Battery Modeling Webinar Series

Challenging Practices of Algebraic Battery Life Models through Statistical Validation and Model Identification via Machine-Learning

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Predictive Battery Lifetime Modeling at the National Renewable Energy Laboratory

Paul Gasper, Kandler Smith

Energy Conversion and Storage Systems Center

Electrochemical Energy Storage

June 1, 2021

Predictive Battery Lifetime Models

Three major applications for battery lifetime models:

Current state-of-health prediction

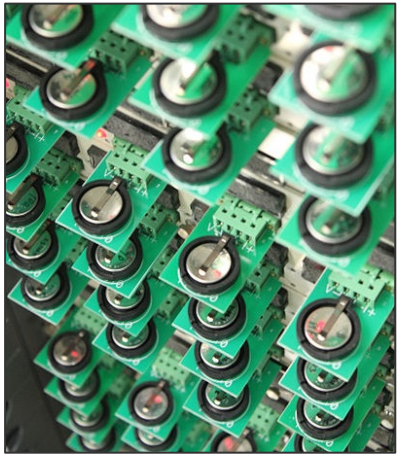
Remaining useful-life prediction

Lifetime simulation models.

Developing Algebraic Lifetime Simulation Models

The Challenge of Battery Lifetime Prediction

Lab Testing:
Predefined loads, controlled environments, 10–100 cells, 1–2 years.



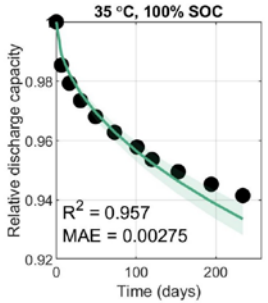
Real-World Applications:
Complex, variable loads, variable environments, ?? cells, and 10–20+ years.

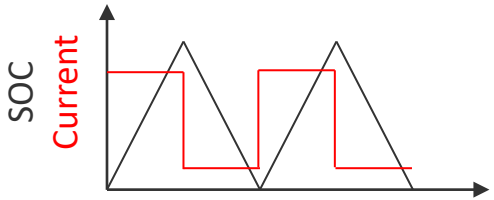
The Challenge of Battery Lifetime Prediction

Data From the Lab:

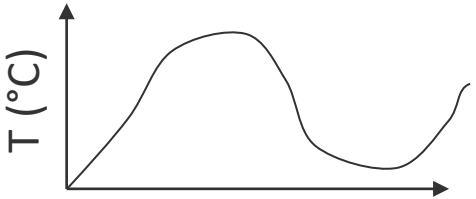
Cell	Temperature (T) (°C)	State of Charge (SOC)	Depth of Discharge (DOD)	C-Rate
1	30	75	0	0
2	30	50	100	1
3	45	75	50	0.5

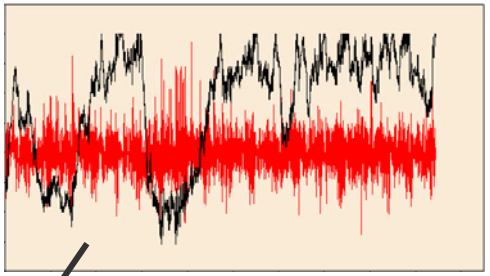
State of health (SOH) (time [t], equivalent full cycles [EFC], etc.)





Real-World Applications:



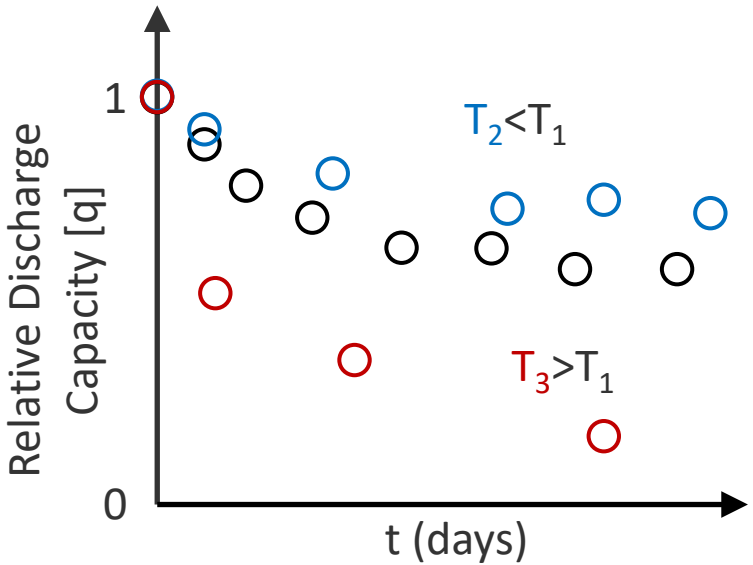


Voltage
Current

SOC(t) → Average SOC
DOD
C-rate
EFC
→ SOH (t, EFC, etc.)

Reduced-Order Model Identification Problem Statement

Lab Testing Data With Constant Experimental Conditions:



What We Are Trying To Find:

The degradation rate for any given battery use case/environmental conditions.

Challenges:

If q(t) is linear, then dq/dt is constant, and predicting changes to SOH is easy.

But both q(t)and dq/dt(t) can be nonlinear, and dq/dt is also dependent on test conditions.

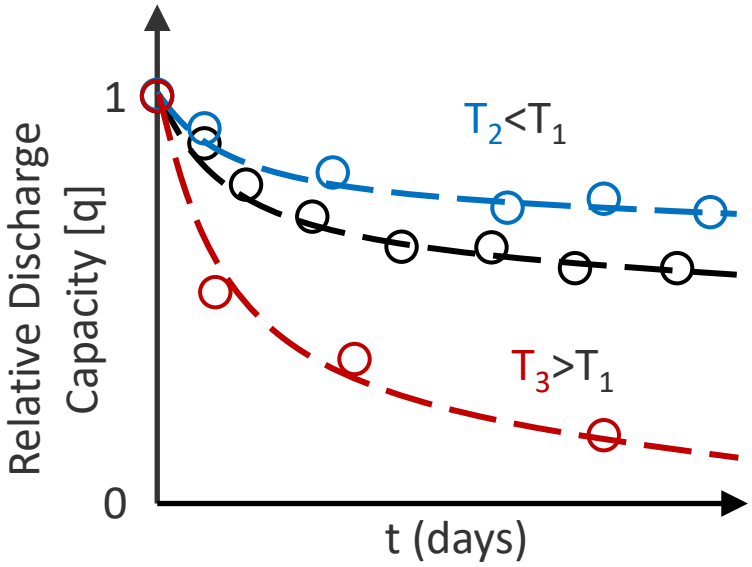
Common Approach:

Defining equations by making physically informed assumptions or using simple, empirically defined models.

Reduced-Order Model Identification Problem Statement

Parameter Submodels (Time-Invariant)

Lab Testing Data With Constant Experimental Conditions:



$$\beta = \gamma_0 \exp\left(\gamma_1 \frac{1}{T}\right)$$

Global Model

$$q = 1 - \gamma_0 \exp\left(\gamma_1 \frac{1}{T}\right) t^{\alpha}$$

$$q_2 = 1 - \boldsymbol{\beta_2} t^{\alpha}, \; T = \mathbf{T_2}$$

$$q_1 = 1 - \boldsymbol{\beta_1} t^{\alpha}, \; T = \mathbf{T_1}$$

$$q_3 = 1 - \boldsymbol{\beta_3} t^{\alpha}, \; T = \mathbf{T_3}$$

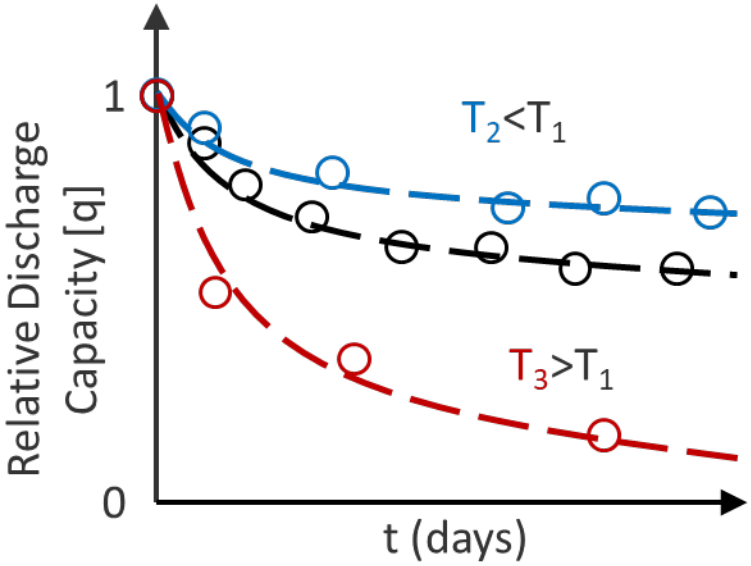
Local Models (Time-Variable)

α, β, γ: fitting parameters

Reduced-Order Model Identification Problem Statement

Parameter Submodels (Time-Invariant)

Lab Testing Data With Constant Experimental Conditions:



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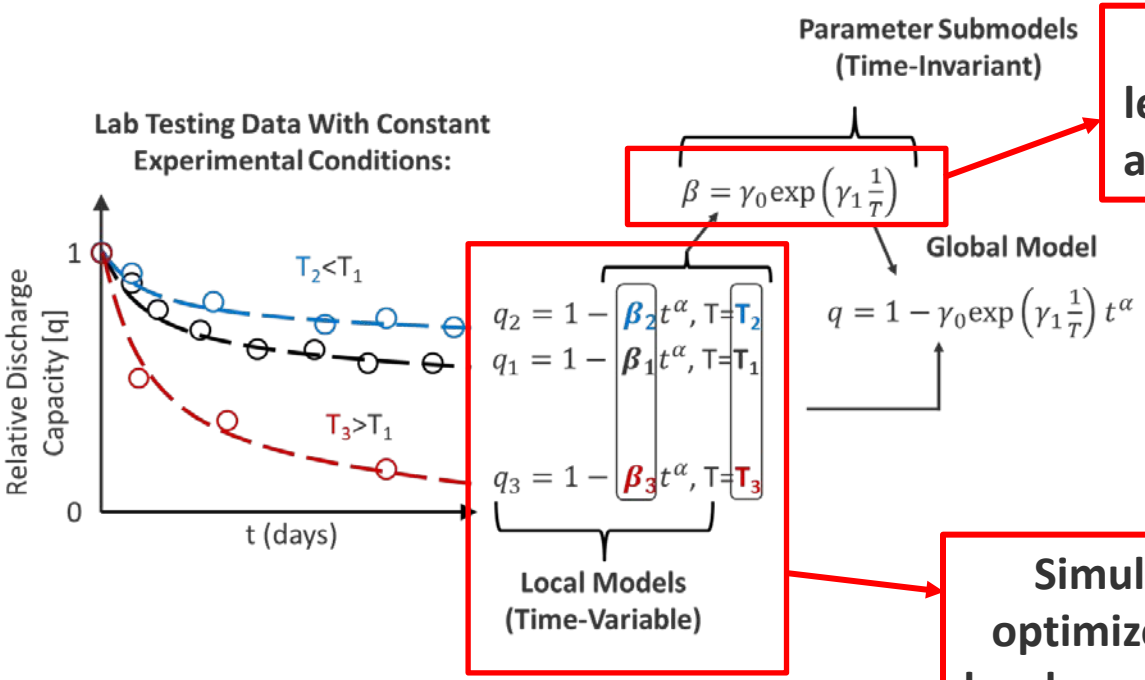
Local Models (Time-Variable)

Reduced-Order Model Identification Problem Statement



Use machine learning (ML) to find accurate submodels.

For all steps, cross-validate, quantify uncertainty, and simulate extrapolations.

Simultaneously optimize global and local parameters using bilevel regression.

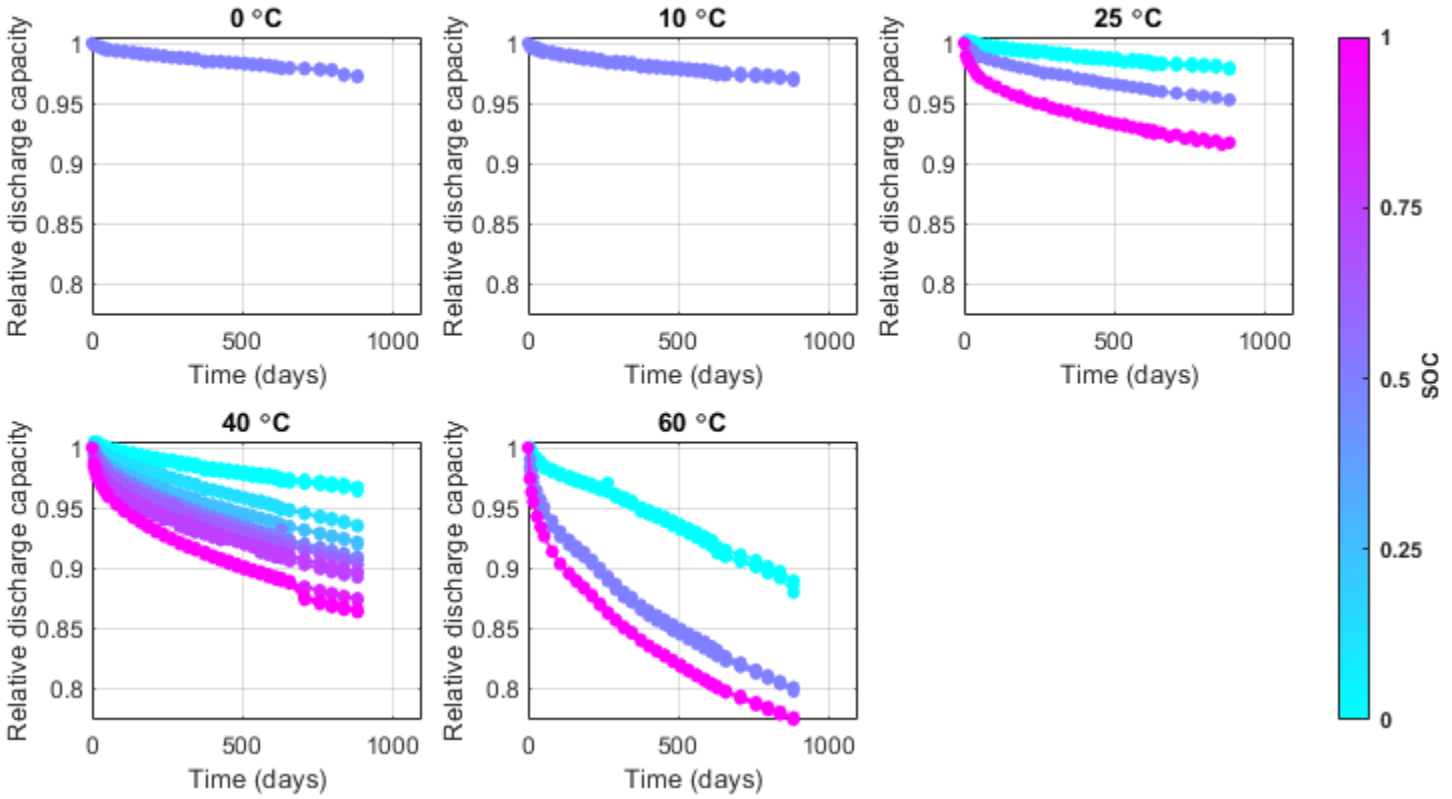
Dataset

Calendar Aging

Naumann, M., F. B. Spingler, A. Jossen. 2020. Analysis and modeling of cycle aging of a commercial $LiFePO_4$/graphite cell. *Journal of Power Sources* 451 (March) 227666. DOI:10.1016/j.jpowsour.2019.227666.

Naumann, M., M. Schimpe, P. Keil, H. C. Hesse, A. Jossen. 2018. Analysis and modeling of calendar aging of a commercial $LiFePO_4$/graphite cell. *Journal of Energy Storage* 17 (June) 153–169. DOI:10.1016/j.est.2018.01.019.

Calendar Aging



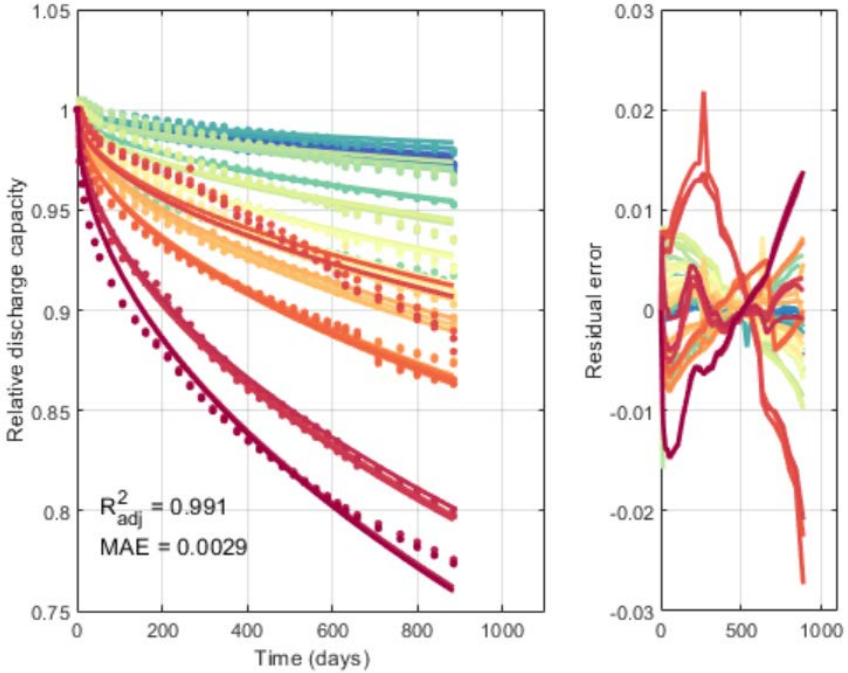
Manual Model Identification

Calendar Capacity Fade

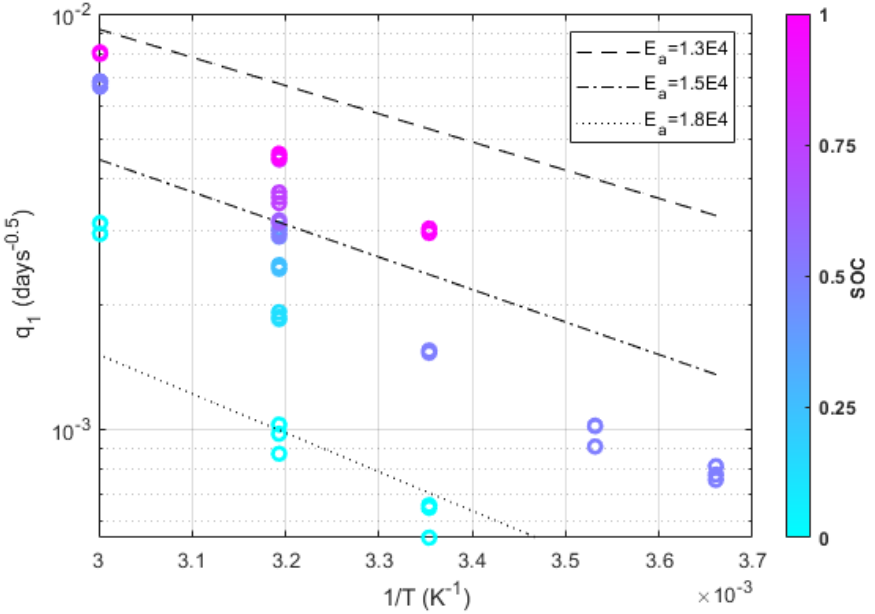
Optimizing a Square Root of Time Model

Local Optimization

$$q = 1 - q_1 \times t^{0.5}$$



Fitted q_1 Values

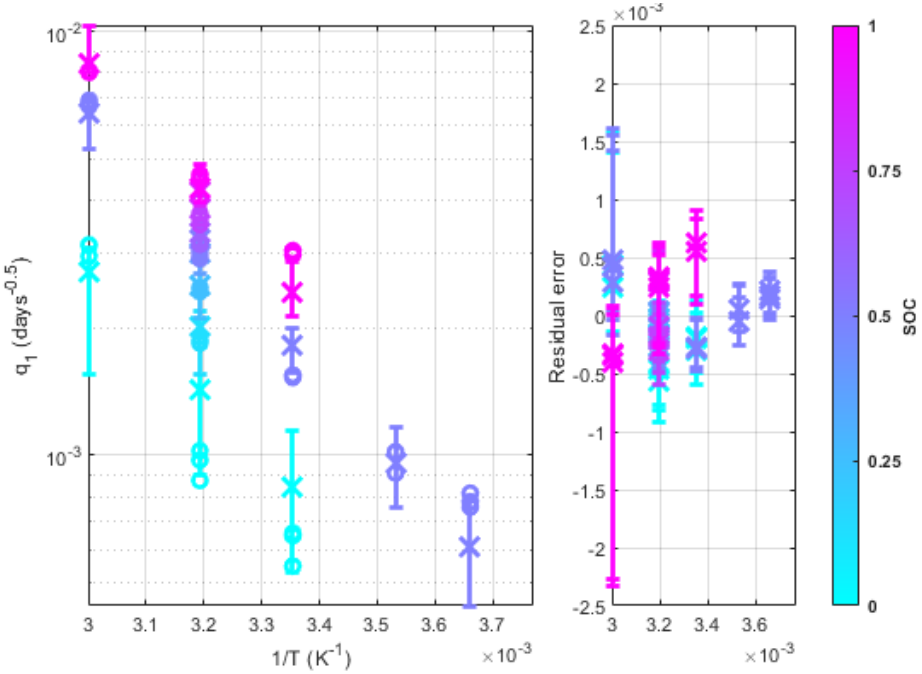


Optimizing a Submodel and Global Model

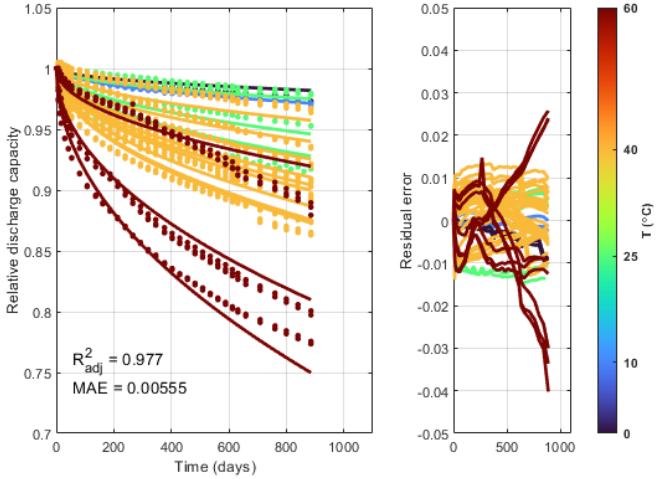
q_1 Submodel

$$q_1 = q_{1,ref} \times \exp(-(E_a/R) \times (\frac{1}{T} - \frac{1}{T_{ref}}) \dots$$

$$\dots \exp((\alpha \frac{F}{R}) \times (\frac{U_a}{T} - \frac{U_{a,ref}}{T_{ref}}))$$

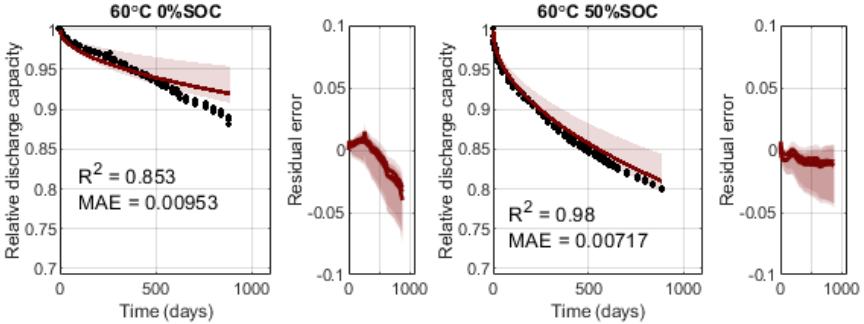


Global



Mean Absolute Error (MAE)= 0.56%

Cross-validation error (MAE_{CV})= 0.84%



Improving the Time-Dependent Model Equation

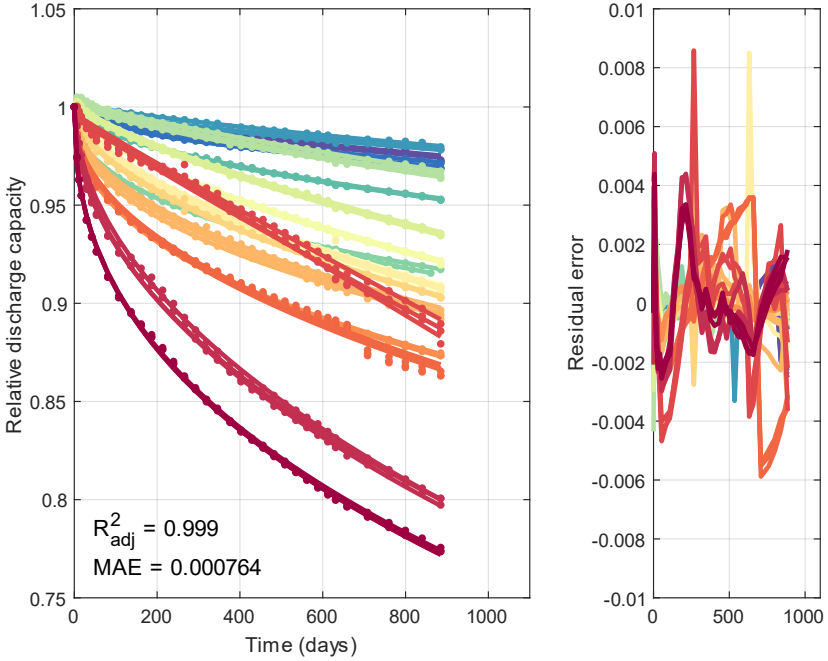
Calendar Capacity Fade

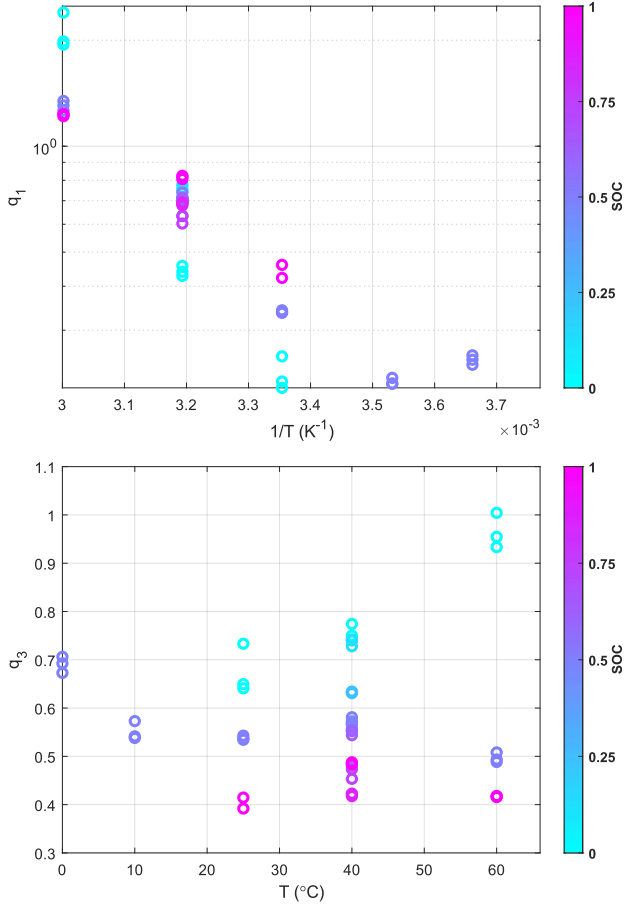
Finding a More Optimal Model Structure

Bilevel Optimization

$$q = 1 - 2 \times q_1 \times \left(\frac{1}{2} - \frac{1}{1 + \exp((q_2 t)^{q^3})}\right)$$

$Global: q_2, \quad Local: q_1, q_3$





Identifying Submodels Through Symbolic Regression

Machine-Learning Approach – Symbolic Regression

1. Input the features.

A: **T**
B: **SOC**

2. Apply the operators to generate new features.

A: {**T**, **T**^{2}}
B: {**SOC**, **SOC**^{2}}

A: {**T**, **T**^{2}}
B: {**SOC**, **SOC**^{2}}
C: {**SOC/T**^{2},…}

Feature matrix is very wide with many highly correlated features.

3. Search for the subset of features that model the data.

$$Y = \beta_0 + \beta_1 \mathbf{SOC} + \beta_2 \mathbf{SOC/T^2} + \cdots$$

This search has combinatorial complexity:
(1,000 choose 5) = $\mathbf{8 \times 10^{12}}$.

Linear:

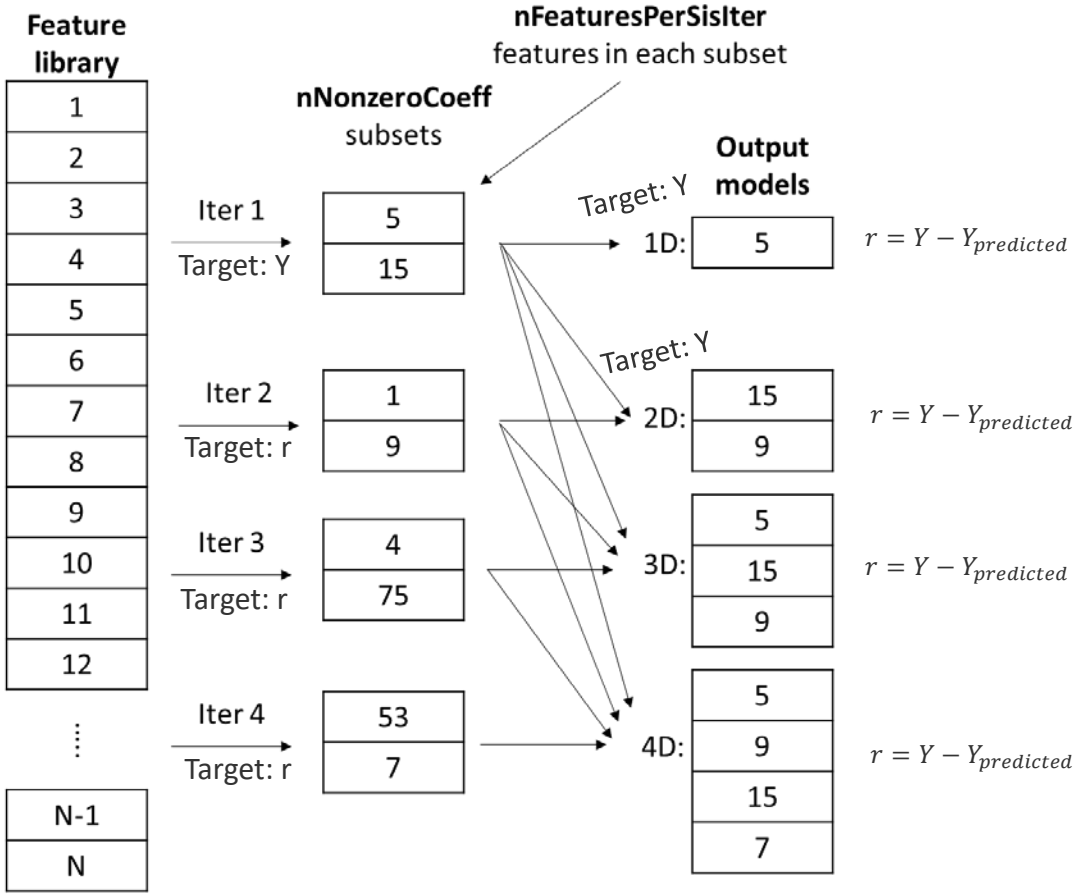
$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 \ldots$$

Multiplicative:

$$\exp(\log(Y)) = exp(\beta_0 + \beta_1 X_1 + \beta_2 \log(X_2) \ldots)$$

$$Y = exp(\beta_0) exp(\beta_1 X_1) \cdot X_2^{\beta_2} \ldots$$

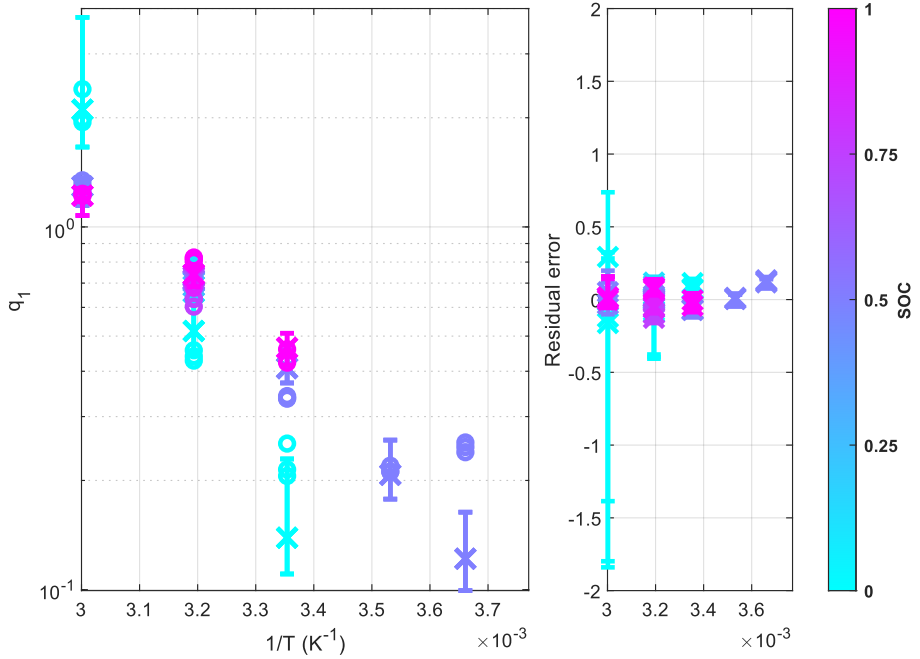
Feature Selection Algorithm: Sure Independence Screening and Sparsifying Operator

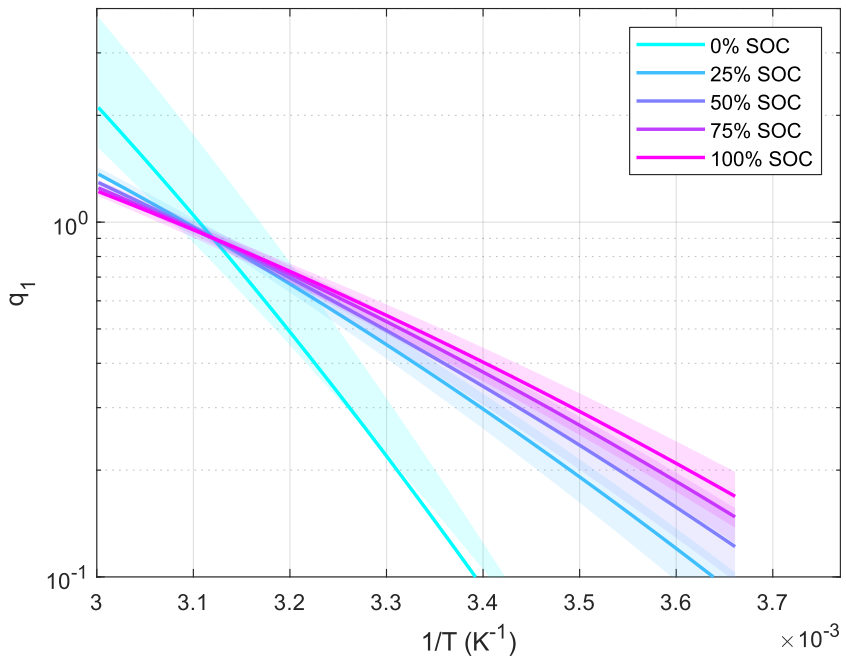


Sure Independence Screening and Sparsifying Operator: Ouyang, R., S. Curtarolo, E. Ahmetcik, M. Scheffler, and L. M. Ghiringhelli. 2018. SISSO: A compressed-sensing method for identifying the best low-dimensional descriptor in an immensity of offered candidates. *Physical Review Materials* **2** (7) 083802. https://doi.org/10.1103/PhysRevMaterials.2.083802.

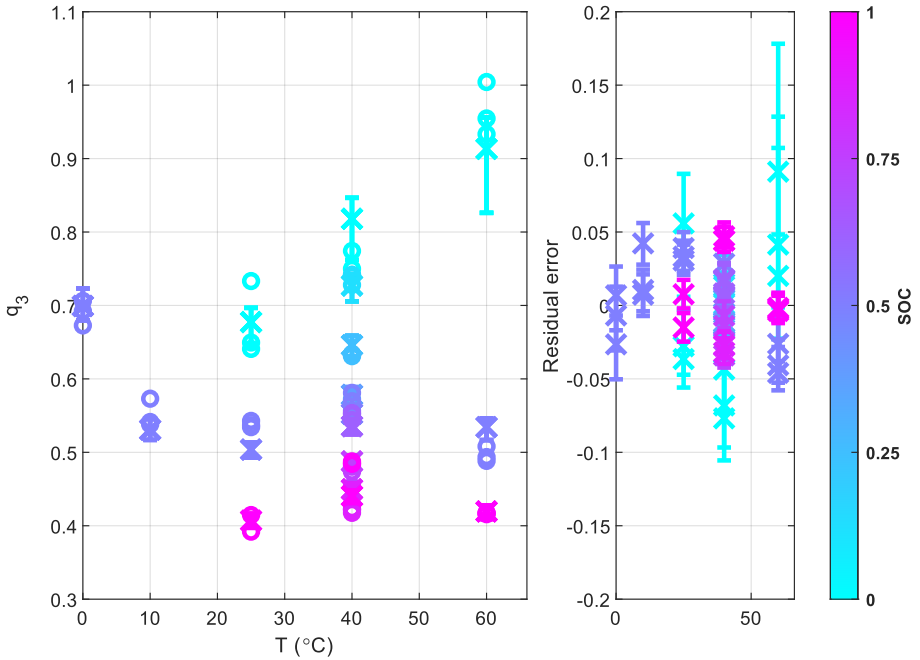
Fortran, MATLAB, Python [1, sklearn: 2]

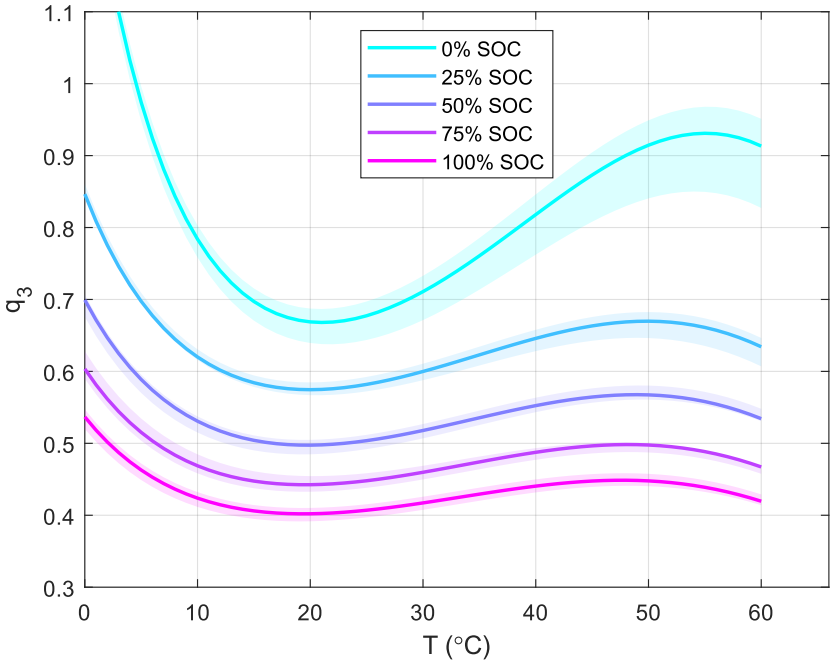
q_1 Submodel Identification



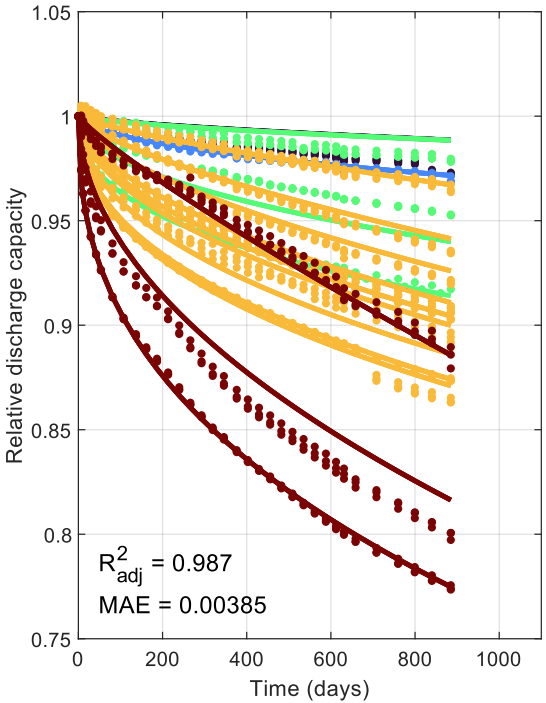


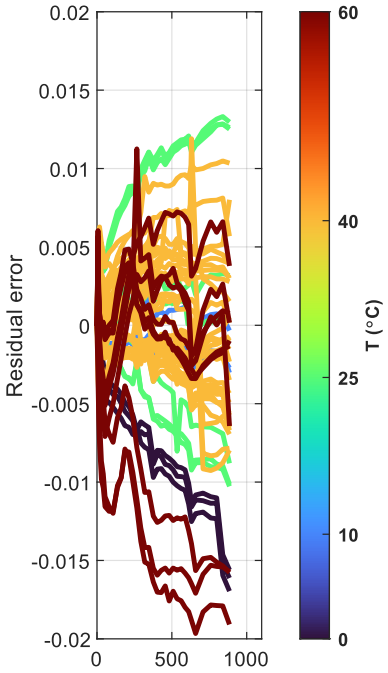
q_3 Submodel Identification





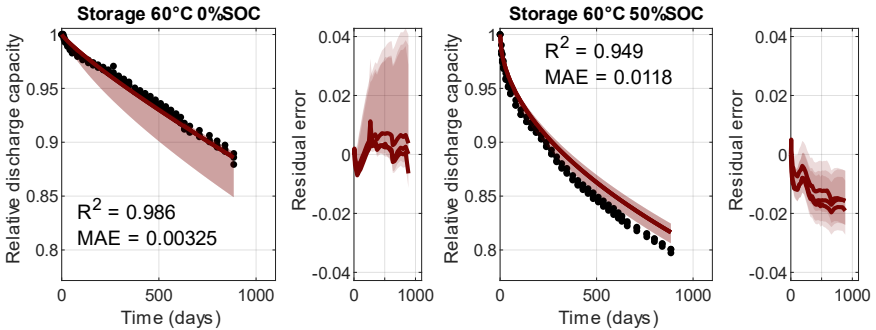
Global Model





Standard Approach:
MAE=0.56%
MAE_{CV}=0.84%

ML-Assisted:
MAE=0.39%
MAE_{CV}=0.51%



Dataset

Cycle Aging

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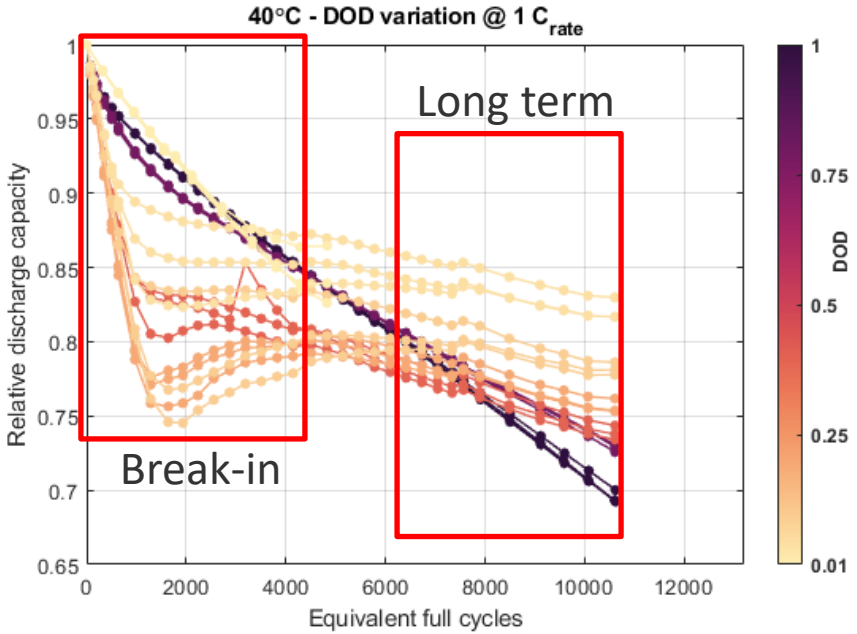
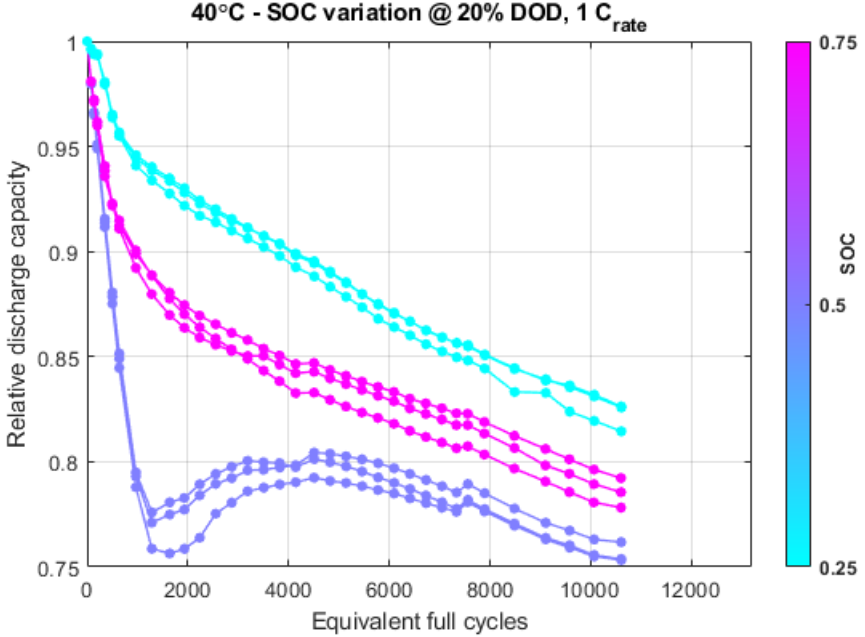
Cycling Aging





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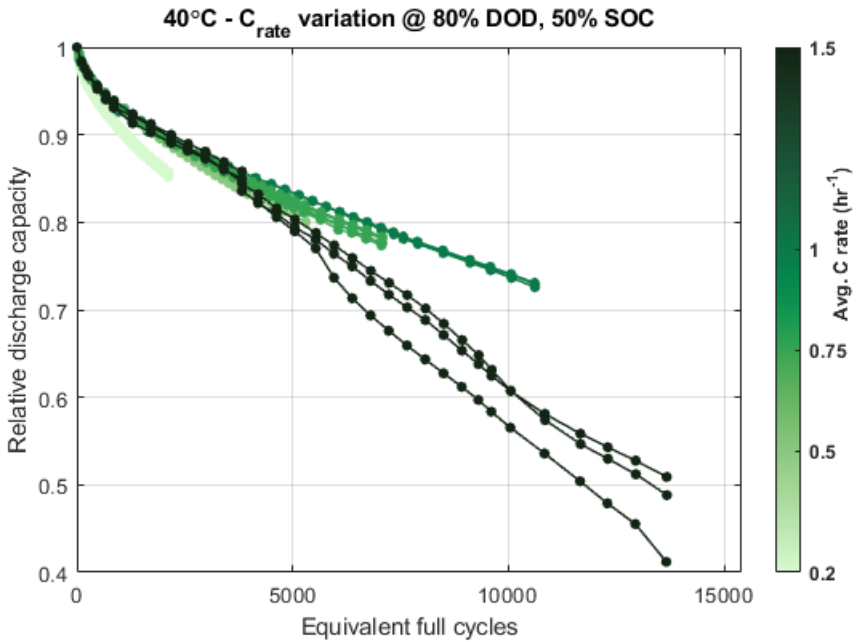
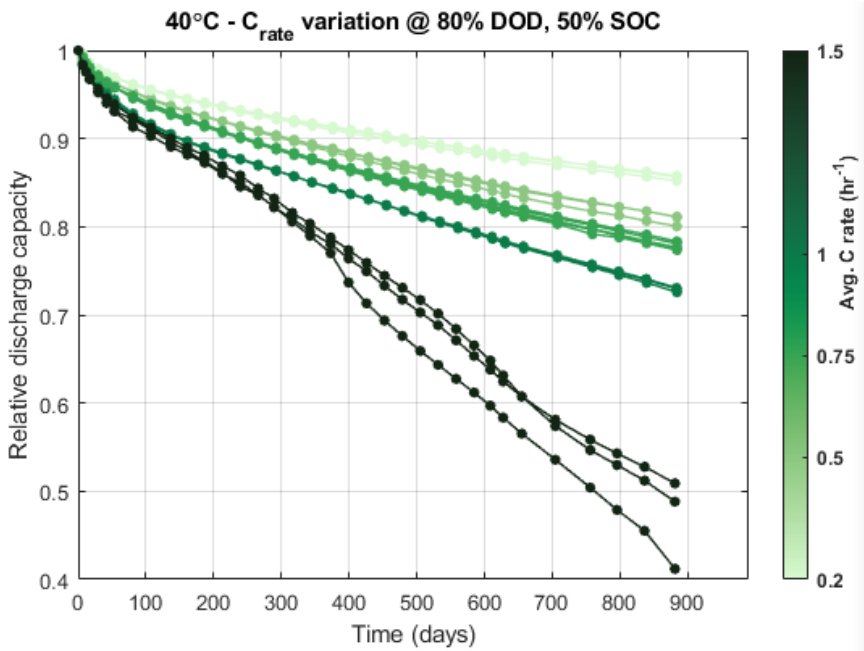
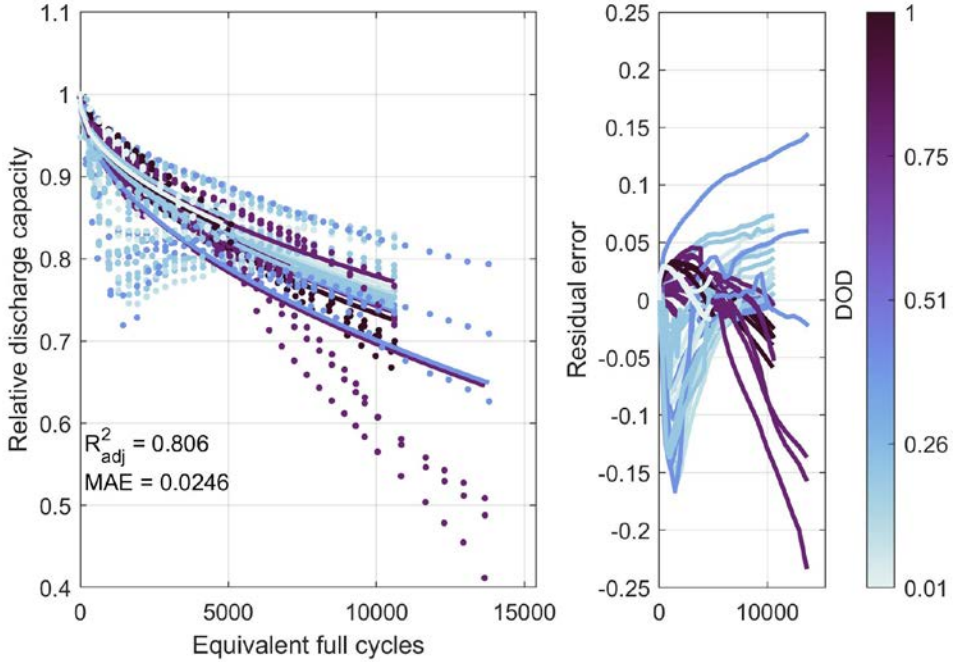


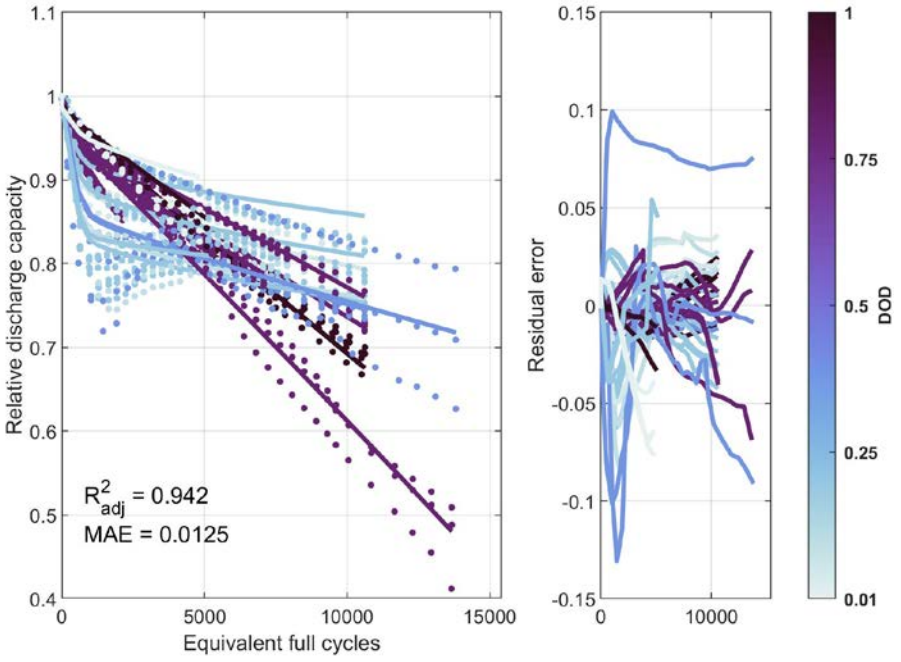


Prior Work vs. ML-Assisted

Prior Work:



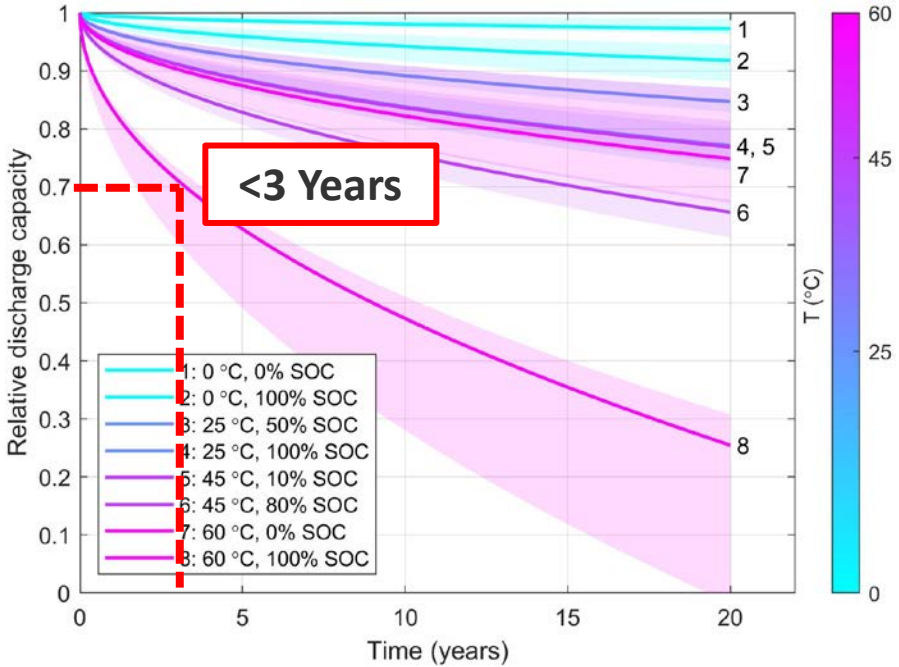
ML-Assisted:



Impact on Simulation

Calendar Aging (20 years)

Standard Approach:



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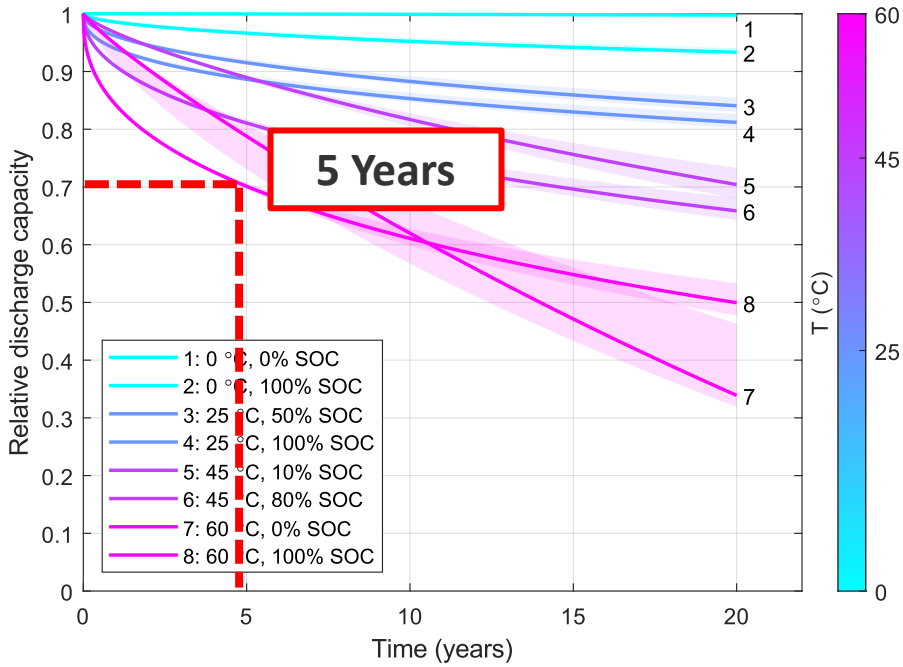
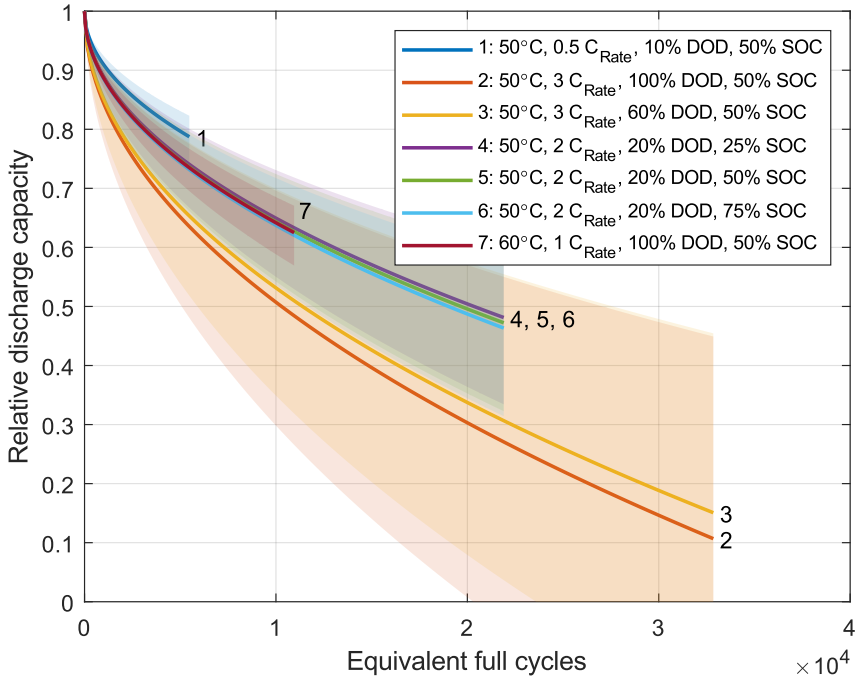
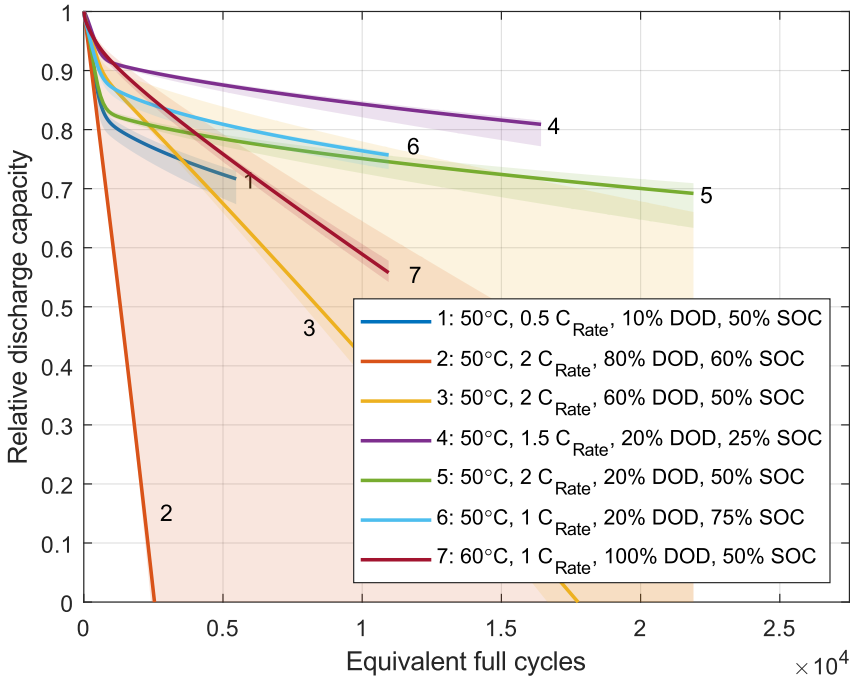


Cycling Aging (3 years)

Standard Approach:



ML-Assisted:



Takeaways

Takeaways

- Accurate models can help inform experimental design and help users make better control decisions or predict technoeconomic impact.
- Do not trust any model, unless…
  - You understand how it relates to its training data (e.g., any systematic errors, impact of test design/setup)
  - Model extrapolations and interpolations “make sense.”
- ML can help identify accurate models, but it does not replace being careful.

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NREL/PR-5700-80158

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Transforming ENERGY

Extra Slides

Current State-of-Health Prediction

Problem Statement:

What is the current state of health (SOH) of my battery?

Input Data:

This includes, basically, any cell measurement (e.g., current-voltage-temperature-time (I-V-T-t data) [charge/discharge, voltage relaxation, random pulses], electrochemical impedance spectroscopy [EIS], ultrasound, pressure).

Assumptions:

You do not have the time/capability to simply measure the SOH metric you care about.

Applications:

This includes real-world SOH detection.

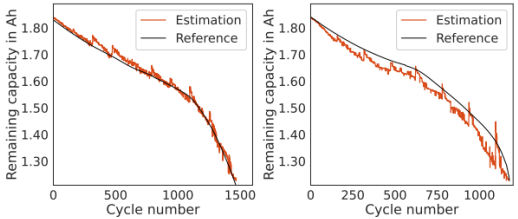
Current State-of-Health Prediction

Examples:

Using Partial Charge Curves:

Online capacity estimation of lithium-ion batteries with deep long short-term memory networks

Weihan Li [a,b,*], Neil Sengupta [a,b], Philipp Dechent [a,b], David Howey [c,f], Anuradha Annaswamy [g], Dirk Uwe Sauer [a,b,c,d]



On the feature selection for battery state of health estimation based on charging–discharging profiles

Yuanyuan Li [a], Daniel-Ioan Stroe [b,*], Yuhua Cheng [a,*], Hanmin Sheng [a], Xin Sui [b], Remus Teodorescu [b]

Deep Gaussian process regression for lithium-ion battery health prognosis and degradation mode diagnosis

Piyush Tagade [a], Krishnan S. Hariharan [a,*], Sanoop Ramachandran [a], Ashish Khandelwal [a], Arunava Naha [a], Subramanya Mayya Kolake [a], Seong Ho Han [b]

Machine learning pipeline for battery state-of-health estimation

Darius Roman, Saurabh Saxena, Valentin Robu, Michael Pecht & David Flynn

Using EIS:

https://doi.org/10.1038/s41467-020-15235-7 OPEN

Identifying degradation patterns of lithium ion batteries from impedance spectroscopy using machine learning

Yunwei Zhang [1,2,6], Qiaochu Tang [2,3,4,6], Yao Zhang [5], Jiabin Wang [2,3,4], Ulrich Stimming [2,3,4,7] & Alpha A. Lee [1,2,7]

Development of a battery real-time state of health diagnosis based on fast impedance measurements

Edoardo Locorotondo [a,*], Vincenzo Cultrera [a], Luca Pugi [a], Lorenzo Berzi [a], Marco Pierini [a], Giovanni Lutzemberger [b]

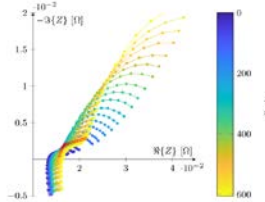


Fig. 2. Nyquist plot of the impedance spectra obtained during cyclic aging ($SoC = 100\%$, $T = 30$ °C).

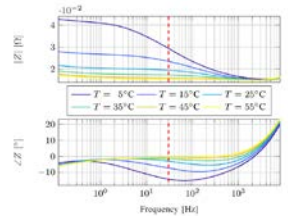


Fig. 3. Bode plot of impedance spectra at different temperatures ($SoH = 100\%$, $SoC = 90\%$).

Sensitivity Analysis of Battery Cell Aging Estimators based on Impedance Spectroscopy regarding Temperature Compensation

Bernhard Liebhart[1], Simon Diehl[1] and Christian Endisch[1]

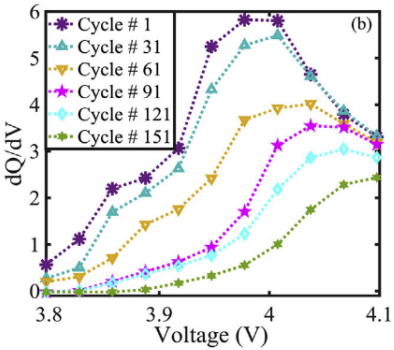
Using $dQdV$:

A quick on-line state of health estimation method for Li-ion battery with incremental capacity curves processed by Gaussian filter

Yi Li [a,b,*], Mohamed Abdel-Monem [a,c], Rahul Gopalakrishnan [a], Maitane Berecibar [a], Elise Nanini-Maury [b], Noshin Omar [a], Peter van den Bossche [a], Joeri Van Mierlo [a]

Prognostic health condition for lithium battery using the partial incremental capacity and Gaussian process regression

Xiaoyu Li [a,b], Zhenpo Wang [a,b,*], Jinying Yan [c]



Remaining Useful-Life Prediction

Problem Statement:

How long will it be until my battery reaches the end of its life?
This is closely related to classifying good/bad cells.

Input Data:

This includes, basically, any cell measurement (e.g., I-V-T-t data [charge/discharge, voltage relaxation, random pulses], EIS, ultrasound, pressure).

Assumptions:

We continue to use the battery in the same manner as it has been historically used (or in the same way that the model was trained on).

Applications:

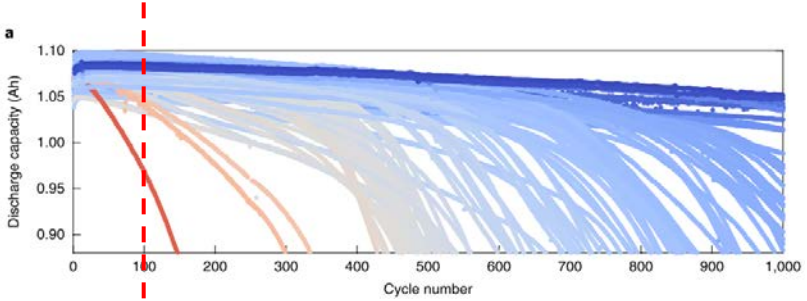
This includes optimization of battery use, classification of bad cells, anticipation of battery replacement.

Remaining Useful-Life Prediction

Examples:

nature energy
ARTICLES
https://doi.org/10.1038/s41560-019-0356-8

Data-driven prediction of battery cycle life before capacity degradation



First 5%–30% of lifetime required (mean=20%).

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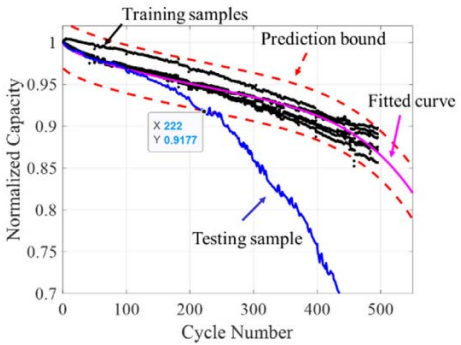
Early detection of anomalous degradation behavior in lithium-ion batteries



First 5%–30% of lifetime required (this is a classifier).

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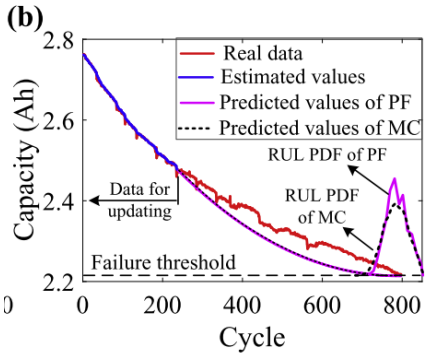
Validation and verification of a hybrid method for remaining useful life prediction of lithium-ion batteries



First 30% of lifetime required (regardless of actual cell lifetime).

Lifetime Simulation Models

Examples:

Algebraic:

Challenging Practices of Algebraic Battery Life Models through Statistical Validation and Model Identification via Machine-Learning

Paul Gasper,[1,z] Kevin Gering,[2] Eric Dufek,[2] and Kandler Smith[1]

Life Prediction Model for Grid-Connected Li-ion Battery Energy Storage System

Kandler Smith, Aron Saxon, Matthew Keyser, Blake Lundstrom, Ziwei Cao, Albert Roc

Comprehensive Modeling of Temperature-Dependent Degradation Mechanisms in Lithium Iron Phosphate Batteries

M. Schimpe,[1,*,z] M. E. von Kuepach,[1] M. Naumann,[1] H. C. Hesse,[1] K. Smith,[2,**] and A. Jossen[1]

Analysis and modeling of calendar aging of a commercial $LiFePO_4$/graphite cell

Maik Naumann*, Michael Schimpe, Peter Keil, Holger C. Hesse, Andreas Jossen

Analysis and modeling of cycle aging of a commercial LiFePO4/ graphite cell

Maik Naumann *, Franz B. Spingler, Andreas Jossen

Single Particle:

Unlocking Extra Value from Grid Batteries Using Advanced Models

Jorn M. Reniers[1,2,3], Grietus Mulder[2,3], David A. Howey[1,4*]

Improving optimal control of grid-connected lithium-ion batteries through more accurate battery and degradation modelling

Jorn M. Reniers[a,b,c], Grietus Mulder[b,c], Sina Ober-Blöbaum[a], David A. Howey[a,*]

Capacity and power fade cycle-life model for plug-in hybrid electric vehicle lithium-ion battery cells containing blended spinel and layered-oxide positive electrodes

Andrea Cordoba-Arenas [a,*], Simona Onori [b,1], Yann Guezennec [a], Giorgio Rizzoni [a]

Realistic lifetime prediction approach for Li-ion batteries

E. Sarasketa-Zabala *, E. Martinez-Laserna, M. Berecibar, I. Gandiaga, L.M. Rodriguez-Martinez [1], I. Villarreal

A holistic aging model for $Li(NiMnCo)O_2$ based 18650 lithium-ion batteries

Johannes Schmalstieg [a,c,*], Stefan Käbitz [a,c], Madeleine Ecker [a,c], Dirk Uwe Sauer [a,b,c]