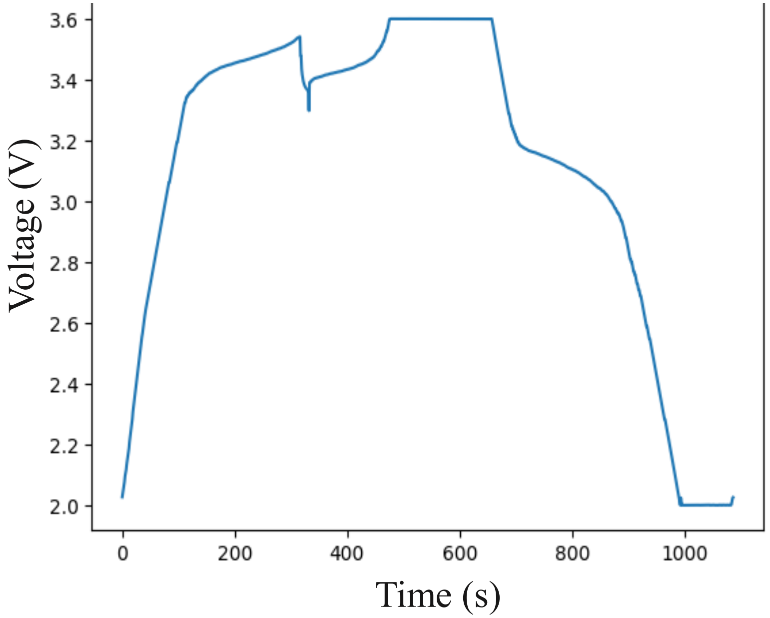
- The combined training and testing data points are 667000

ML Model 1 – Raw Data

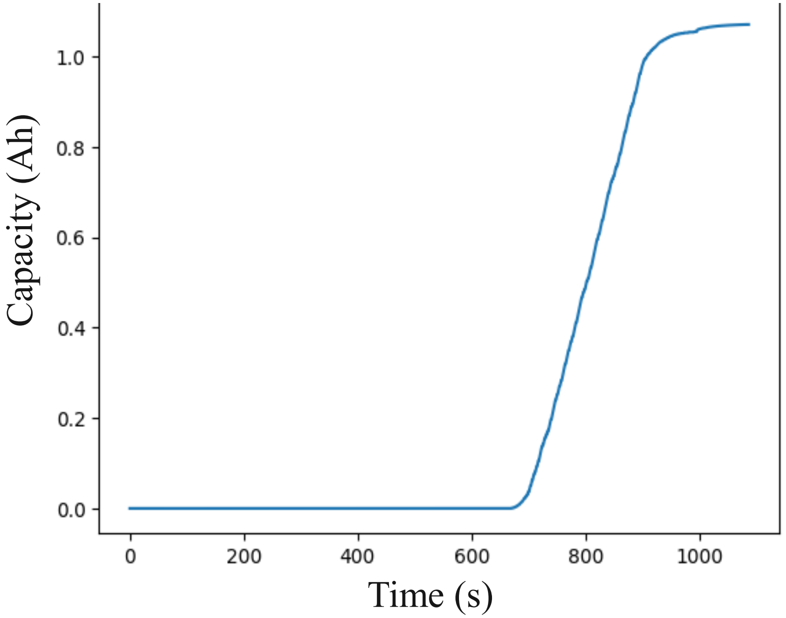
Current Profile for 1 Cycle



Voltage Profile for 1 Cycle

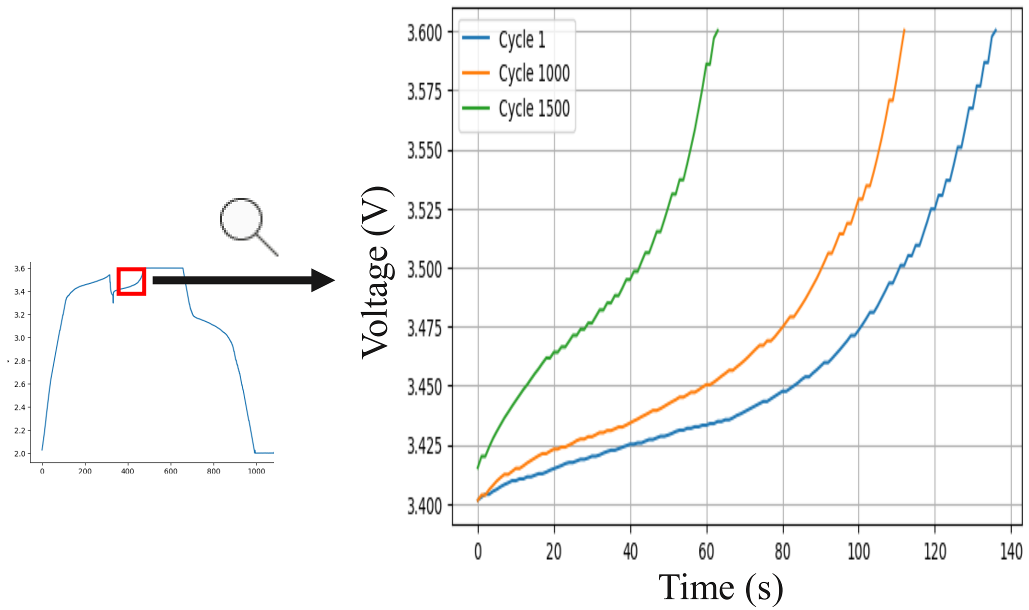


Discharge Capacity Profile for 1 Cycle

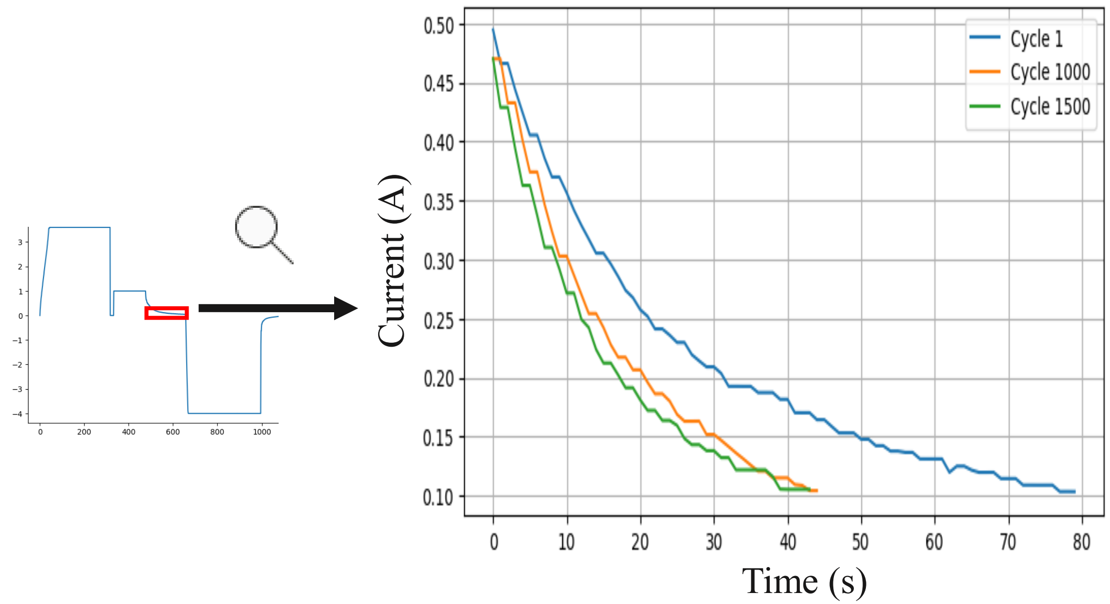


ML Model 1 – Feature Extraction

Voltage Curve

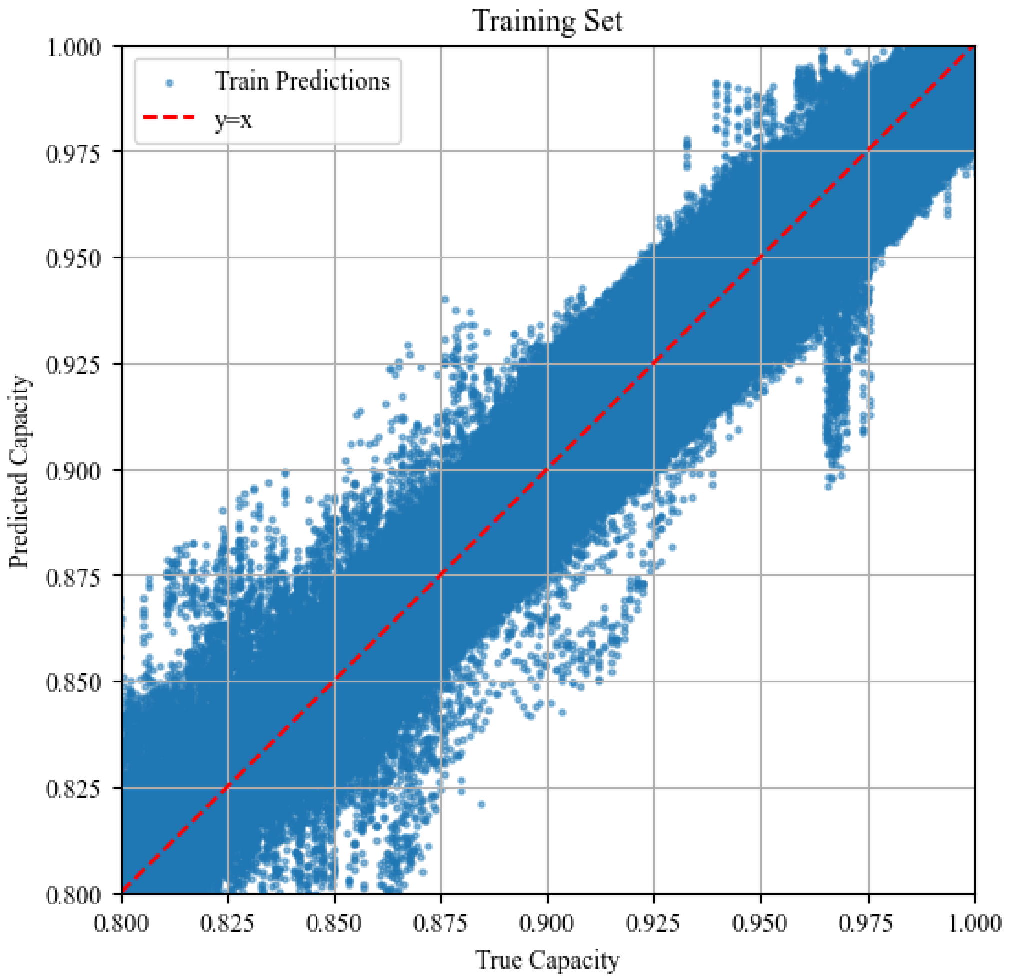


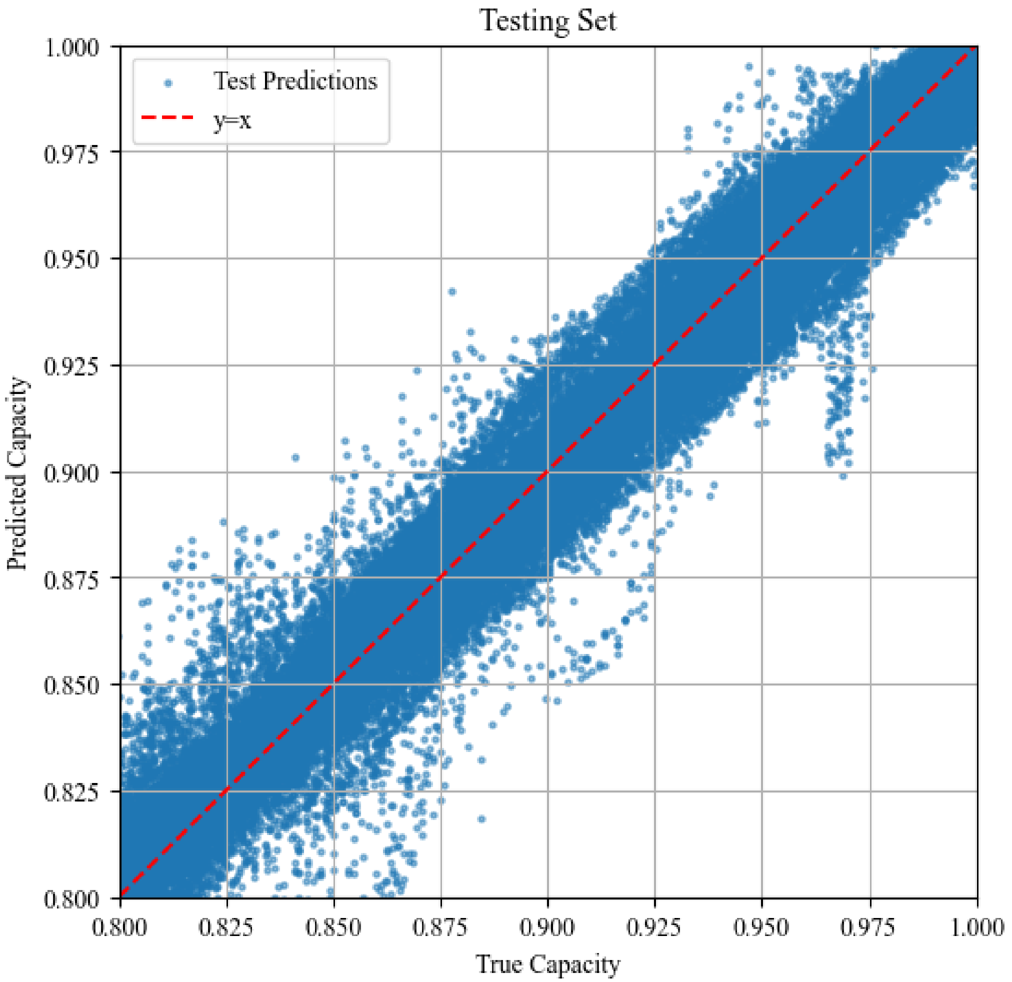
Current Curve



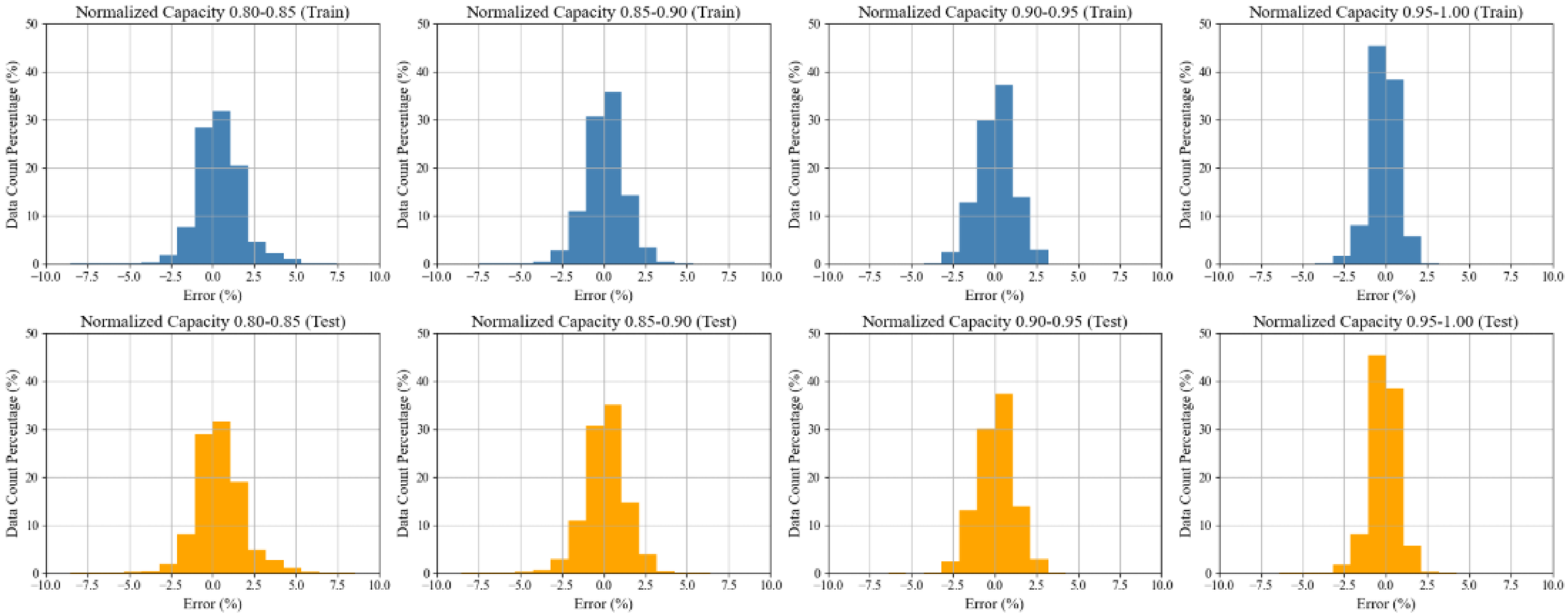
- Features are extracted from the current and voltage curves during a short period before battery is fully charged
- 8 features are extracted from each curve: mean, standard deviation, kurtosis, skewness, duration, accumulated charge, curve slope and curve entropy

ML Model 1 – Modeling Result





ML Model 1 – Modeling Result



- Error is calculated as (predicted capacity – true capacity)/true capacity x 100
- The maximum error for both the training and testing sets is approximately 8.5%

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4 **Current Challenges and Future Work**

Current Challenges and Future Work

Challenges

- Due to the lengthy process of conducting battery life cycle tests, it is challenging to gather a dataset with large number of battery cells from either lab or field

- Physics-based models require electrochemical parameters that are often unavailable from field data. Methods must be developed to calibrate these parameters obtained from online sources and the literature

Future Work

- Continue calibrating the ML model 1 of the Physics-informed ML model

- Process newly obtained field data and apply the physics model to it

- Integrate calendar aging into the Physics-informed ML model

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Appendix - Principle Equations

	Doyle-Fuller-Newman Model (DFN)	Single Particle Model (SPM)
Lithium Diffusion in Solid Particles	$\frac{\partial c_s(x,r,t)}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(D_s(c_s,T)\, r^2 \frac{\partial c_s}{\partial r}\right)$	$\frac{\partial c_s(r,t)}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(D_s(c_s,T)\, r^2 \frac{\partial c_s}{\partial r}\right)$
Lithium Transport in Electrolyte	$\frac{\partial(\varepsilon_e c_e)}{\partial t} = \nabla \cdot (D_e^{\text{eff}} \nabla c_e) + \frac{1-t^+}{F} a j_{\text{tot}}(x,t)$	Not included for SPM
Charge Conservation (electrolyte)	$\nabla \cdot (\kappa^{\text{eff}} \nabla \phi_e + 2\kappa^{\text{eff}}(1-t^+)\frac{RT}{F} \nabla \ln c_e) = a\, j_{\text{tot}}(x,t)$	Not included for SPM
Charge Conservation (solid)	$(\sigma^{\text{eff}} \nabla \phi_s) = -a\, j_{\text{tot}}(x,t)$	Not included for SPM
SEI growth	$\frac{\partial L_{\text{SEI}}(x,t)}{\partial t} = \frac{M_{\text{SEI}}}{\rho_{\text{SEI}} F} j_{\text{SEI}}(x,t)$	$\frac{dL_{\text{SEI}}(t)}{dt} = \frac{M_{\text{SEI}}}{\rho_{\text{SEI}} F} j_{\text{SEI}}(t)$
Lithium plating	$j_{\text{pl}}(x,t) = i_{0,\text{pl}}(x,t)\left[\exp\left(\frac{\alpha F \eta_{\text{pl}}(x,t)}{RT}\right) - \exp\left(-\frac{(1-\alpha) F \eta_{\text{pl}}(x,t)}{RT}\right)\right]$	$j_{\text{pl}}(t) = i_{0,\text{pl}}(t)\left[\exp\left(\frac{\alpha F \eta_{\text{pl}}(t)}{RT}\right) - \exp\left(-\frac{(1-\alpha) F \eta_{\text{pl}}(t)}{RT}\right)\right]$
Loss of Active Material	$j_{\text{int,eff}}(x,t) = f_{\text{LAM}}(x,t)\, a(x)\, i_0 \left[e^{\alpha_a F\eta/RT} - e^{-\alpha_c F\eta/RT}\right]$	$j_{\text{int,eff}}(t) = f_{\text{LAM}}(t)\, a\, i_0 \left[e^{\alpha_a F\eta/RT} - e^{-\alpha_c F\eta/RT}\right]$