Identification of Life Models for Li-Ion Batteries Using Penalized Regression and Bilevel Optimization

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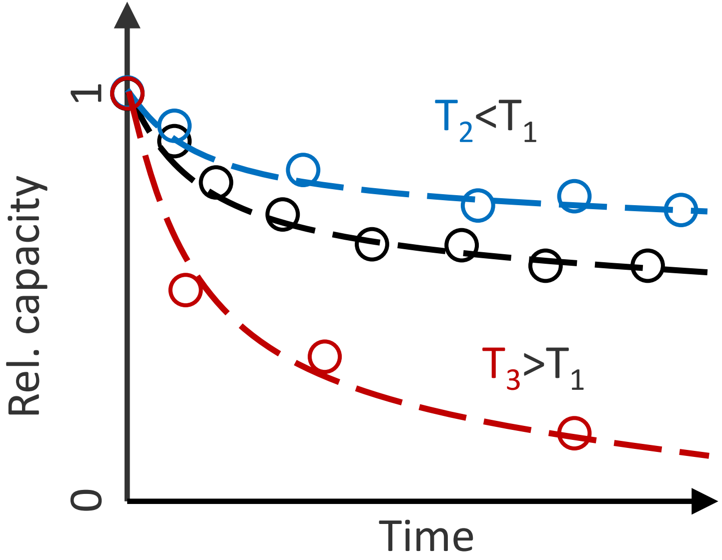
Reduced-order battery degradation models



Parameter sub-model (Time-invariant)

$$\beta_1 = \gamma_0 \exp\left(\gamma_1 \frac{1}{T}\right)$$

$$q_2 = 1 - \boxed{\beta_{1,2}} t^{0.5}, \; T = T_2$$

$$q_1 = 1 - \boxed{\beta_{1,1}} t^{0.5}, \; T = T_1$$

$$q_3 = 1 - \boxed{\beta_{1,3}} t^{0.5}, \; T = T_3$$

Local models (Time-varying)

Global model

$$q = 1 - \gamma_0 \exp\left(\gamma_1 \frac{1}{T}\right) t^{0.5}$$

Reduced-order battery degradation models

- \+ Inherently interpretable
- \+ Can extrapolate well from extremely small data sets
- \+ Fast computing
- – Do not model internal dynamics (E.g., pseudo-2D numerical models)
- – **Difficult to identify accurate models**

Reduced-order battery degradation models

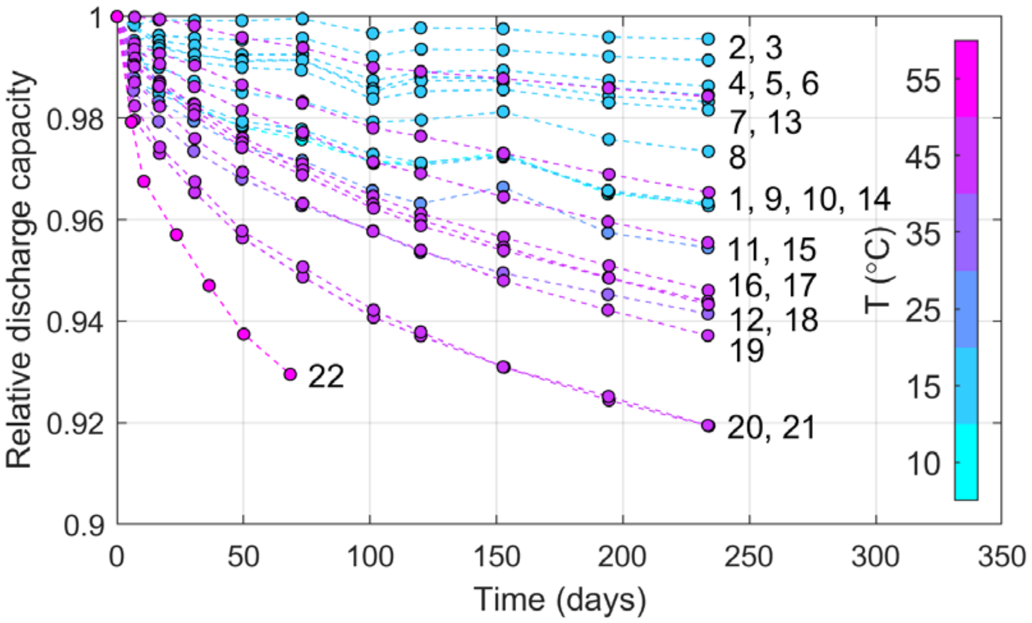
Two pathways for identifying reduced-order models exist in the literature:

1. Analytically derived relationships from simple systems
2. Empirical relationships based on trends in plotted data

Example follows…

Manual model identification

1. Fit each cell locally with the equation $q = 1 - \beta_1 t^{0.5}$, resulting in a vector of β_1 values.



[1] M. Schimpe, M. E. von Kuepach, M. Naumann, H. C. Hesse, K. Smith, and A. Jossen, *J. Electrochem. Soc.*, 165, A181–A193 (2018). https://doi.org/10.1149/2.1181714jes

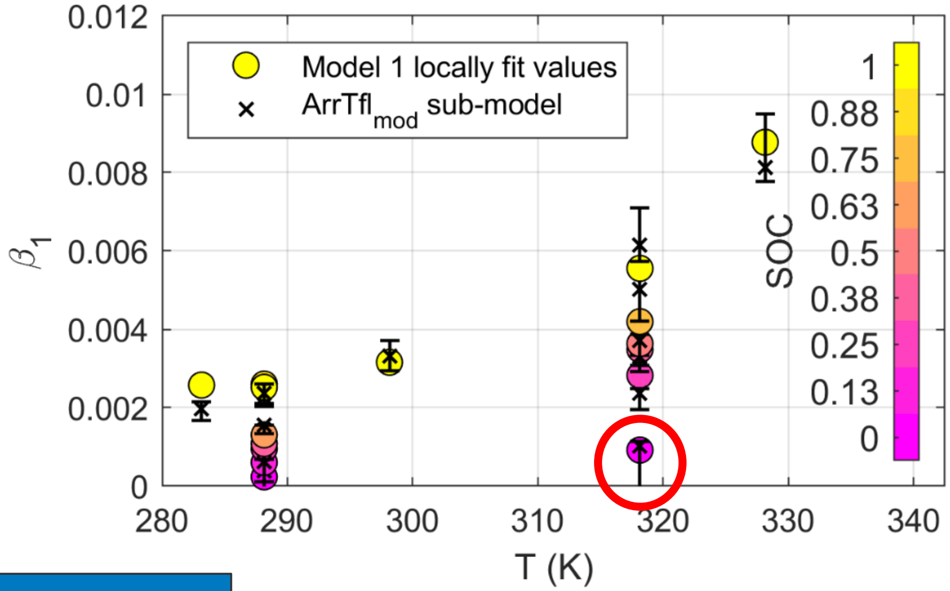
Manual model identification

1. Fit each cell locally with the equation $q = 1 - \beta_1 t^{0.5}$, resulting in a vector of β_1 values.
2. Fit β_1 values with a physically informed or empirically derived sub-model.

ArrTfl

$$\boldsymbol{\beta}_1(\boldsymbol{\gamma}, \boldsymbol{T}, \boldsymbol{U}_a) = \gamma_0 \exp\left(\gamma_1 \frac{1}{\boldsymbol{T}}\right) exp\left(\gamma_2 \frac{\boldsymbol{U}_a}{\boldsymbol{T}}\right)$$

R^2_{adj} = 0.943, MAPE = 24.3%



$ArrTfl_{mod}$

R^2_{adj} = 0.958, MAPE = 14.4%

$$\boldsymbol{\beta}_1(\boldsymbol{\gamma}, \boldsymbol{T}, \boldsymbol{U}_a) = \gamma_0 \exp\left(\gamma_1 \frac{1}{\boldsymbol{T}}\right)\left(\boxed{\gamma_2 +} exp\left(\gamma_3 \frac{\boldsymbol{U}_a}{\boldsymbol{T}}\right)\right) \text{[1]}$$

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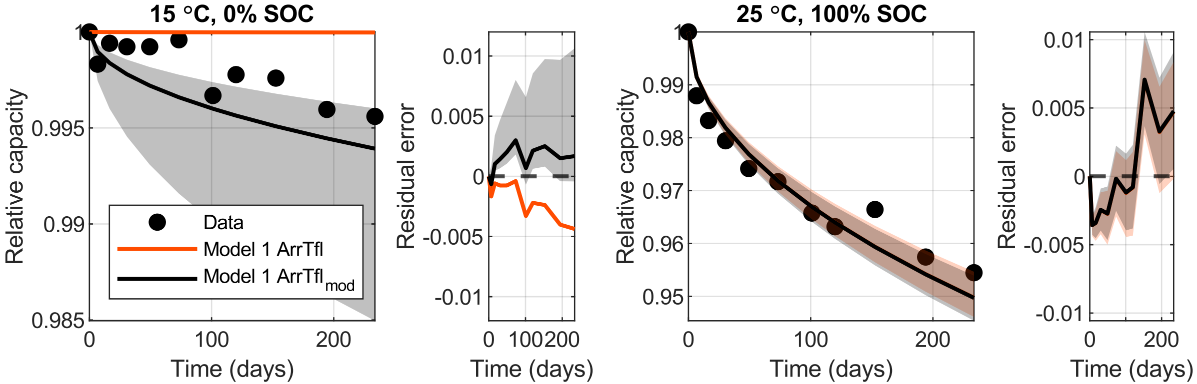
Manual model identification

1. Fit each cell locally with the equation $q = 1 - \beta_1 t^{0.5}$, resulting in a vector of β_1 values
2. Fit β_1 values with a physically informed or empirically derived sub-model
3. Construct a global model

ArrTfl

$$\boldsymbol{\beta}_1(\boldsymbol{\gamma}, \boldsymbol{T}, \boldsymbol{U}_{\boldsymbol{a}}) = \gamma_0 \exp\left(\gamma_1 \frac{1}{\boldsymbol{T}}\right) exp\left(\gamma_2 \frac{\boldsymbol{U}_{\boldsymbol{a}}}{\boldsymbol{T}}\right)$$



Few obvious pathways to improvement.

ArrTfl$_{mod}$

$$\boldsymbol{\beta}_1(\boldsymbol{\gamma}, \boldsymbol{T}, \boldsymbol{U}_{\boldsymbol{a}}) = \gamma_0 \exp\left(\gamma_1 \frac{1}{\boldsymbol{T}}\right)\left(\gamma_2 + exp\left(\gamma_3 \frac{\boldsymbol{U}_{\boldsymbol{a}}}{\boldsymbol{T}}\right)\right) [1]$$

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Methods and Models

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Automatic identification procedure

Local

Global
(assumed constant)

$$q = 1 - \boxed{\beta_1} t^{\boxed{0.5}}$$

1. Bi-level (nested) optimization
   - Local parameters correspond to unique behaviors of each cell
   - Global parameters correspond to behaviors shared by all cells
2. Symbolic regression [2,3]
   - Algorithmically generate descriptors from input features
   - Find optimal subset of descriptors using LASSO regularization
   - Both linear and multiplicative models are searched

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

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

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

Models investigated

Each model type was tested with various combinations of local and global parameters, growing increasingly complex as more parameters are fit locally, for a total of 15 models.

As local params are added, model DOF decreases:

DOF = # data points – # parameters

1 parameter

3 parameters

Square-root: $q = 1 - \beta_1 t^{0.5}$

4 parameters, $\lim_{t\to\infty} q = \beta_1$

Power law [4]: $q = \alpha_0 - \beta_1 t^{\alpha_1}$

Stretched exp. [5]: $q = \alpha_0 - \beta_1\left(1 - 1/exp\left((\alpha_1 t)^{\alpha_2}\right)\right)$

Sigmoidal [6]: $q = \alpha_0 - 2\beta_1\left(\frac{1}{2} - \frac{1}{1 + exp\left((\alpha_2 t)^{\alpha_3}\right)}\right)$

4 parameters, $\lim_{t\to\pm\infty} q = \pm\beta_1$

Results

Identification of Life Models for Li-Ion Batteries Using Penalized Regression and Bilevel Optimization

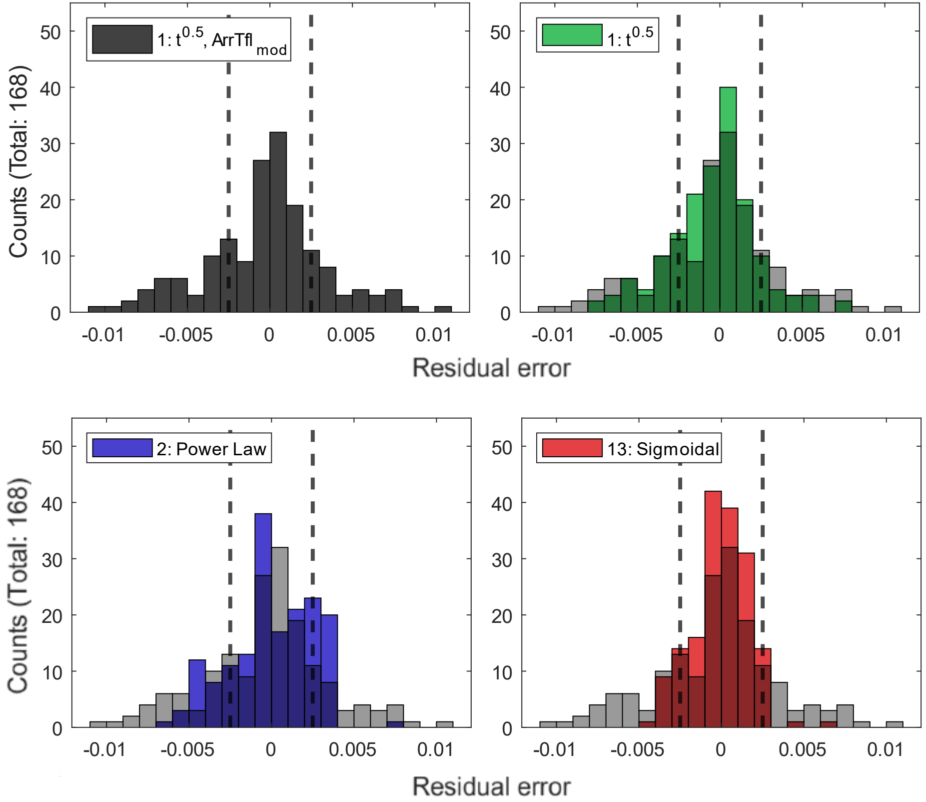
Models of interest

Compared to physically-informed/empirically identified models, automatically identified models demonstrate:

- Improved accuracy
- Reduced systematic deviation
- Lower predictive uncertainty

MAE: 0.26%

MAE: 0.19%



MAE: 0.2%

MAE: 0.13%

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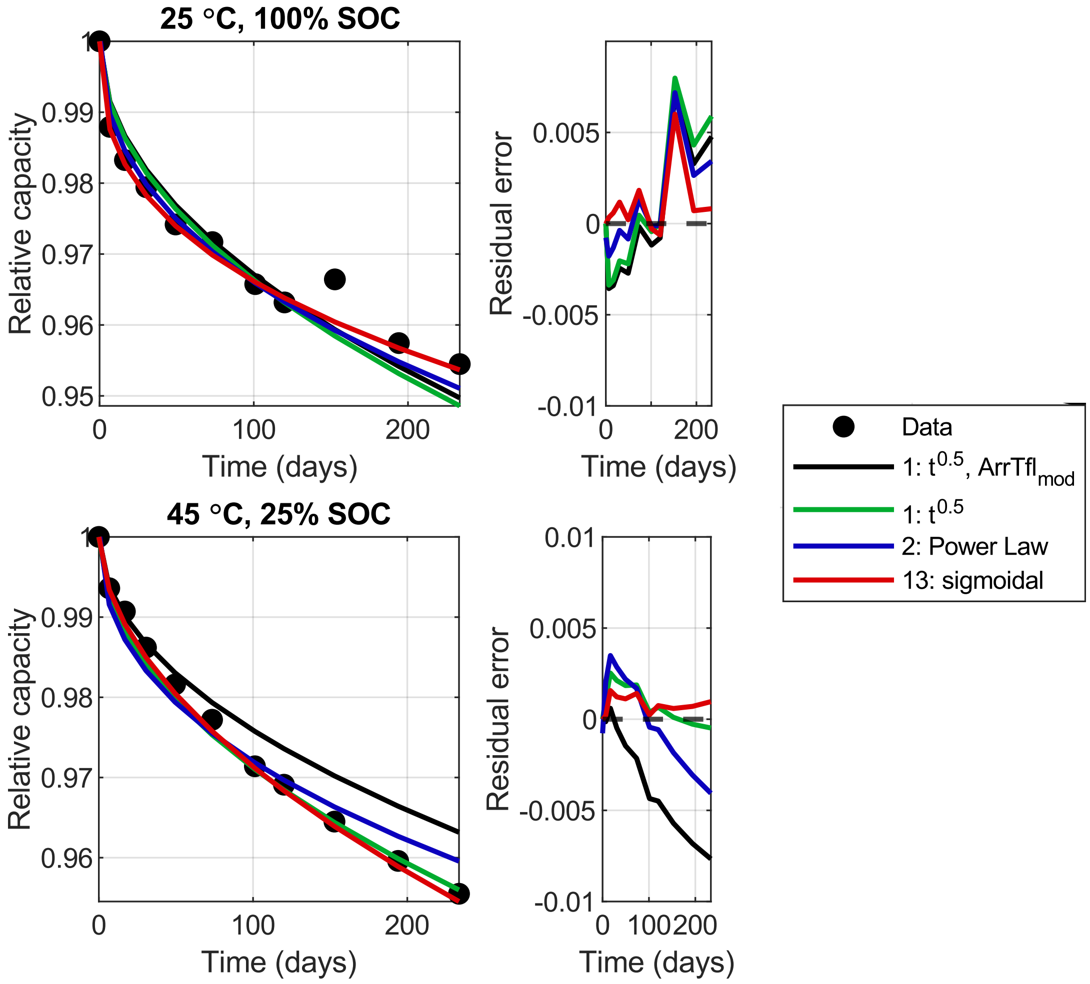

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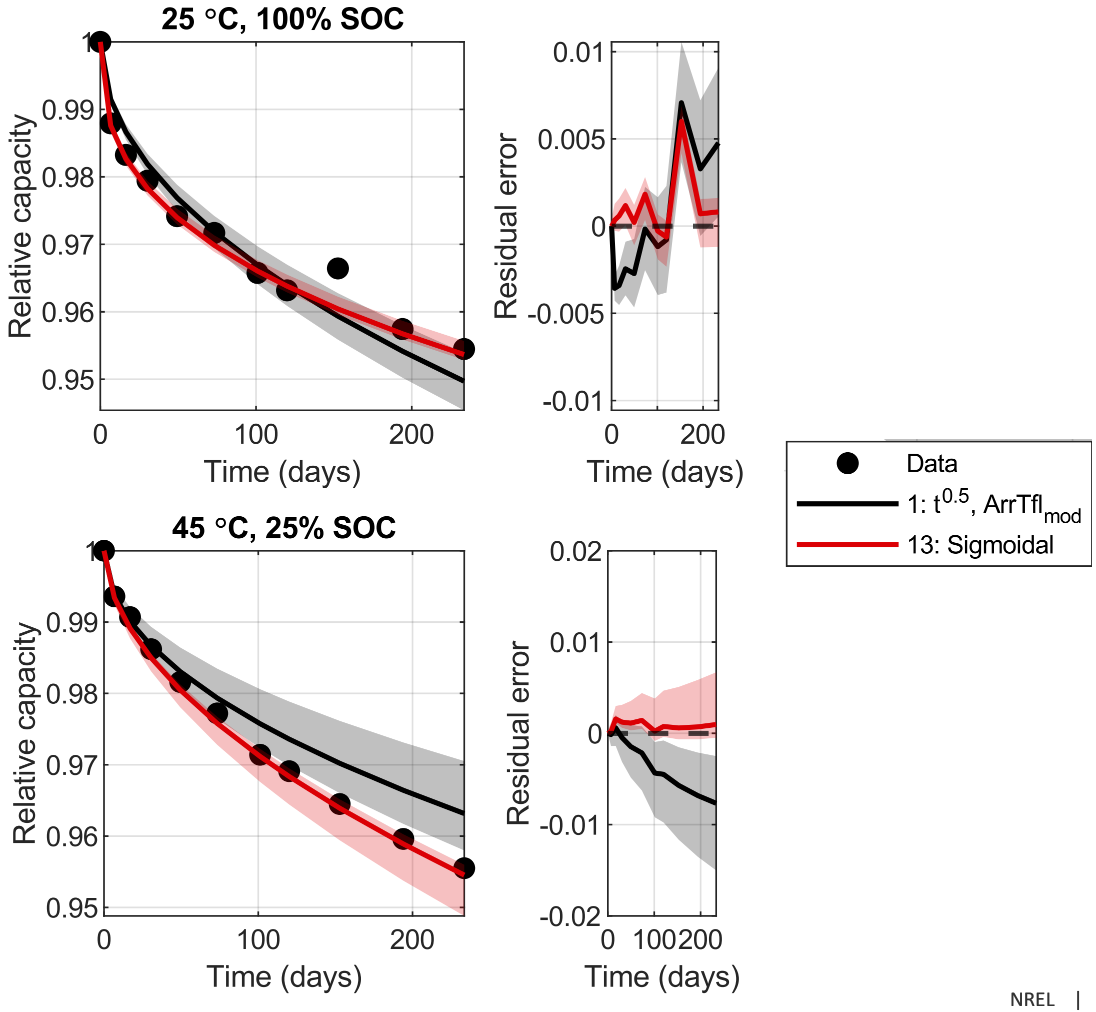

Model Convergence

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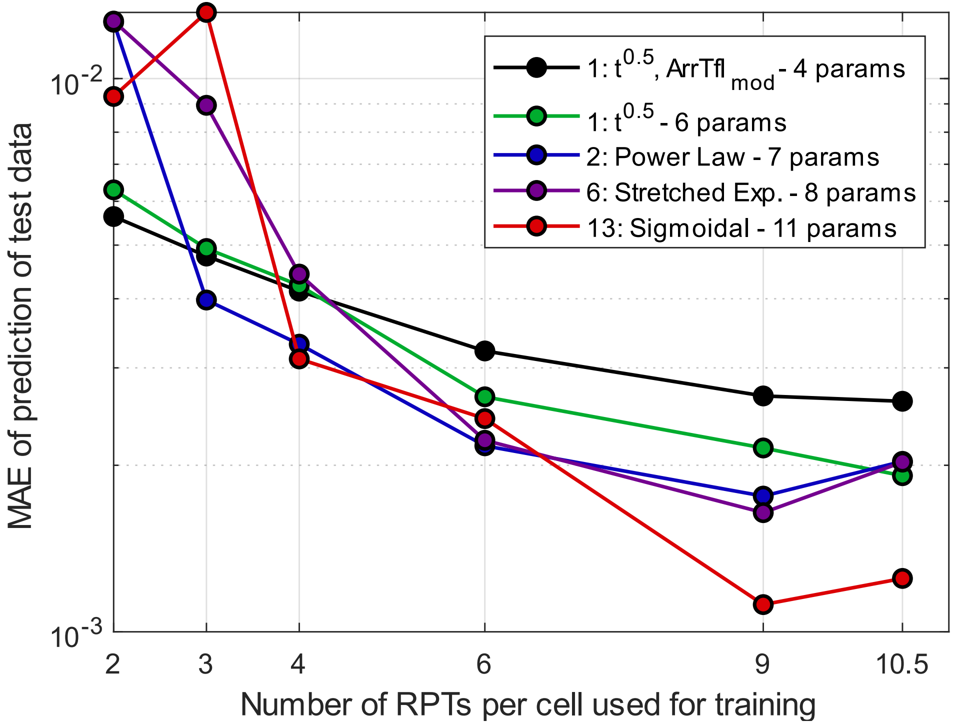
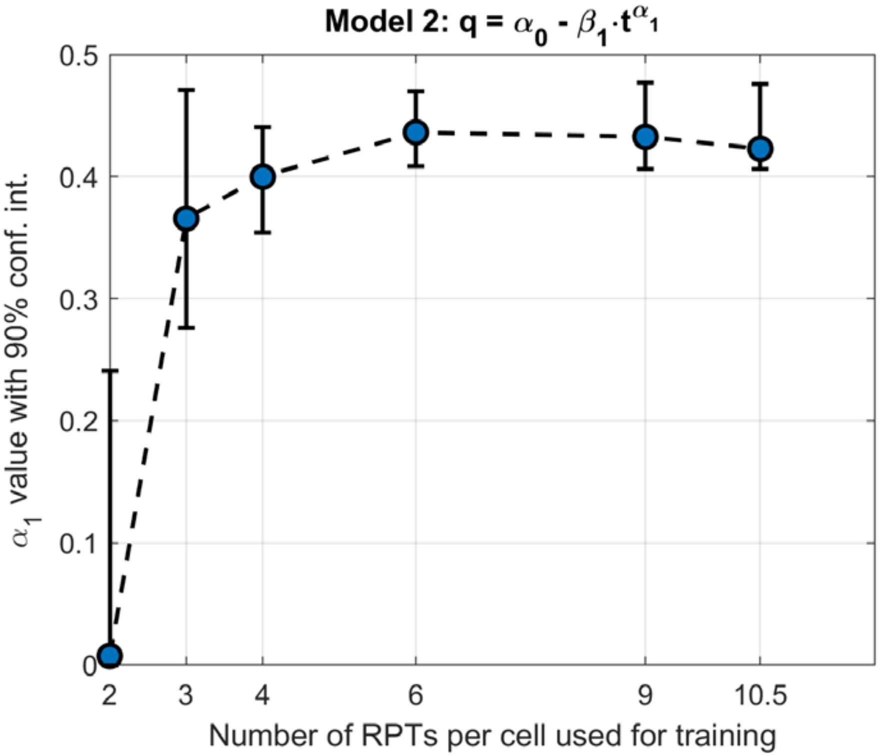
Convergence: Global model error

Automatically identified models converge with less data than the manually identified models



Convergence: Parameter values

Power exponent converges by 6 RPTs (~75 days out of 230)



Convergence: Sub-model structure

# of RPTs	Sub-model type	MAPE (test)	Power Law: LASSO identified β_1 sub-model descriptors				
			γ_1	γ_2	γ_3	γ_4	γ_5
2	Linear	332%	$T^2 SOC$	T^2/U_a	$T^2/\sqrt{U_a}$		
3	Mult.	48%	$exp(T/\sqrt{U_a})$	$exp(T^2 U_a)$	$exp(T^2/\sqrt{U_a})$		
4	Mult.	15%	$exp(T/\sqrt{U_a})$	$exp(T^2 U_a^2)$	$exp(T^2/\sqrt{U_a})$	$exp(\sqrt{U_a}/T)$	
6	Mult.	6.2%	$exp(T^2)$	$exp(T^2 SOC)$	$exp(T^2\sqrt{U_a})$	$exp(U_a/T^2)$	$exp(\sqrt{U_a}/T^2)$
9	Mult.	5.8%	$exp(T^2)$	$exp(T^2\sqrt{U_a})$	$exp(T^2 SOC^2)$	$exp(\sqrt{U_a}/T^2)$	$exp(1/(U_a^2 T^2))$
All (10.5)	Mult.	7.7%	$exp(T^2)$	$exp(\sqrt{U_a}/T^2)$	$exp(1/(U_a^2 T^2))$	$exp(1/(U_a^3 T^2))$	

Convergence: Sub-model structure

Sub-model accuracy converges by 6 RPTs (~75 days out of 230)

# of RPTs	Sub-model type	MAPE (test)	Power Law: LASSO identified β_1 sub-model descriptors				
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Convergence: Sub-model structure

Symbolic regression 'discovers' Tafel-like behavior – SOC/U_a are **never** used without temperature interactions in well-fitting models.

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Model Simulations

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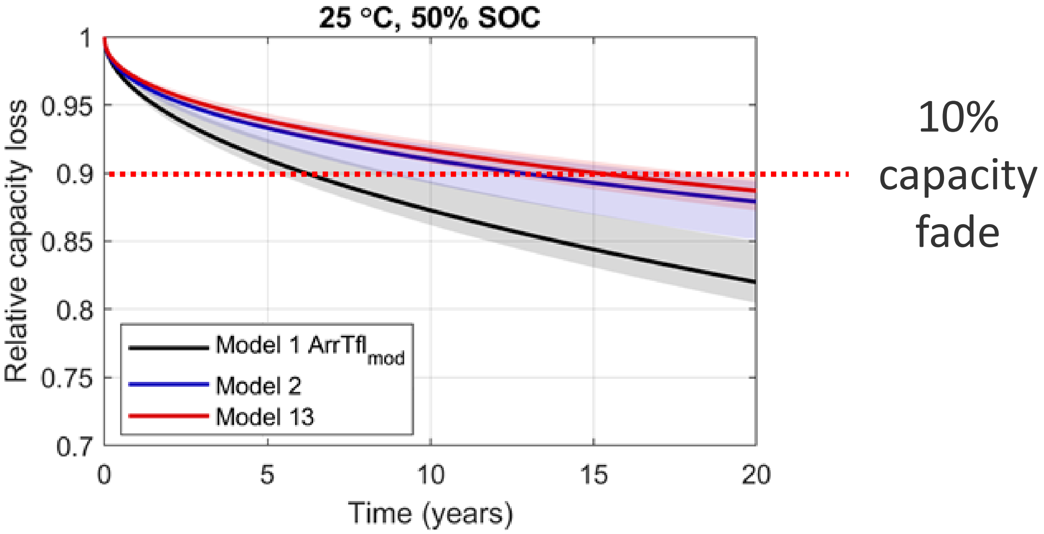
20-year simulation

Application relevant case

(25 °C, 50% SOC)

Model predictions of time to 10% capacity fade vary from 6.5 years to 15 years, differing by a factor of 2.3.



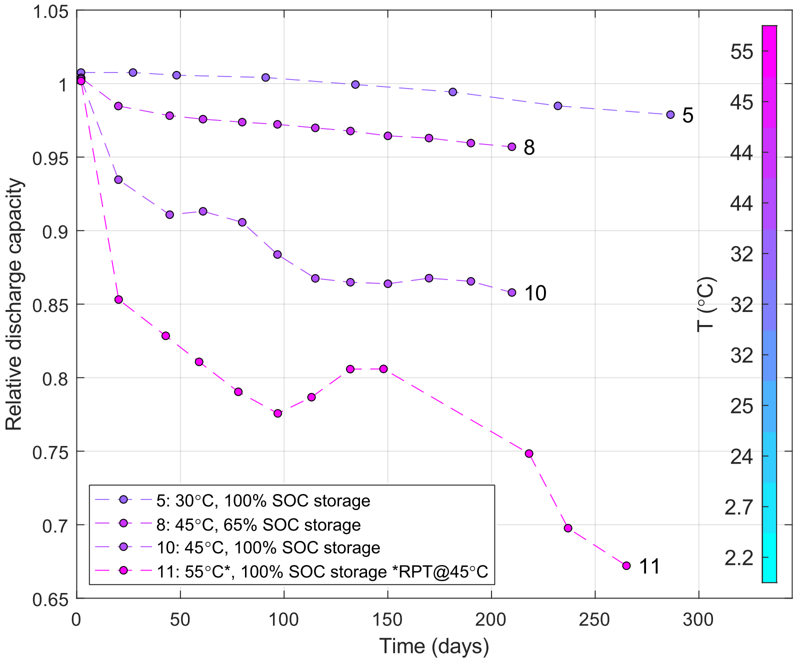
Small data sets

Identification of Life Models for Li-Ion Batteries Using Penalized Regression and Bilevel Optimization

[7] K. Smith, A. Saxon, M. Keyser, B. Lundstrom, Z. Cao, and A. Roc, Proc. Am. Control Conf., 4062–4068 (2017) https://doi.org/10.23919/ACC.2017.7963578.

Kokam 75 Ah, NMC/Gr

Even with extremely small data sets, procedure identifies a more accurate and lower uncertainty model than manual search.



Models fit to data:

- Sqrt(t), Arrhenius·Tafel β_1 sub-model
- Power law models
- Sigmoidal models

Kokam 75 Ah, NMC/Gr

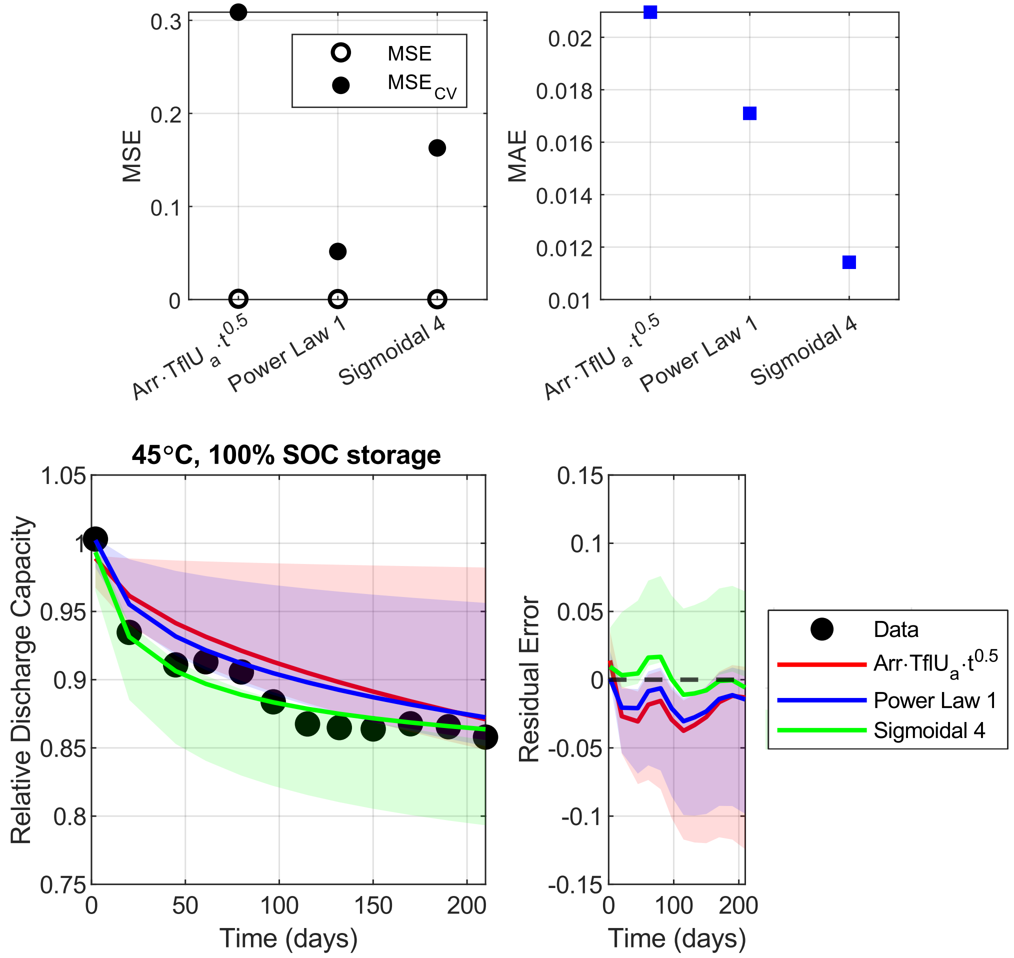
Best model: Power Law 1

Optimal power exponent of time deviates substantially from square-root:

0.23 (90% CI: 0.22, 0.32)

Tafel-like behavior is identified, even with only two sampled SOCs:

$$\beta_1 = \gamma_0 \, exp\left(\frac{\gamma_1}{T^2}\right) exp\left(\gamma_2 \frac{T^2}{U_a^{0.5}}\right)$$



Implications

Identification of Life Models for Li-Ion Batteries Using Penalized Regression and Bilevel Optimization

Implications for modeling

- Model optimality is only proven by comparison
- Confidence intervals / uncertainty quantification are crucial for interpreting model behavior
- Extrapolation of $t^{0.5}$ models may be overpredicting degradation by almost 100%

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https://www.nrel.gov/transportation/energy-storage.html

https://www.nrel.gov/transportation/energy-storage-publications.html

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Thanks for listening!

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