

# Online Co-Estimation of State of Charge and Voltage Dynamics of Li-ion Batteries via Physics-Inspired Modeling

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Introduction	Review Objective	Method	Simulation	Noise Mitigation	Experiment	Estimation	Conclusion
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#### Introduction

- Li-ion batteries (LiBs) in modern life
  - High energy density
  - Low self-discharge
  - Rechargeable
- Battery Management Systems (BMS)
  - Performance
  - Safety
  - Reliability
- BMS need State-of-Charge (SOC)
  - SOC is the remaining charge in battery
  - Not measurable (Need to be estimated)
  - Complex dynamics (Need to be predicted)
  - Current technology limits the operating range of batteries
- Objective
  - Create accurate, efficient, and control-oriented SOC model
  - Develop algorithm to estimate SOC





Introduction	Review	Objective	Method	Simulation	Noise Mitigation	Experiment	Estimation	Conclusion	
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#### Outline

- Literature Review on SOC Estimation and Modeling
- Objectives
- Methods
  - o Interpretable data-driven model
  - o Physics-inspired model
  - o Tuning parameters
  - Noise mitigation
  - Framework to estimate SOC
  - o Experiments
- Results and Discussion
- Conclusion and Future work



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### **Battery Dynamics Modeling**

#### SOC and Voltage have Complex Dynamics





#### Introduction Review Objective Method Simulation Noise Experiment Estimation Conclusion

### **Battery Dynamics Modeling: Empirical Models**

- Historical data
- Statistical methods
- Coulomb counting; e.g. Ghoulam et al., 2022
- SOC-voltage mapping; e.g. Xing et al., 2014



- ×Very sensitive to operating condition
- ×Require large and high-quality datasets to build model







## Battery Dynamics Modeling: Mechanistic Models (1)

- Express the process inside the battery with analytical equations
  - Electrochemical reactions
  - Heat and mass transport



- > Bimplifed of 2001 en Tole by Newman's Group)
  - Birgle & Avrice Di Moedesi (SBM) P. 200) anordechi Dogle, 2004 0, 1993
  - Birguen Poletiowet Mooding with no bedates letter an 2000 An perature (SPMeT); Park et al., 2021
  - Diovytiep Teu Plantik kerwinoathe (IDMI RIV) P. 24 Dajolia bablie et nall, d2/01 a 5 nics); Thomas et al., 2002
- ✓ Suitable for construction and optingizasion





- $\checkmark$  Capture the dynamics of the modeled processes, detailed insight
- $\checkmark$  High interpretability, allow for design and performance optimization
- ✓ Extrapolatable to a wide range of conditions for complex models
- ★ Require many parameters, several not available
- ×Based on idealized principles, not always apply
- $\times$ Only predict the modeled phenomena
- $\times$ Computationally expensive with added complexity

Model	Number of parameters	Computational Complexity
DFN	33	High
SPMeT	31	Medium
SPM	20	Low

Conclusion



### Introduction Review Objective Method Simulation Noise Experiment Estimation Conclusion

## Battery Dynamics Modeling: ECMs (1)

#### Equivalent Circuit Model (ECM)

• Express the battery's dynamic with electrical components



- ECM with simple passive electrical elements; e.g. Schmidt et al., 2016
  - Determine Open circuit voltage (OCV) from voltage and current
  - Estimate SOC via SOC-OCV mapping
- ECM with fractional-order or distributed elements; Wildeuer et al., 2021
  - Using impedance spectra







Experiment

## Battery Dynamics Modeling: ECMs (2)

#### **♦ ECM**

- ✓ Use measurable data (current and voltage)
- ECM with passive electrical components:
  - $\checkmark$  Simple with low computational cost
  - X Narrow operating range due to lack of physics-based information
  - X Need to use look-up tables with many sets, still limited due to being linear
- ECM with fractional-order or distributed elements:
  - $\checkmark\,$  Connections to internal processes of LiBs
  - ✓ Larger operating conditions
  - × Require impedance spectra
  - imes Need specific devices with careful experimental control
  - imes Not suitable for real-time applications





#### Review Objective Method Introduction

Simulation

Noise

Mitigation

## Battery Dynamics Modeling: ML (1)

#### Data-driven Model/Machine Learning

- Express the battery's dynamic from measurable data •
- Black box modeling •
- Support vector machine (SVM); Feng et al., 2019
- Clustering with genetic algorithm; Hu et al., 2016 •
- Neural network (NN); How et al., 2020
  - Recurrent NN; Vidal et al., 2022 •
  - Long short-term memory recurrent NN; Chemali et al., 2018 •







Noise

Mitigation

Experiment

## Battery Dynamics Modeling: ML (2)

#### Data-driven Model/Machine Learning

- ✓ No need for internal parameters (using measurable data)
- $\checkmark$  Adaptable to new chemistries or conditions by retraining
- ✓ Can use novel features instead of traditional metrics (e.g., voltage, current)
- ✓ Low implementation cost, suitable for real-time applications
- ×Require rich and informative dataset to capture operating conditions
- ×Needs an extensive set of data to build model
- imesRisk of overfitting with complex algorithms
- ×Can lead physically inconsistent results and lack interpretability (no connection to physics)
- ×Too many features reduce stability (ill-conditioned problem due to correlated terms)





Noise

Mitigation

Experiment

## Battery Dynamics Modeling: Hybrid Models (1)

- ECM: Increasing operating range and accuracy
  - ECM + Machine learning
    - ECM + deep learning; Su et al., 2023
    - ECM + NN; Borah et al., 2024
  - ECM + Kalman filter; Yao et al., 2024
- $\checkmark$  Refine estimates; suitable for aggressive input
- ✓ Mitigate noise effect
- ✓ Extend ECM operating range
- $\times$ Lack of interpretability
- $\times$ Require large datasets for training
- $\boldsymbol{\times}$  Limited accuracy in low SOC regions



#### Introduction Review Objective Method

Simulation

Noise

Mitigation

Experiment

# Battery Dynamics Modeling: Hybrid Models (2)

- Mechanistic: Increasing accuracy and reducing computational time <sup>Inpu</sup>
  - SPM + Machine learning
    - SPM + recurrent NN; Saehong Park et al., 2017
    - SPM with thermal dynamics + feed forward NN; Tu et al., 2023
  - Mechanistic models + Kalman filter
    - SPM + Kalman filter; Fang et al., 2014
    - P2D + Kalman filter; Smiley et al., 2018
  - Physics-informed NN, Hofmann et al., 2023
  - Solving SPM with electrolyte equations with NN; Xue et al., 2023
- $\checkmark$  Improve accuracy by capturing complex unmodeled dynamics with ML
- ✓ Extend operating range of simplified model (ECM and SPM)
- ×Require large datasets for training machine learning
- $\textbf{\times}$  Need many internal parameters for mechanistic models
- Increase complexity in balancing mechanistic and machine learning components







### **Proposed Approach**

- Desired Model:
- ✓ Interpretable and control-oriented data-driven model
  - Uncover governing equations not fitting data only
- ✓ Connection to physics
- ✓ Perform well in unseen data
- Interpretable input/output modeling techniques:
- Dynamic mode decomposition (DMD); Tu, 2013
  - Approximate linear system
- Sparse identification of nonlinear dynamics (SINDy); Brunton et al., 2016
  - Nonlinear reduced order model through sparsification of a library of potential terms
  - Require remarkably less data comparing to NN

➤Dynamics of LiB is highly nonlinear

SINDy challenges:Selecting library termsSelecting sparsification parameters



Introduction	> Review	Objective	Method	Simulation	Noise Mitigation	Experiment	Estimation	Conclusion	
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#### Objective

- Main objective: Develop a tractable data-driven model to discover the governing equations of Li-ion batteries
- Hypothesis: Voltage and SOC dynamics can be represented by a few terms from the measured data, and SOC levels can be accurately estimated via these learned dynamics

#### > Aim 1: Discovering Battery's Voltage and SOC dynamics

- Create a nonlinear interpretable data-driven model for Li-ion battery
- Enhance the modeling technique by including physics-inspired terms
- Formulate a multi-objective cost function to capture the dynamics

#### Aim 2: Robust Modeling with Noisy Data

- Extend data-driven model using a Joint Unscented Kalman Filter to mitigate noise effects
- Develop a co-estimation framework to update model parameters using measurement data

#### > Aim 3: Data Generation and Model Development

- Generate data from a detailed cylindrical cell battery model
- Design experiments on a single cell at different temperatures
- Conduct experimental studies and collect data



Introduction Review Objective	Method Simulation	Noise Mitigation	Experiment	Estimation	Conclusion	
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#### Roadmap

- Discover governing equation of Li-ion batteries
  - Using the measurable data
  - Physics-inspired
  - Generalizability
- Reduce measurement noise effect
  - Using Joint Unscented Kalman Filter
- Co-estimation framework





## Sparse Identification of Nonlinear Dynamics

- SINDy is based on sparse linear regression; Brunton et al., 2016
  - Results in reduced order nonlinear model
  - Detect the governing equation
- Notable extensions to SINDy
- SINDy with control (SINDyC); Brunton et al., 2016
- AIC-inspired on training data; Mangan et al., 2017
- Constraint dynamics; Loiseau & Brunton, 2018
- Including switching dynamic; Li et al., 2019; Mangan et al., 2019
- PDE; Messenger & Bortz, 2021
- MPC; Fasel et al., 2021
- Sensitivity analysis: Naozuka et al., 2022
- Ensemble model; Fasel et al., 2022
- There are several extensions; however, they mostly left the choice of library terms and sparsification parameters which based on the original formulation overfits the model



Estimation

Conclusion

Library:  $\Theta(X, U)$ 

• By defining sparse vector of coefficients  $\Xi$ :

$$X' = \Theta(X, U) \Xi$$

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## Identifying Sparse Vector of Coefficients $\boldsymbol{\Xi}$

 $\boldsymbol{\Xi} = [\xi_1 \quad \xi_2 \quad \cdots \quad \xi_n]^T$ 

• Ridge Regularization problem:

 $\Xi^* = \operatorname{argmin}_{\Xi} \| X' - \Theta \Xi \|_2 + \lambda \| \Xi \|_2 + \xi_{th} \| \Xi \|_0$ 

 $\lambda$ : regularization parameter

• Suitable for correlated terms

Promoting sparsity: Sequentially thresholded ridge regression (STRidge)

•  $\xi_{th}$ : if  $|\xi_i| < \xi_{th} \Rightarrow \xi_i = 0$ 



Conclusion



#### Introduction Review Objective Method Simulation Noise Experiment Estimation Conclusion

# Tuning Sparsification Parameters ( $\lambda, \xi_{th}$ )

• **Original Approach:** Akaike information criterion (AIC)-inspired loss function:

 $AIC = 2N - 2\ln(\hat{L})$ ,  $\hat{L}$  is the maximum value of the likelihood function

$$\mathcal{L}(\Xi) = N \ln\left(\frac{\|X' - \Theta(X, U)\Xi\|_2^2}{N} + \epsilon\right) + 2K$$

k is the number of nonzero coefficients in  $\Xi$ , and N is the number of measured data in time.  $\epsilon \ll 1$  to avoid overfitting the data.

• Goal is to balance accuracy and complexity

 $\Xi^* = \operatorname{argmin}_{\Xi} \| \dot{X} - \Theta \Xi \|_2 + \lambda \| \Xi \|_2 + \xi_{th} \| \Xi \|_0$ 



## Limitations of Generic Model

Preliminary results using SINDy: predict voltage with generic terms and AIC cost function

- Very limited operating condition
  - Lack of connection to physics
  - Exact terms to be included in the library
    - Adding too many terms results in ill-conditioned problems with correlated terms
  - Cost function using only training data

#### Next Steps

- $\checkmark$  Create physics-inspired library
- ✓ Design multi-objective cost function
- $\checkmark$  Predict both voltage and SOC simultaneously





#### NL Control-Oriented Model of Batteries

- Measurable data
  - Voltage and SOC are the states ([V SOC]  $\equiv X$ )
  - Current is the input  $(I \equiv U)$

$$[V_{k+1}, \text{SOC}_{k+1}] = f(V_k, \text{SOC}_k, I_k)$$
$$V_{k+1} = \Theta(V_k, \text{SOC}_k, I_k)\Xi_1$$
$$\text{SOC}_{k+1} = \Theta(V_k, \text{SOC}_k, I_k)\Xi_2$$



- Data to create the data-driven models
  - Python Battery Mathematical Modelling (PyBaMM)
  - 21700 cylindrical Li-ion cell with material NMC 811 parameters set (5000 mAh)
  - DFN Model
- First step: determine a library based on battery physics



### Physics-Informed Library (1)

• DFN model

• Solid and electrolyte concentrations:







## Physics-Informed Library (2)

- DFN model:  $sin(\cdot)$ ,  $exp(\cdot)$
- Overpotential (Butler-Volmer):







• SOC:

## Physics-Informed Library (3)

- DFN model:  $sin(\cdot)$ ,  $exp(\cdot)$ ,  $sinh(\cdot)$
- Electrolyte's electric potential:
- Solid electric potential:

$$\frac{\partial \phi_e}{\partial x}(x,t) = \frac{2RT}{F} \left(1 - t_c^0\right) \left(1 + \frac{d \ln f_c}{d \ln c_e}(x,t)\right) \partial \ln \frac{c_e}{\partial x}(x,t) - \frac{i_e^{\pm}(x,t)}{\kappa}$$



$$\phi_{s}^{\pm}(x,t) = \eta^{\pm}(x,t) + \phi_{e}(x,t) + U^{\pm}(c_{ss}^{\pm}) - FR_{f}^{\pm}j_{n}^{\pm}(x,t)$$

$$V(t) = \phi_s^+(0^+, t) - \phi_s^-(0^-, t)$$

$$SOC(t) = SOC(0) - \frac{1}{C_a} \int_0^t \eta I d\tau$$



# Automated Optimization Algorithm

- Three datasets for modeling:
- Training dataset:
  - Building the model
  - Input and output of this set are known
- Validation dataset:
  - Optimizing the hyperparameters of the identified model
- Test dataset:
  - Evaluating the performance of the identified model

 $\Xi^* = \operatorname{argmin}_{\Xi} \| X' - \Theta \Xi \|_2 + \lambda \| \Xi \|_2 + \xi_{th} \| \Xi \|_0$ 





## **Training Dataset**

- Electrical current is employed to generate data
- Stochastic current signal up to 2C/4C-rate charge/discharge with 50 ms sampling time





#### Validation Dataset

EPA aggressive highway drive cycles for validation





#### **Test Dataset**

#### EPA urban drive cycles for test

• Urban Dynamometer Driving Schedule (UDDS)







#### Introduction Review Objective Method Simulation Noise Experiment Estimation Conclusion

### Introducing Hyperparameter Formulation

• The sparsification parameters are tuned with the training, validation set and number of terms





## Optimal Voltage Dynamics Model

- Number of active terms depends on the hyperparameters ( $\lambda$ ,  $\xi_{th}$ )
- Red region suggests diminishing returns





## Simulation Results (1)

- Voltage and SOC are calculated simultaneously
- Training data NRMSE
  - Voltage: 3.2×10<sup>-4</sup>
  - SOC: 10<sup>-8</sup>





## Simulation Results (2)

- US06 validation data NRMSE:
  - Voltage: 6.1×10<sup>-3</sup>
  - SOC: 2.2×10<sup>-5</sup>



- UDDS test data NRMSE:
  - Voltage: 6.3×10<sup>-3</sup>
  - SOC: 2.8×10<sup>-3</sup>





## **Enhancing Model**

- Current Model
  - ✓ Works for perfect measurement
  - ✓ No uncertainty (e.g., with simulated data)
- Issue on actual implementation
  - Noisy data both in training and validation
  - Error in estimations
- Solution for noisy data and improve estimation
  - Kalman Filter  $\rightarrow$  Adapt the model
    - ✓ Mitigate noise effect
    - ✓ Connect SOC dynamics and SOC-Voltage map





## Joint Unscented Kalman Filter

- Avoid needs for linearization, suitable for nonlinear systems
- Address uncertainty in voltage state and coefficients concurrently

 $\Xi_{r,1}[k+1] = \Xi_{r,1}[k] + w_{\Xi}[k]$  $V[k+1] = \theta_{r,1}[k]\Xi_{r,1}[k] + w_{V}[k]$ 

•  $V_o[k] = V[k] + v_V[k]$ 

Nonzero sparse coefficients

Voltage dynamics

Noisy voltage data

- Update V and  $\Xi_{r,1}$  with the noisy output (Voltage)
- Utilize the updated voltage for the SOC prediction
- SOC[k + 1] =  $\theta_{r,2}[k] \Xi_{r,2}[k]$





## Simulation Results with Added Noise (1)

- Voltage data has 5% Gaussian noise as a measurement noise
- Training data NRMSE
  - Voltage:  $10^{-3}$
  - SOC: 1.008×10<sup>-7</sup>







#### Simulation Results with Added Noise (2)

- US06 validation data NRMSE:
  - Voltage: 1.1×10<sup>-3</sup>
  - SOC: 5.0963×10<sup>-5</sup>



- UDDS test data NRMSE:
  - Voltage: 9.0568×10<sup>-4</sup>
  - SOC: 1.1585×10<sup>-4</sup>





## Selecting Battery for Experiment

- NMC batteries: Efficient, dependable
  - Less Cobalt: Reduce price
  - Increasing Nickel: Higher capacity and lower weight
- LGM50 21700 cylindrical cell with NMC 811 cathode





Conclusion

#### Average cost structure of Li-ion cell

https://www.bloomberg.com/news/newsletters/2021-09-14/evbattery-prices-risk-reversing-downward-trend-as-metals-surge



## **Designing Experiment**

- Electrical current is employed to generate data
- 1C-rate: 4.8 A, fully charge the battery in 1 hour with constant current
- Max current for constant current charging: 0.3C-rate
- *T* = 10°C, 25°C, 40°C











#### **Experimental Results**

• Stochastic electrical current signal up to 1C/2C-rate charge/discharge with 50 ms sampling time





### Introduction Review Objective Method Simulation Noise Experiment Estimation Conclusion

## **Tuning Sparsification Hyperparameters**

• Multi-objective cost function

$$\min_{\lambda,\xi_{th}} \mathcal{J}(\Xi) \coloneqq \rho_1 \mathcal{E}_t(x,\hat{x}) + \rho_2 \mathcal{E}_v(x,\hat{x}) + \rho_3 K$$



	Value for SOC	Value for Voltage		
Number of terms	9	9		



Introduction Review Objective Method Simulation Noise Experiment Estimation Conclusion

## Model Using Experimental Data (1)

calculate SOC with Coulomb counting:

 $SOC(t) = SOC(0) - \frac{1}{Q} \int_0^t \eta_c I d\tau$ 

- $\eta_c: \frac{Q_{discharged}}{Q_{charged}}$
- Training data RMSE
  - Voltage:  $2.1 \times 10^{-3}$ V
  - SOC: 8.6×10<sup>-3</sup>







#### Model Using Experimental Data (2)

- Aggressive highway validation data RMSE:
  - Voltage:  $8 \times 10^{-4}$  V
  - SOC: 9.9×10<sup>-3</sup> (ECM+EKF: 6.3×10<sup>-2</sup>)



- City test data RMSE:
  - Voltage:  $6 \times 10^{-4}$  V
  - SOC: 1.2×10<sup>-2</sup>





### Introduction Review Objective Method Simulation Noise Experiment Estimation Conclusion

### SOC Estimation: Co-estimation Framework

- Adding uncertainty in SOC dynamics due to noisy current and unknown initial value
- Address uncertainty in both states and coefficients concurrently
- $\Xi_{r,1}[k+1] = \Xi_{r,1}[k] + w_{\Xi}[k]$
- $V[k+1] = \theta_{r,1}[k] \Xi_{r,1}[k] + w_V[k]$
- $|\operatorname{SOC}[k+1] = \theta_{r,2}[k]\Xi_{r,2}[k] + w_S[k]|$  SOC
- $V_o[k] = V[k] + v_V[k]$

- Nonzero sparse coefficients
- SOC-Voltage map
- SOC dynamics
- Noisy voltage data
- Update V, SOC and  $\Xi_{r,1}$  with the noisy output (Voltage)





## **Co-estimation Results (1)**

- US06 Validation data
- Initial SOC: 0.8 (20% uncertainty)
- SOC RMSE after convergence: 0.0102
- ECM+EKF fails to estimate SOC
- Voltage RMSE: 0.0008V





## **Co-estimation Results (2)**

- UDDS Test data
- Initial SOC: 0.8 (20% uncertainty)
- SOC RMSE after convergence: 0.0130
- ECM+EKF fails to estimate SOC
- Voltage RMSE: 0.0006V

- Battery tester voltage accuracy: ±0.02% full-scale range (±0.0004V)
- Similar to maximum absolute error of voltage (0.0004V)





#### **Co-estimation Result on Different Conditions**

Evaluate the transferability of the model to cold and warm environments by only adjusting the coefficients





Introduction	Review	Objective	Method	Simulation	Noise Mitigation	Experiment	Estimation	Conclusion	
--------------	--------	-----------	--------	------------	---------------------	------------	------------	------------	--

#### Conclusion



- Formulating nonlinear sparse modeling with hyperparameters
- Tuning of sparsification hyperparameters via a novel cost function
- Augmented the technique with a joint unscented Kalman filter to work with noisy data and co-estimation

Contributions to energy storage systems:

- Detailed analysis of complex electrochemical models of Li-ion batteries to determine physics-informed library terms
- Validated the modeling technique on DFN models
- Designed and conducted experiments to generate modeling data
- Created a control-oriented, tractable, interpretable battery model
- Developed a technique to determine voltage-SOC mapping to replace the currently used look-up tables from extensive experiments
- Online SOC estimation via introduced co-estimation framework
- Validated performance across diverse operating ranges, proving robustness and adaptability





#### **Future Work**

- **Testing in other Operating Conditions**: Assess model performance in extreme conditions
- Fast Charging: Design optimal current profile using the model to reduce charging time
- **Applications to other Cell Chemistries**: Evaluate and extend the model to other chemistries (e.g., sodium-ion)
- Ensemble Machine Learning: Improve model accuracy and generalizability
- Adaptive Modeling: Evaluate model's online adaption on aged cells



#### **Publications**

#### Journals:

- "Augmented Sparse Nonlinear Identification of Nonlinear Dynamics (aSINDy)," SIAM Journal on Optimization, (In Preparation)
- "Online Co-Estimation of State of Charge and Voltage Dynamics of Li-ion Batteries via Physics-Inspired Modeling," IEEE Trans. Transp. Electrif, (Under Review), IF: 7.2
- "Homogenized Mechanical-Electrochemical-Thermal Model of a Lithium-ion Cell," eTransportation, (Under Review), IF: 15
- "The Impact of Lightweighting and Battery Technologies on the Sustainability of Electric Vehicles: A Comprehensive Life Cycle Assessment," *Environmental Impact Assessment Review* (2024), **IF: 9.8**
- "A Data-Driven Framework for Learning Governing Equations of Li-ion Batteries and Co-Estimating Voltage and State-of-Charge," Journal of Energy Storage (2024), IF: 8.9
- "Data-driven Discovery of Lithium-Ion Battery State of Charge Dynamics," Journal of Dynamic Systems, Measurement, and Control (2023)

#### **Conferences:**

- "Bootstrap-Based Sparse Modeling for Temperature-dependent State-Of-Charge Prediction of Batteries," 2025 American Control Conference (ACC'25), (Under Review)
- "Real-time Internal Short Circuit Detection in Li-ion Battery Modules During Field Use," ACC'24
- "A Physic-Inspired Machine Learning Nonlinear Model of Li-ion Batteries," ACC'23
- "Sparse Modeling of Energy Storage Systems in Presence of Noise," *IFAC-PapersOnLine* (2023)
- "Discovering Governing Equations of Li-ion Batteries Pertaining State of Charge Using Input-Output Data," ACC'23
- "Modeling of Li-ion batteries for real-time analysis and control: A data-driven approach," ACC'22