NREL
Transforming ENERGY

Battery Modeling Webinar Series

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]

Predictive battery lifetime modeling at NREL

Dr. Paul Gasper, Dr. Kandler Smith
Energy Conversion and Storage Systems Center
Electrochemical Energy Storage

June 1st, 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

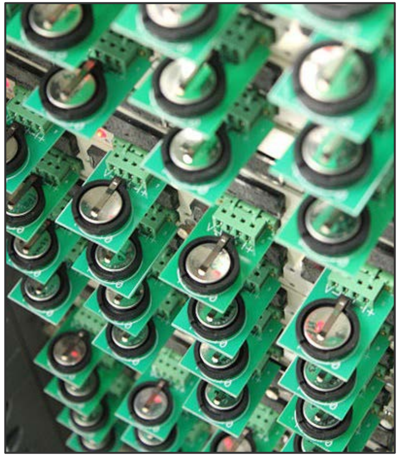
The challenge for battery lifetime prediction

Lab testing:

Pre-defined loads

Controlled environments

10-100 cells, 1-2 years



Real-world applications:

Complex, varying loads; varying environments

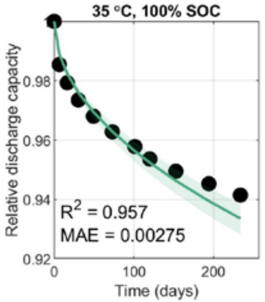
?? cells, 10-20+ years

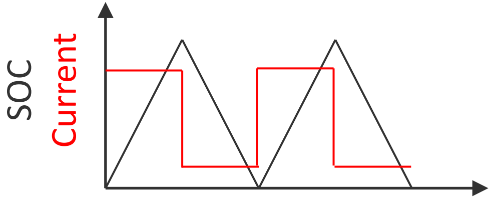
The challenge for battery lifetime prediction

Your data from the lab:

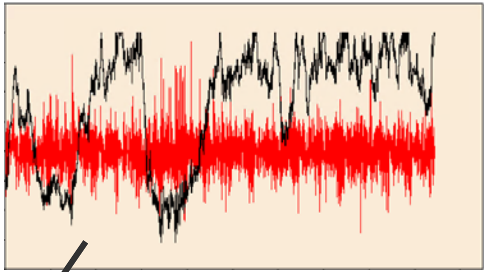
Cell	T (°C)	SOC	DOD	C-rate
1	30	75	0	0
2	30	50	100	1
3	45	75	50	0.5

SOH(t,EFC, …)





Real-world applications:

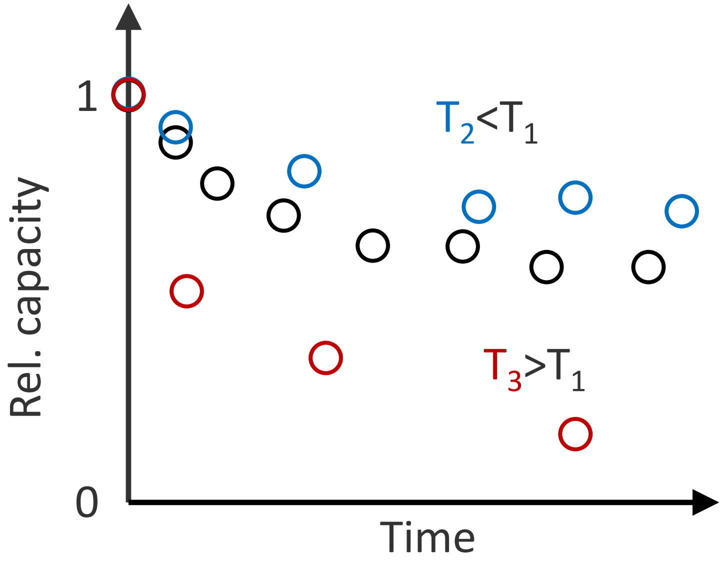


Voltage
Current

SOC(t) → Avg. SOC, DOD, C-rate, EFC → SOH(t,EFC, …)

Reduced order model identification
Problem statement

Lab testing data, with constant experimental conditions



What we are trying to find:

Degradation rate for any given battery use case / environmental conditions.

Challenges:

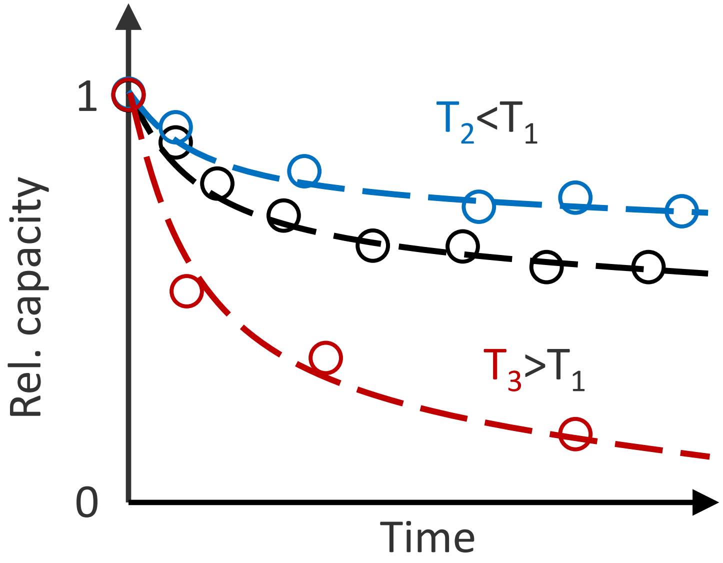
If q(t) is linear, then dq/dt is constant, and predicting changes to SOH is easy. But, both q(t)and dq/dt (t) can be non-linear, and dq/dt is also dependent on test conditions.

Common approach:

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

Reduced order model identification
Problem statement

Lab testing data, with constant experimental conditions



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

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

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

Local models (Time-varying)

Parameter sub-models (Time-invariant)

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

Global model

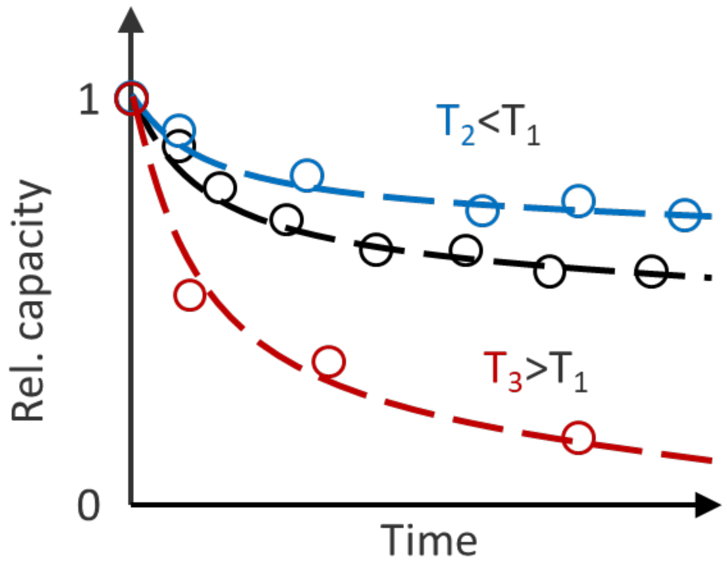
$$q = 1 - \gamma_0 \exp\left(\gamma_1 \frac{1}{T}\right) t^{\alpha}$$

Reduced order model identification
Problem statement

Parameter sub-models (Time-invariant)

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

Lab testing data, with constant experimental conditions



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

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

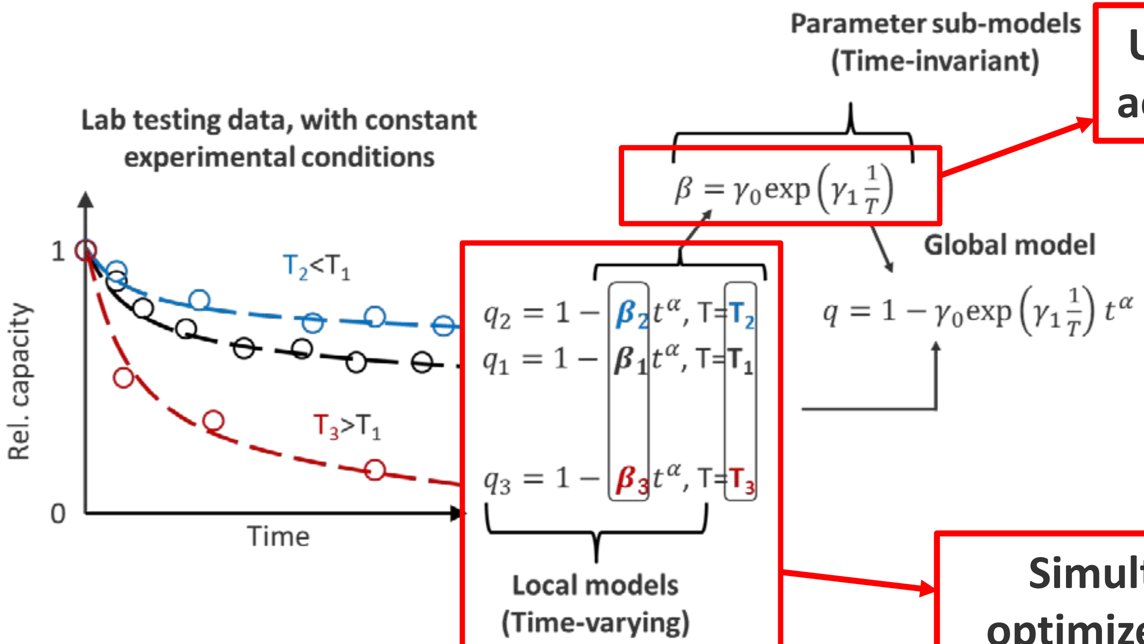
$$q_3 = 1 - \boldsymbol{\beta_3} t^{\alpha},\ \mathrm{T} = \mathbf{T_3}$$

Global model

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

Local models (Time-varying)

Reduced order model identification
Problem statement



Use ML to help find accurate sub-models

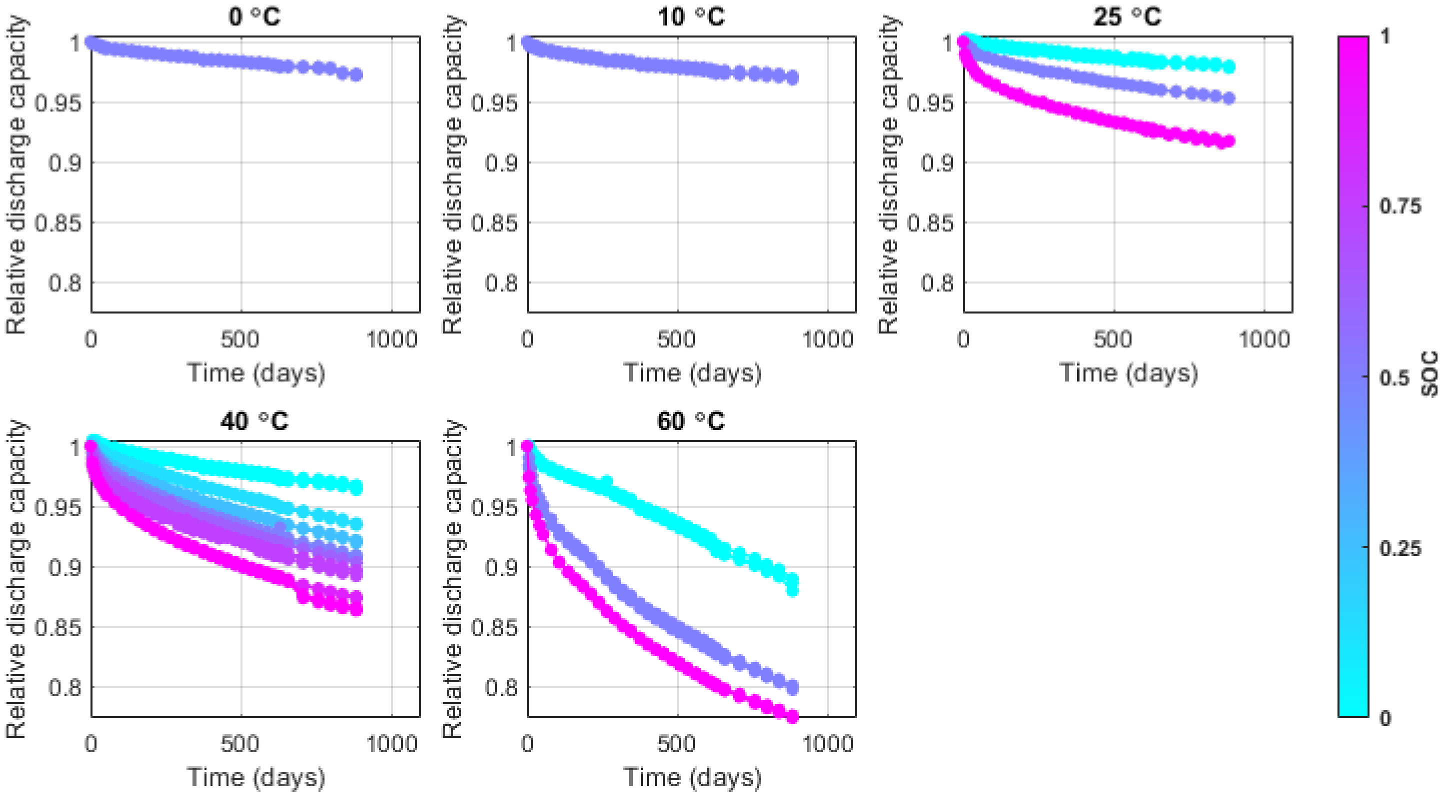
For all steps:
Cross-validate, quantify uncertainty, and simulate extrapolations

Simultaneously optimize global and local parameters using bilevel regression

Data set
Calendar aging

J. of Energy Storage **17** (2018) 153-169. DOI:10.1016/j.est.2018.01.019
J. of Power Sources **451** (2020) 227666. DOI:10.1016/j.jpowsour.2019.227666

Calendar aging



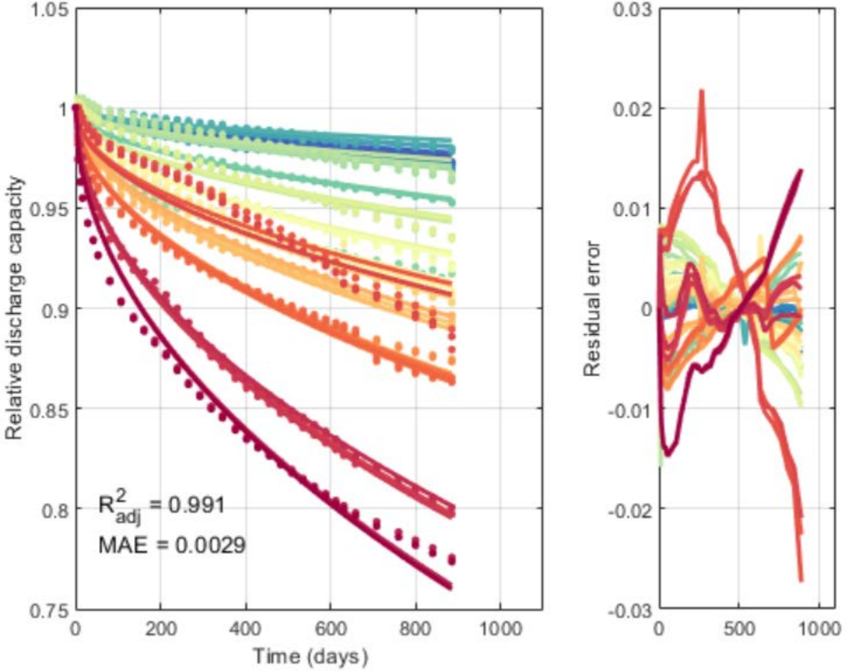
Manual model identification

Calendar capacity fade

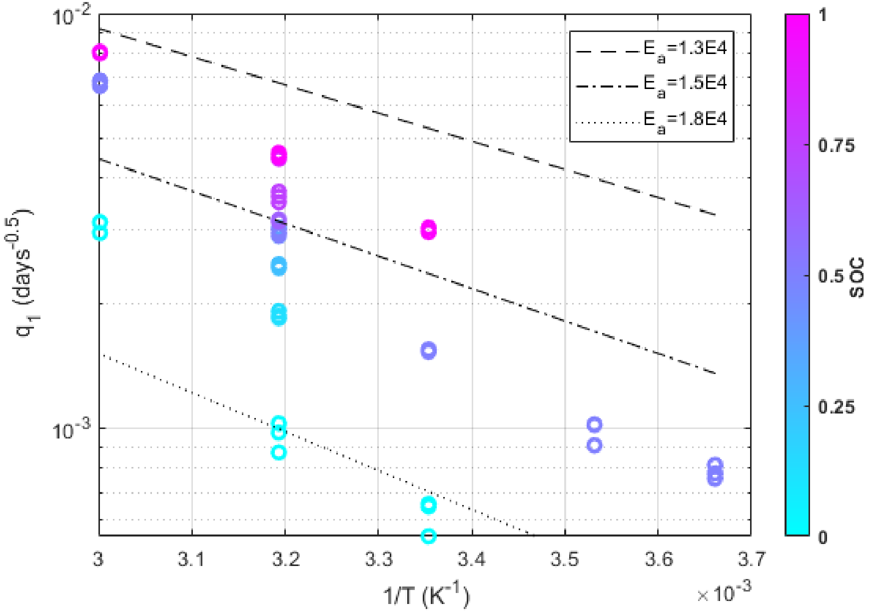
Optimizing a square-root of time model

Local optimization

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



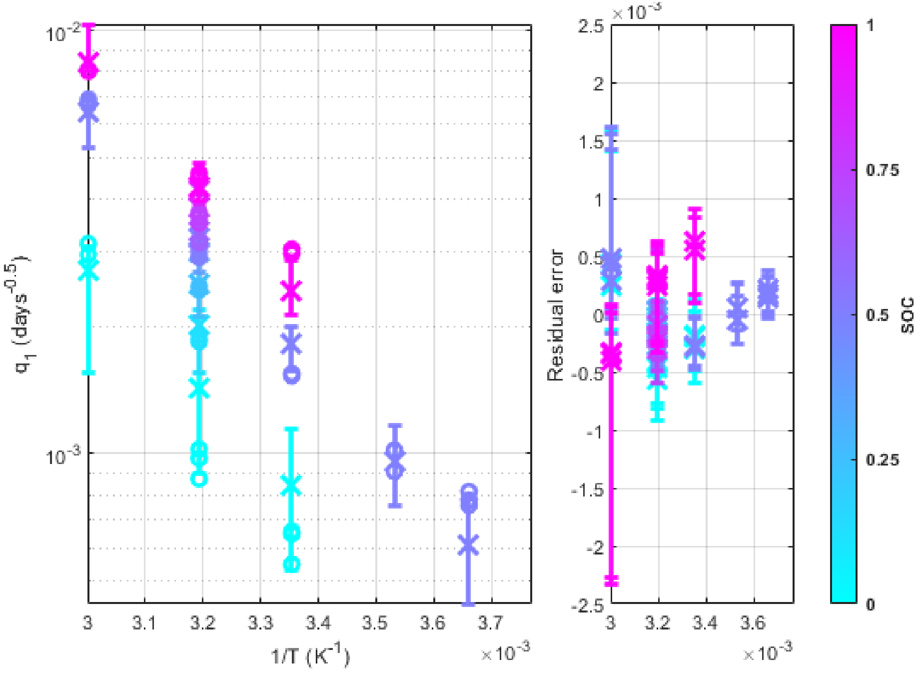
Fitted q_1 values



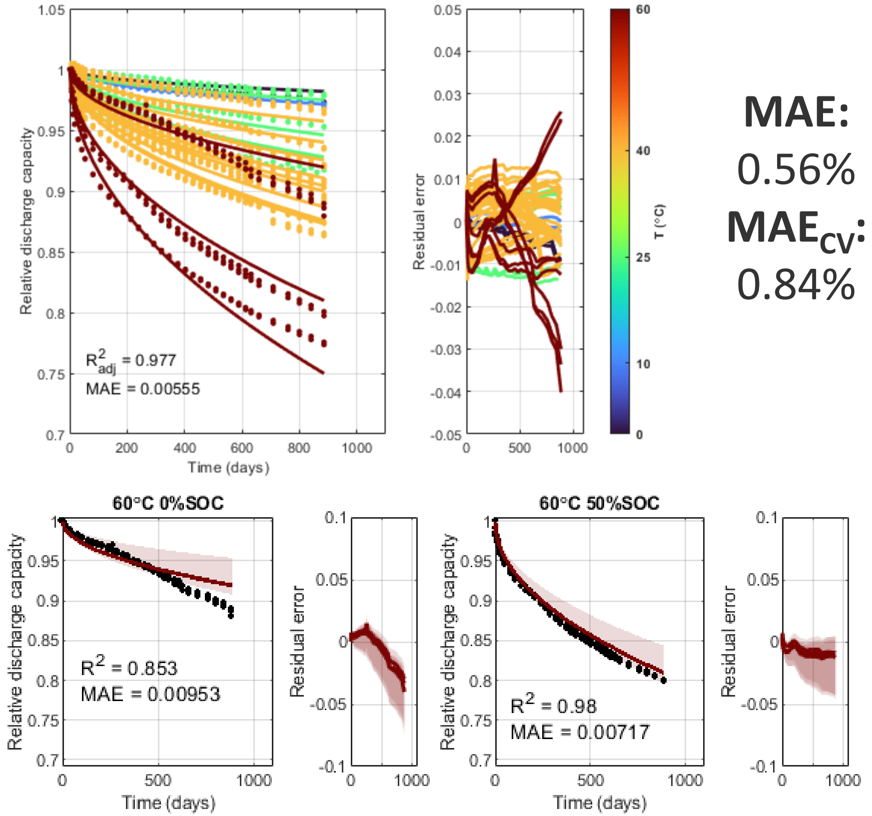
Optimizing a sub-model and global model

q_1 sub-model

$$q_1 = q_{1,ref} \cdot \exp(-(E_a/R) \cdot (1/T - 1/T_{ref})) \cdot \ldots$$
$$\ldots \exp((\alpha F/R) \cdot (U_a/T - U_{a,ref}/T_{ref}))$$



Global



MAE:
0.56%
MAE_{CV}:
0.84%

Improving the time-dependent model equation

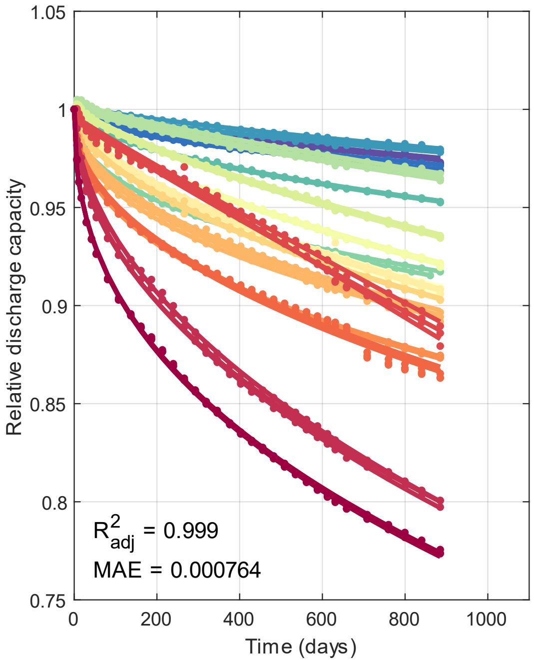
Calendar capacity fade

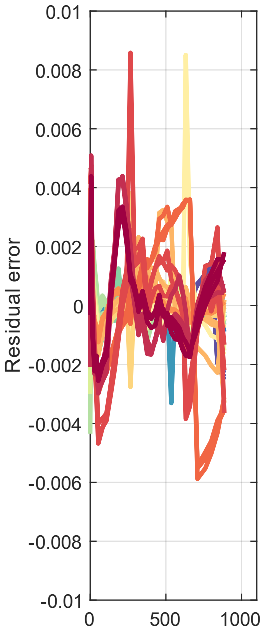
Finding a more optimal model structure

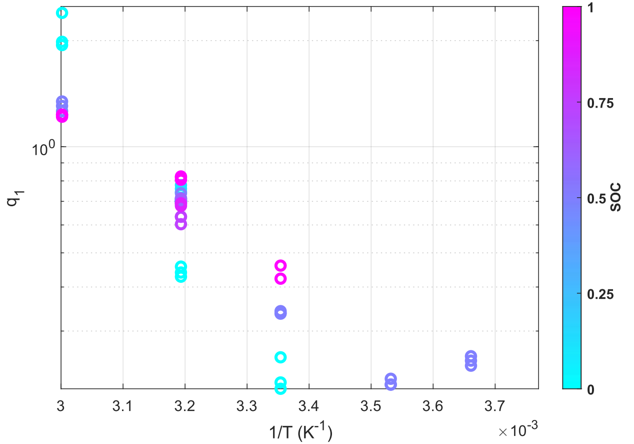
Bilevel optimization

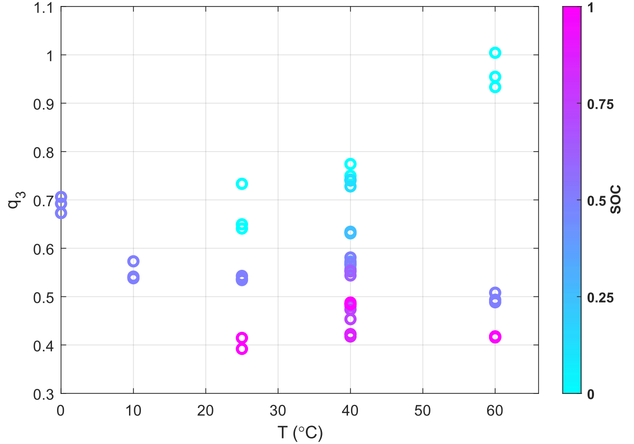
$$q = 1 - 2 \cdot q_1 \cdot (1/2 - 1/(1 + \exp((q_2 \cdot t)^{q_3})))$$

Global: q_2, Local: q_1, q_3









Identification of sub-models through symbolic regression

ML approach – Symbolic regression

1: Input features

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

2: Apply 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:
(1000 choose 5) = **8·10^{12}**

Linear

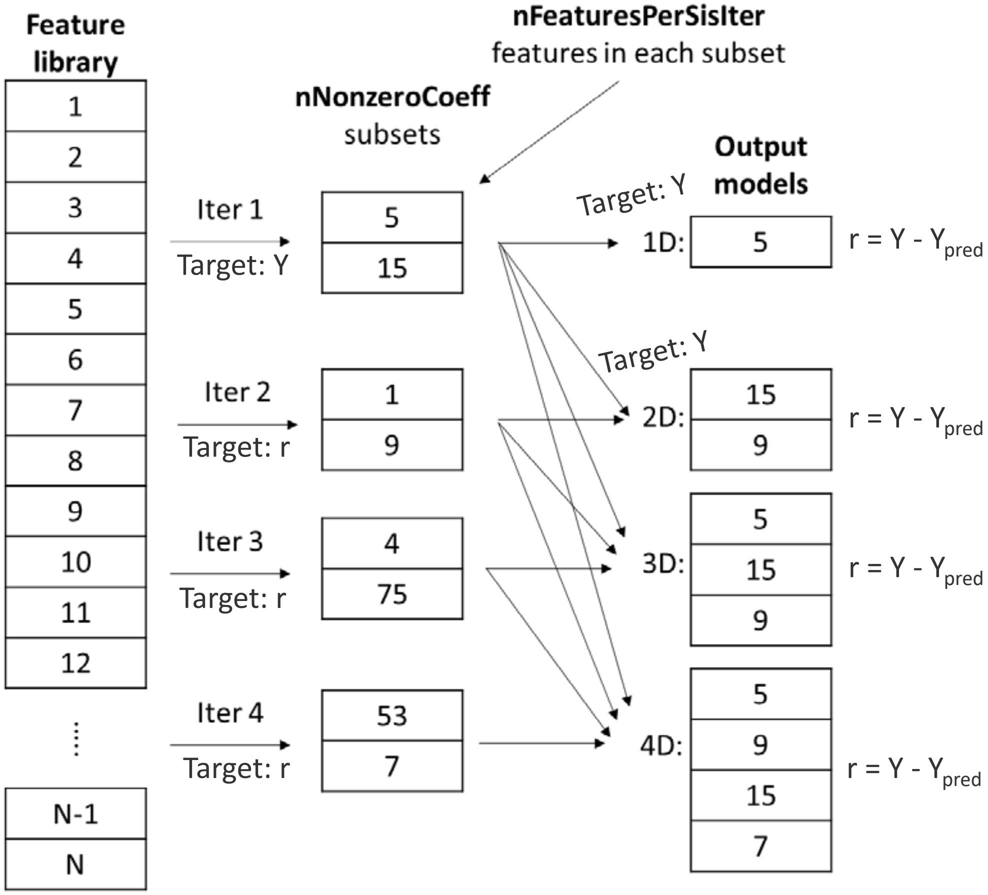
$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots$$

Multiplicative

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

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

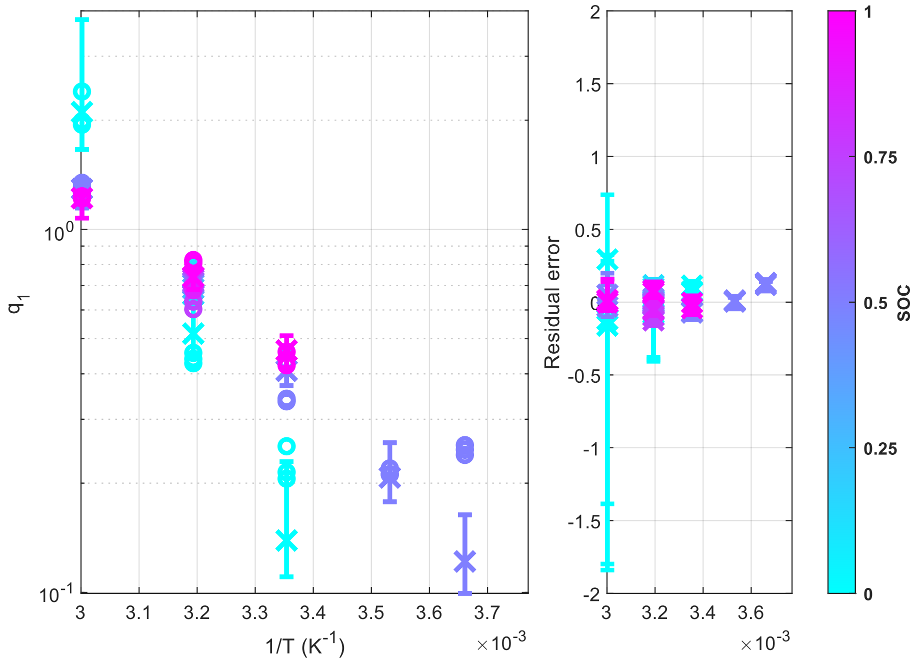
Feature selection algorithm: SISSO

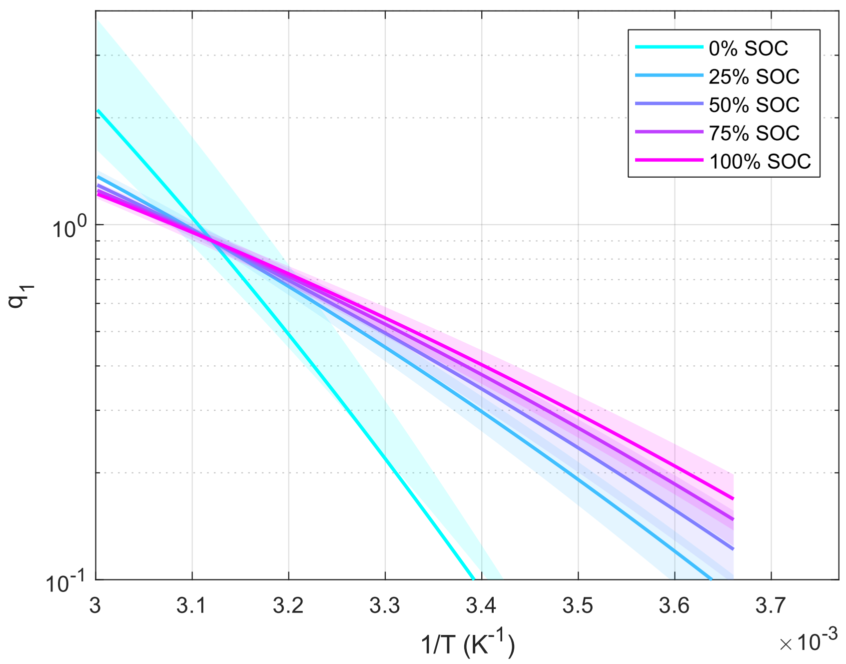


SISSO: Ouyang et. al.: https://doi.org/10.1103/PhysRevMaterials.2.083802

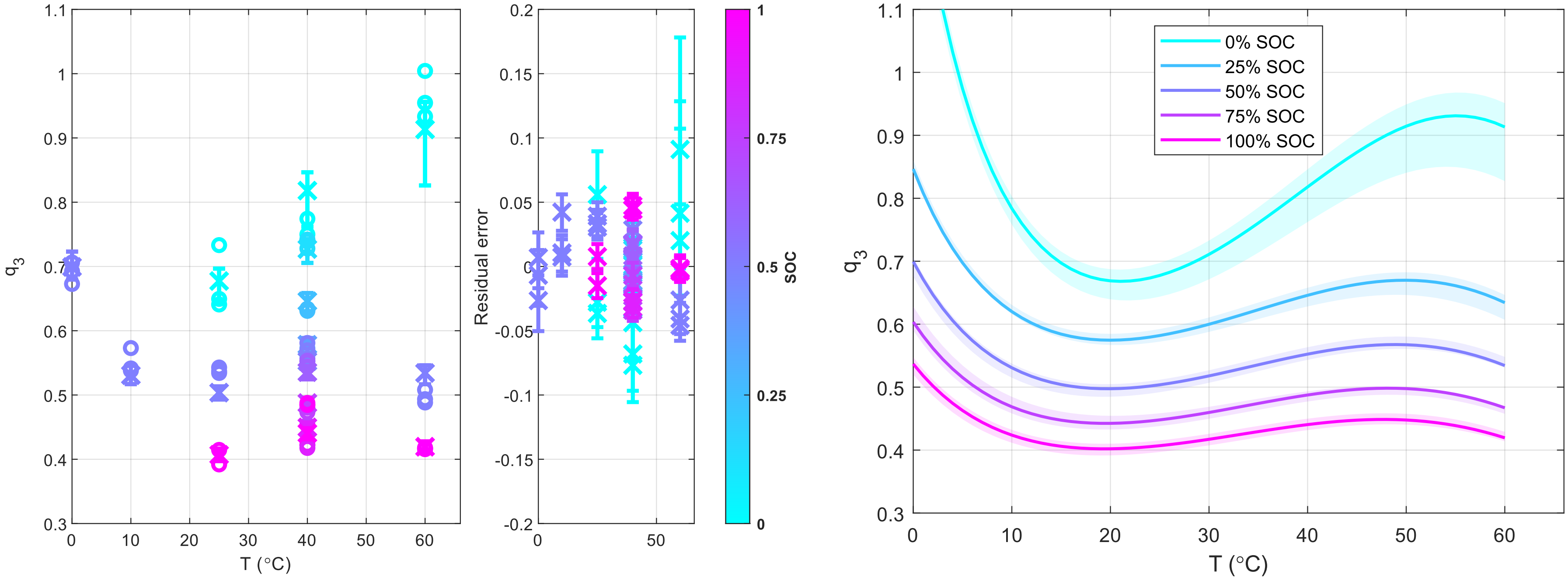
[Fortran](), [Matlab](), Python [[1](), sklearn: [2]()]

q_1 sub-model identification

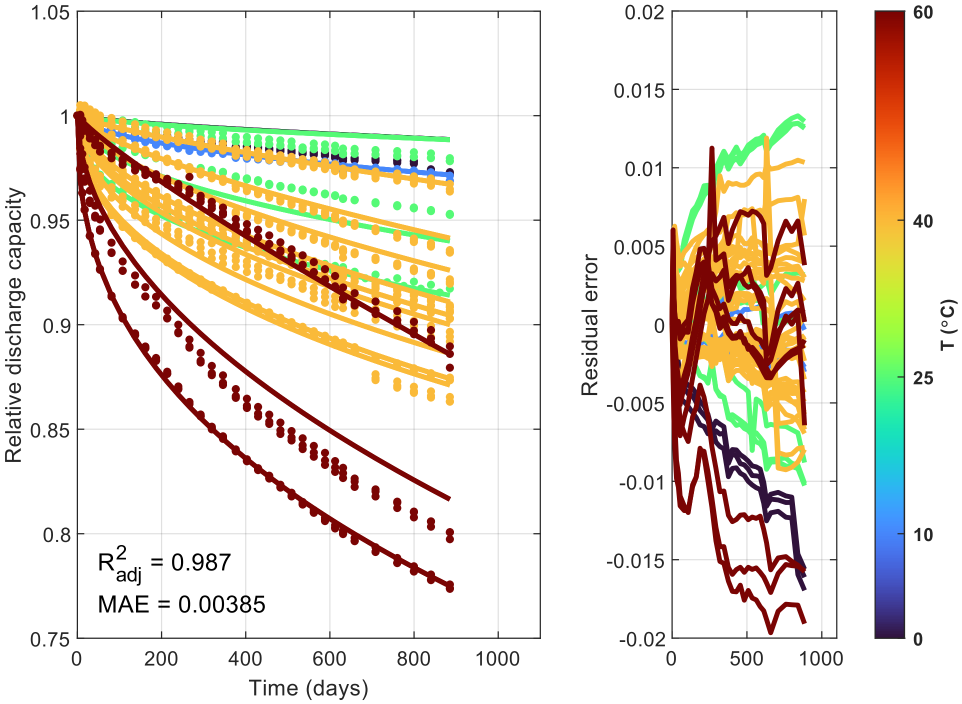




q_3 sub-model identification



Global model



Standard approach

MAE:

0.56%

MAE_{CV}:

0.84%

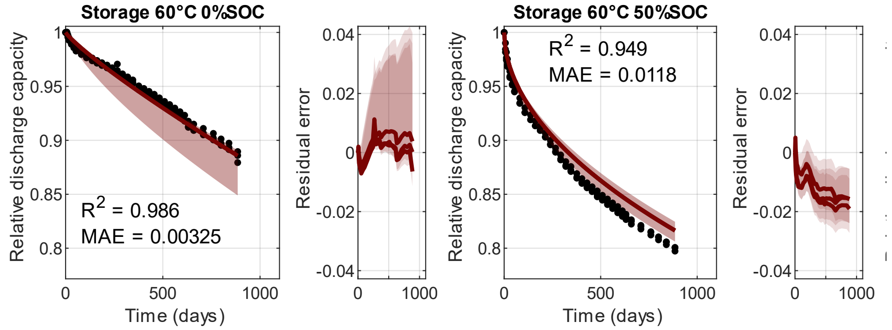
ML-assisted

MAE:

0.39%

MAE_{CV}:

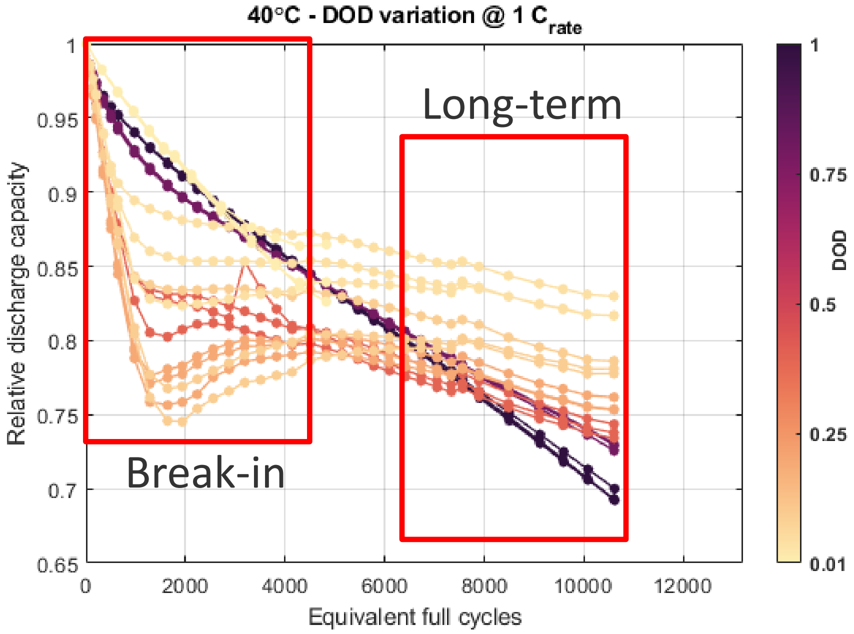
0.51%

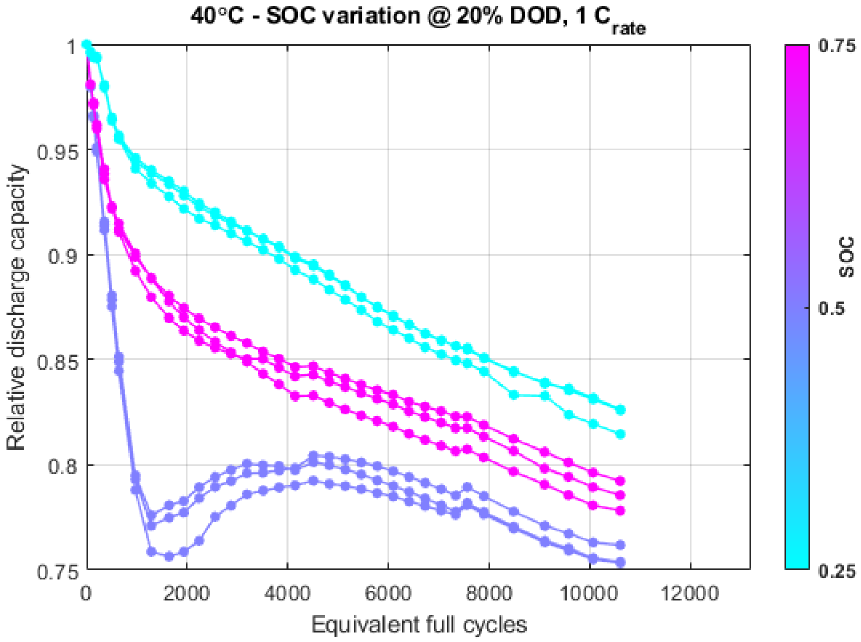


Data set
Cycle aging

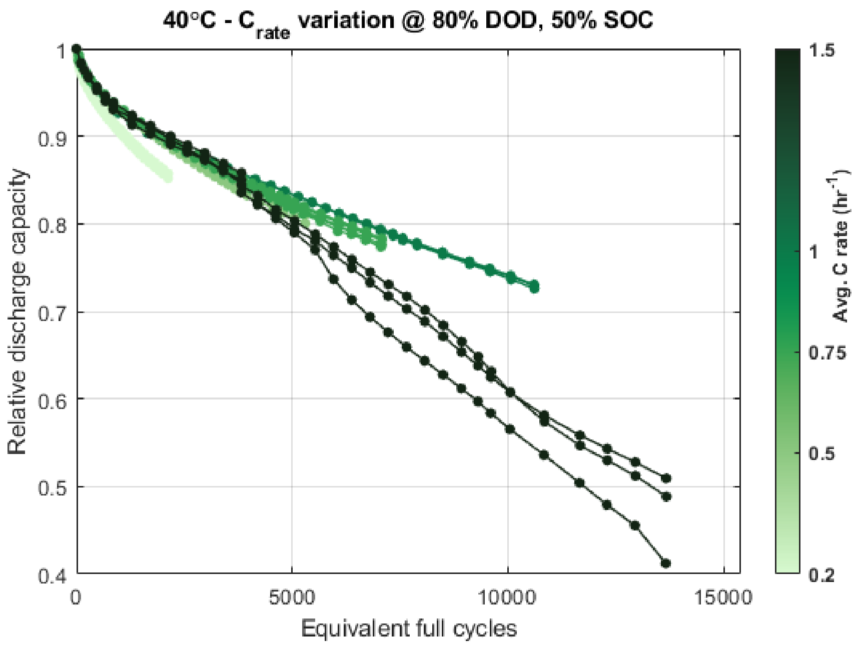
J. of Energy Storage **17** (2018) 153-169. DOI:10.1016/j.est.2018.01.019
J. of Power Sources **451** (2020) 227666. DOI:10.1016/j.jpowsour.2019.227666

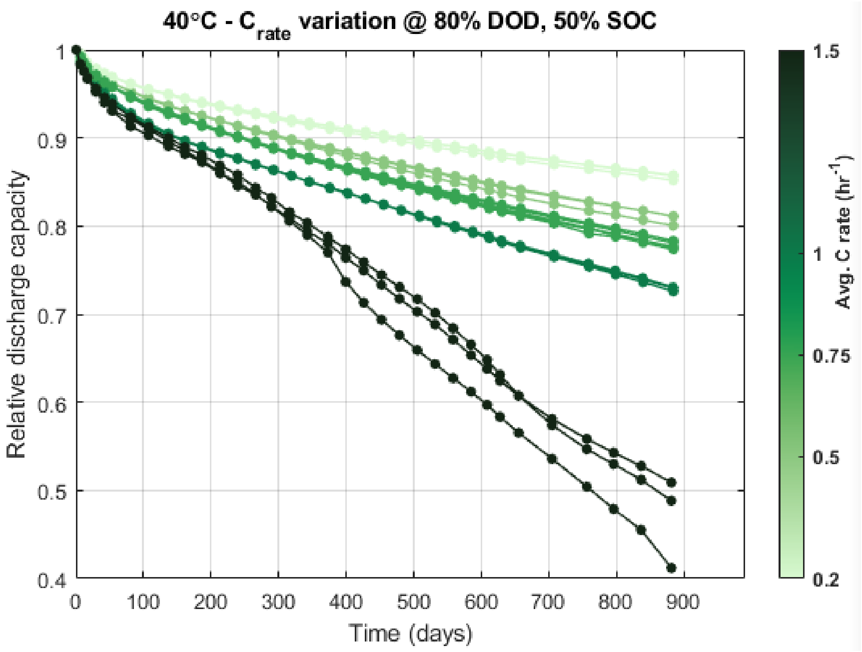
Cycling aging





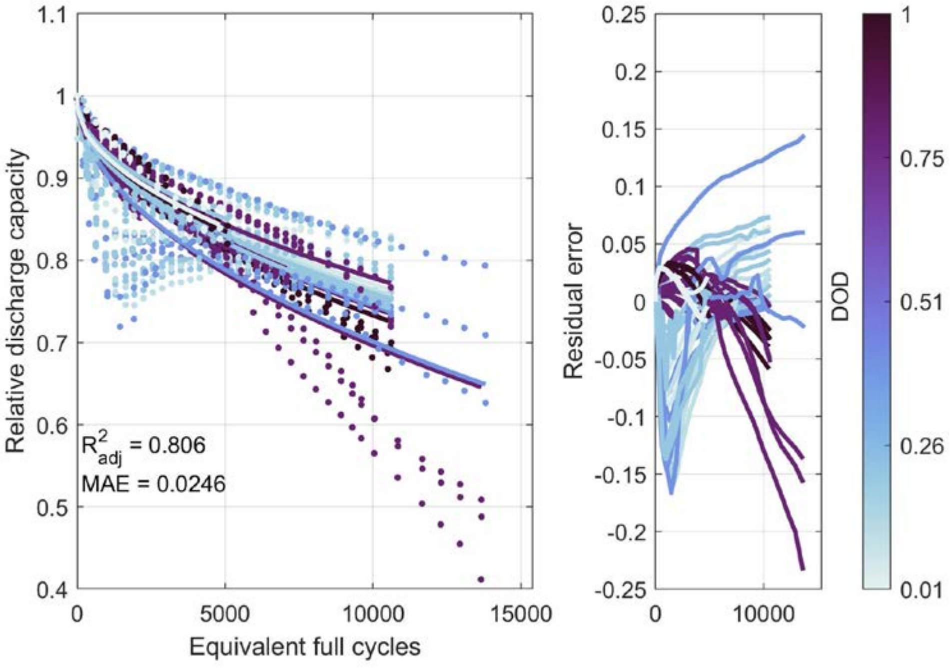
Cycling aging



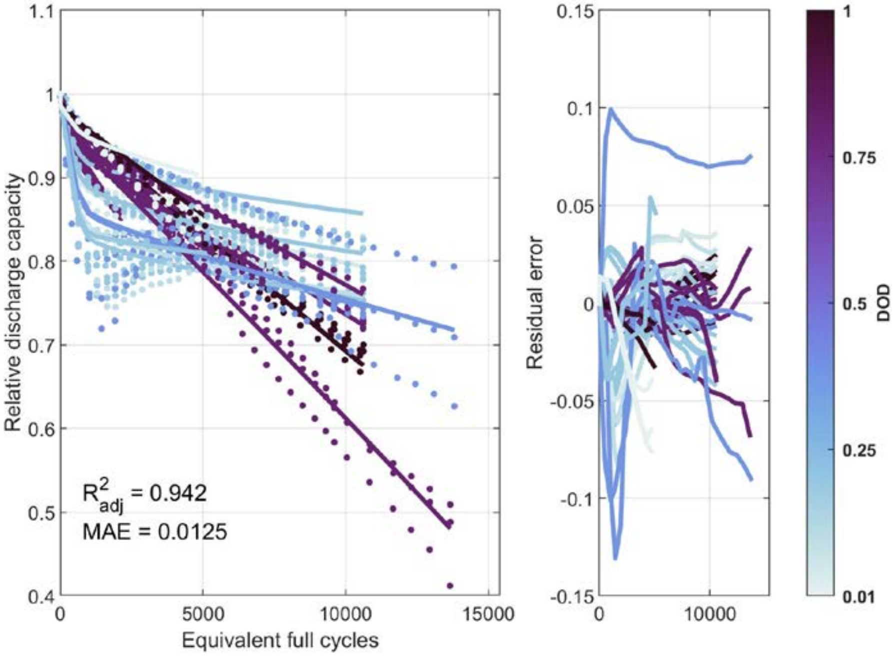


Prior work vs. ML-assisted

Prior work



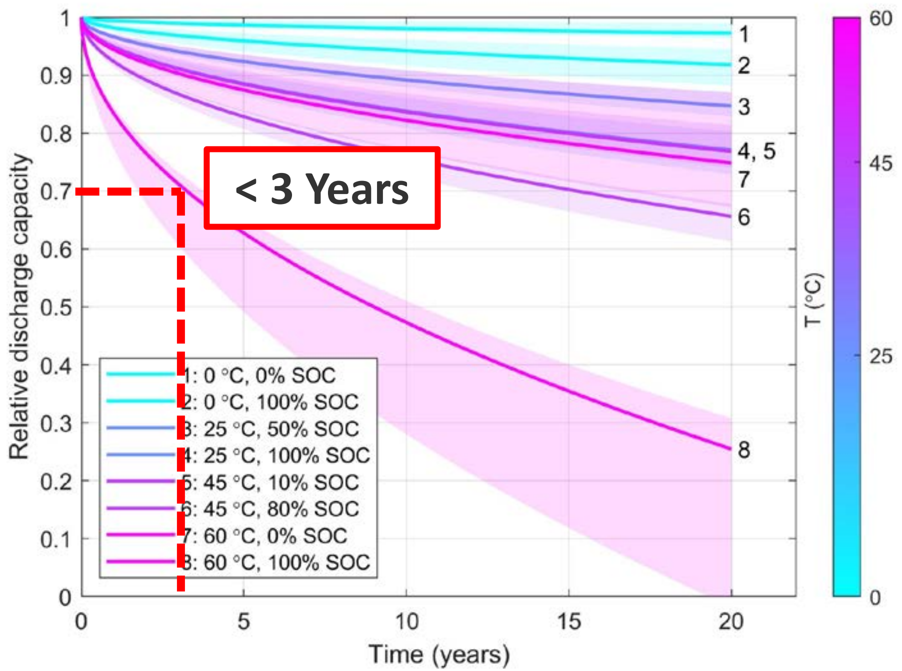
ML-assisted



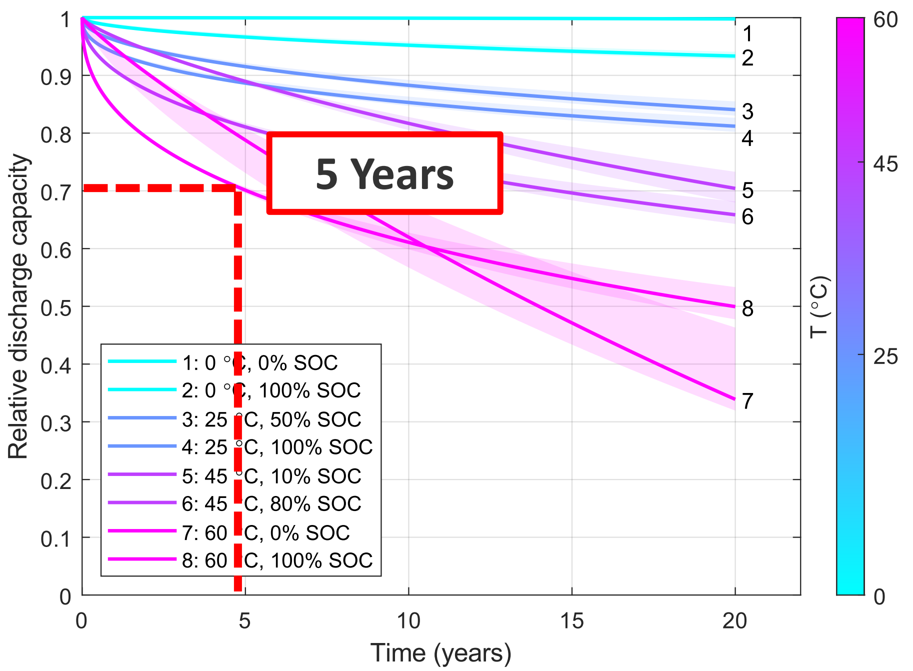
Impact on simulation

Calendar aging (20 years)

Standard approach

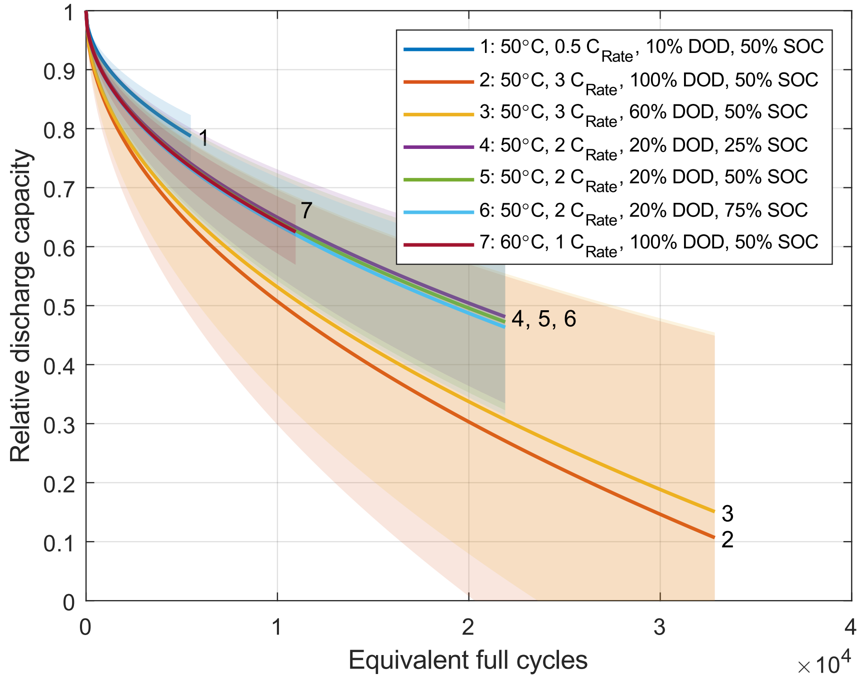


ML-assisted

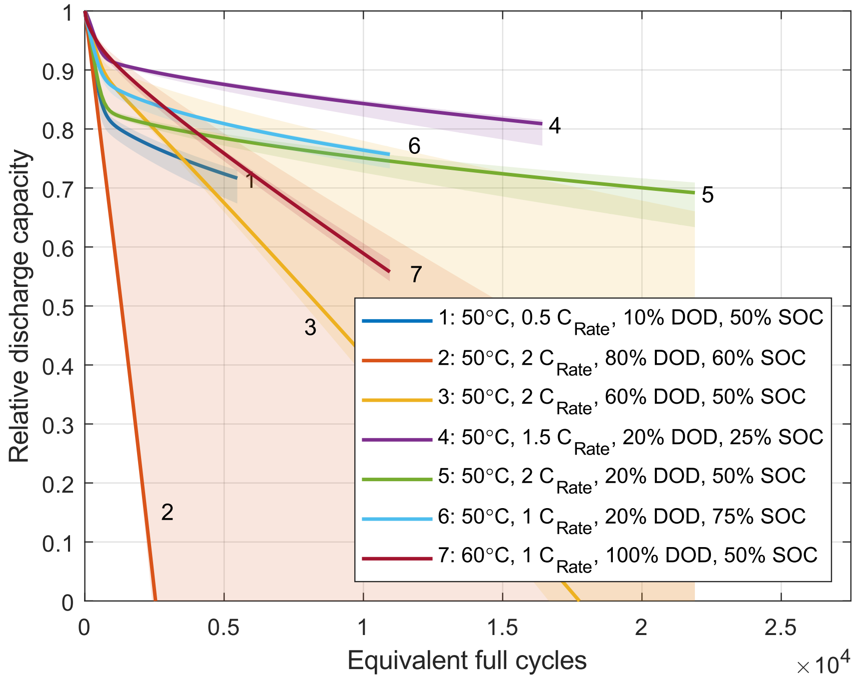


Cycling aging (3 years)

Standard approach



ML-assisted



Takeaways

Takeaways

- Accurate models can help inform experimental design, make better control decisions, or predict technoeconomic impact
- Don’t trust any model unless…
  - You understand how it relates to its training data (any systematic errors, impact of test design/setup, …)
  - Model extrapolations and interpolations ‘make sense’
- ML can help find accurate models, but it doesn’t replace being careful

Thanks to DOE VTO support from Simon Thompson, Samuel Gillard, Steven Boyd, and David Howell

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NREL/PR-5700-80161

This work was authored in part by the National Renewable Energy Laboratory, operated by Alliance for Sustainable Energy, LLC, for the U.S. Department of Energy (DOE) under Contract No. DE-AC36-08GO28308. Funding provided by the U.S. Department of Energy Vehicle Technologies Office, program manager Samuel Gillard. The views expressed in the article do not necessarily represent the views of the DOE or the U.S. Government. The U.S. Government retains and the publisher, by accepting the article for publication, acknowledges that the U.S. Government retains a nonexclusive, paid-up, irrevocable, worldwide license to publish or reproduce the published form of this work, or allow others to do so, for U.S. Government purposes.

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Extra slides

Current state-of-health prediction

Problem statement:

What is the current state-of-health of my battery?

Input data:

Basically any cell measurement: I-V-T-t data (Charge/discharge, voltage relaxation, random pulses), EIS, ultrasound, pressure, ….

Assumptions:

You don’t have the time/capability to simply measure the SOH metric you care about

Applications:

Real-world SOH detection

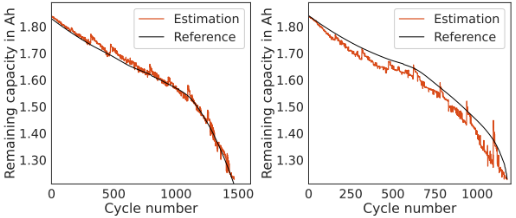
Current state-of-health prediction

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[e,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]

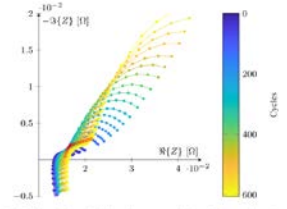


Fig. 2. Nyquist plot of the impedance spectra obtained during cyclic aging ($SoC = 100\%$, $T = 30$ °C).

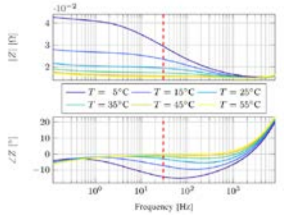


Fig. 3. Bode plot of impedance spectra at different temperatures ($SoH = 100\%$, $SoC = 90\%$).

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]

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

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

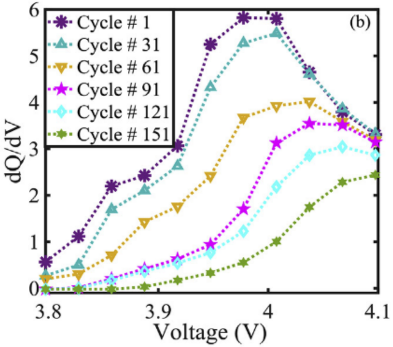
Using dQdV

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 end-of-life?

This is closely related to classifying good/bad cells.

Input data:

Basically any cell measurement: 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:

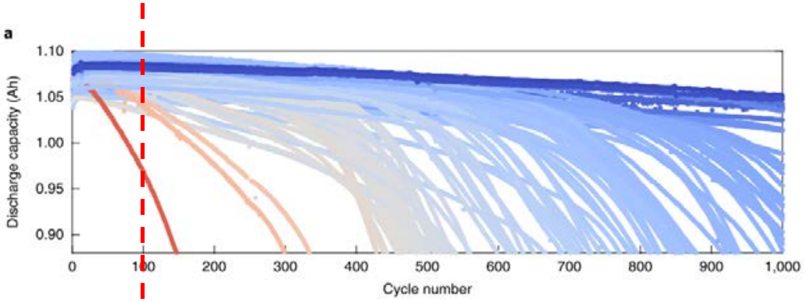
Optimization of battery use, classification of bad cells, anticipation of battery replacement

Remaining useful life prediction

Examples:

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

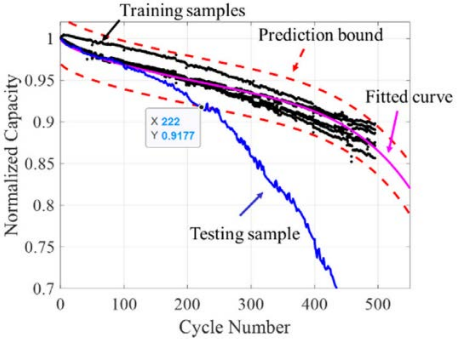
Data-driven prediction of battery cycle life before capacity degradation



First 5%-30% of lifetime required (mean 20%)

Contents lists available at ScienceDirect
Journal of Energy Storage
journal homepage: www.elsevier.com/locate/est

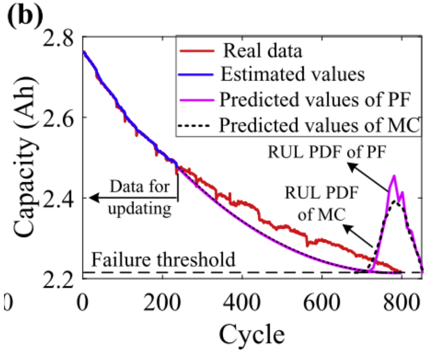
Early detection of anomalous degradation behavior in lithium-ion batteries



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

Journal of Cleaner Production 212 (2019) 240–249
Contents lists available at ScienceDirect
Journal of Cleaner Production
journal homepage: www.elsevier.com/locate/jclepro

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

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]

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

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