Predicting Rapid Degradation Onset in Lithium-Ion Batteries during Real-Time Operation Using Machine Learning

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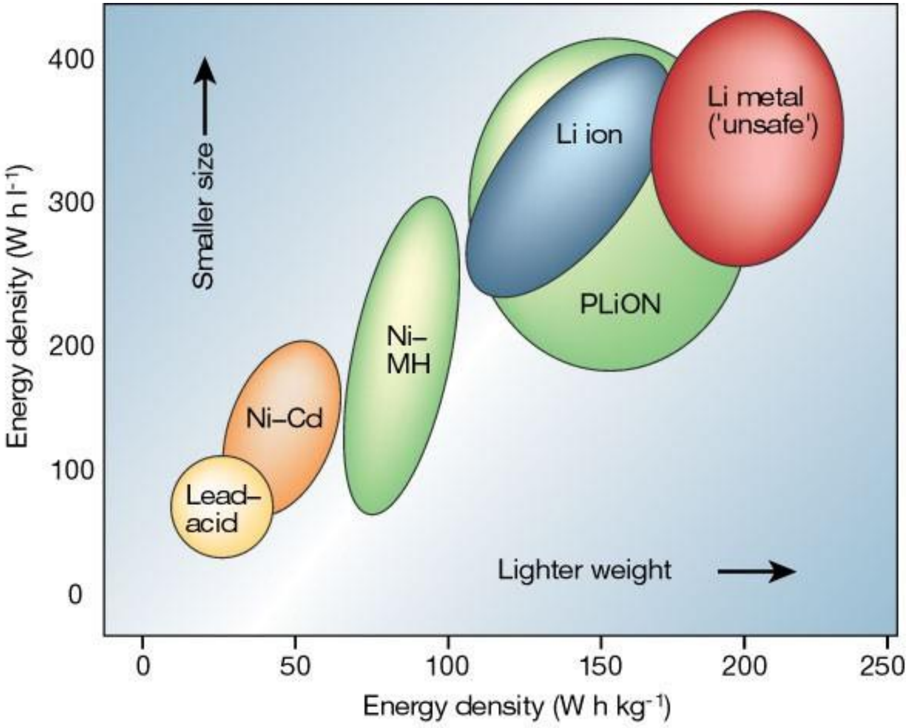
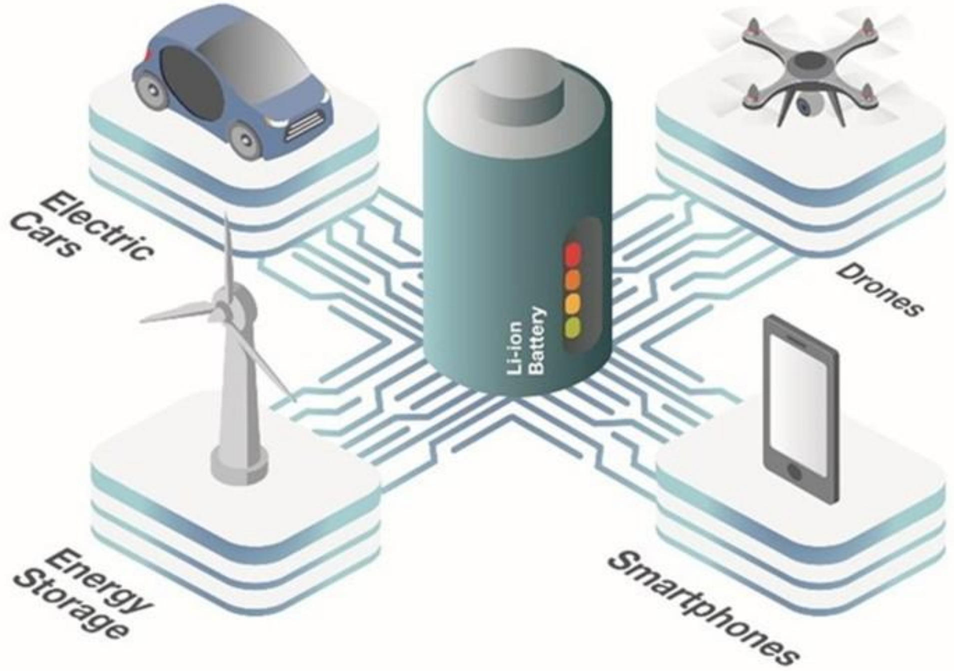
Benefits of Li-ion Batteries





- Li-ion batteries have higher energy densities and greater design flexibility
- Used in various applications like energy storage, transportation, and electronic devices.

Tarascon, J. M., and Armand, M., 2001, “Issues and challenges facing rechargeable lithium batteries,” Nature, **414**(6861), pp 359-367.

Potential Hazards of Li-ion Batteries

LIB shipment fire [1]

USS Bonefish [3]

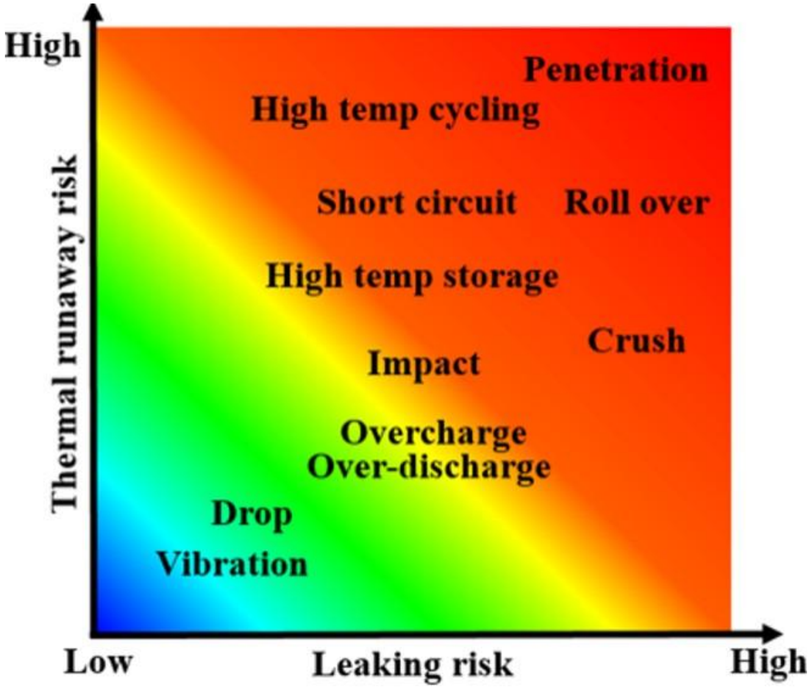
Samsung Galaxy Note 7 [4]

Boeing 787 [2]

EV crash fire [5]

[1] "Lithium battery fire hazard in the aviation industry," from http://www.lithiumsafe.com/lithium-battery-fires-in-aircraft/
[2] Lau, K., "Why the Boeing 787 Lithium-ion Battery System caught fire in 2013," from https://everspring.net/?p=686
[3] NavSource Online: Submarine Photo Archive, from http://www.navsource.org/archives/08/08582.htm
[4] Lopez, R., 2017, "Here's Why the Samsung Galaxy Note 7 Caught Fire," from https://www.revu.com.ph/2017/01/samsung-galaxy-note-7-fire-reason/
[5] Isidore, C., 2018, "Are electric cars more likely to catch fire?," from https://money.cnn.com/2018/05/17/news/companies/electric-car-fire-risk/index.html

Safety Map of Li-ion Batteries



- Various operating conditions affect the safety of batteries.

Objectives

- **Develop Machine Learning Models for Li-ion Battery Degradation Prediction:** Construct ML models to accurately predict the degradation trajectory and estimate the end-of-life (EOL) of Li-ion batteries based on operational and environmental conditions.

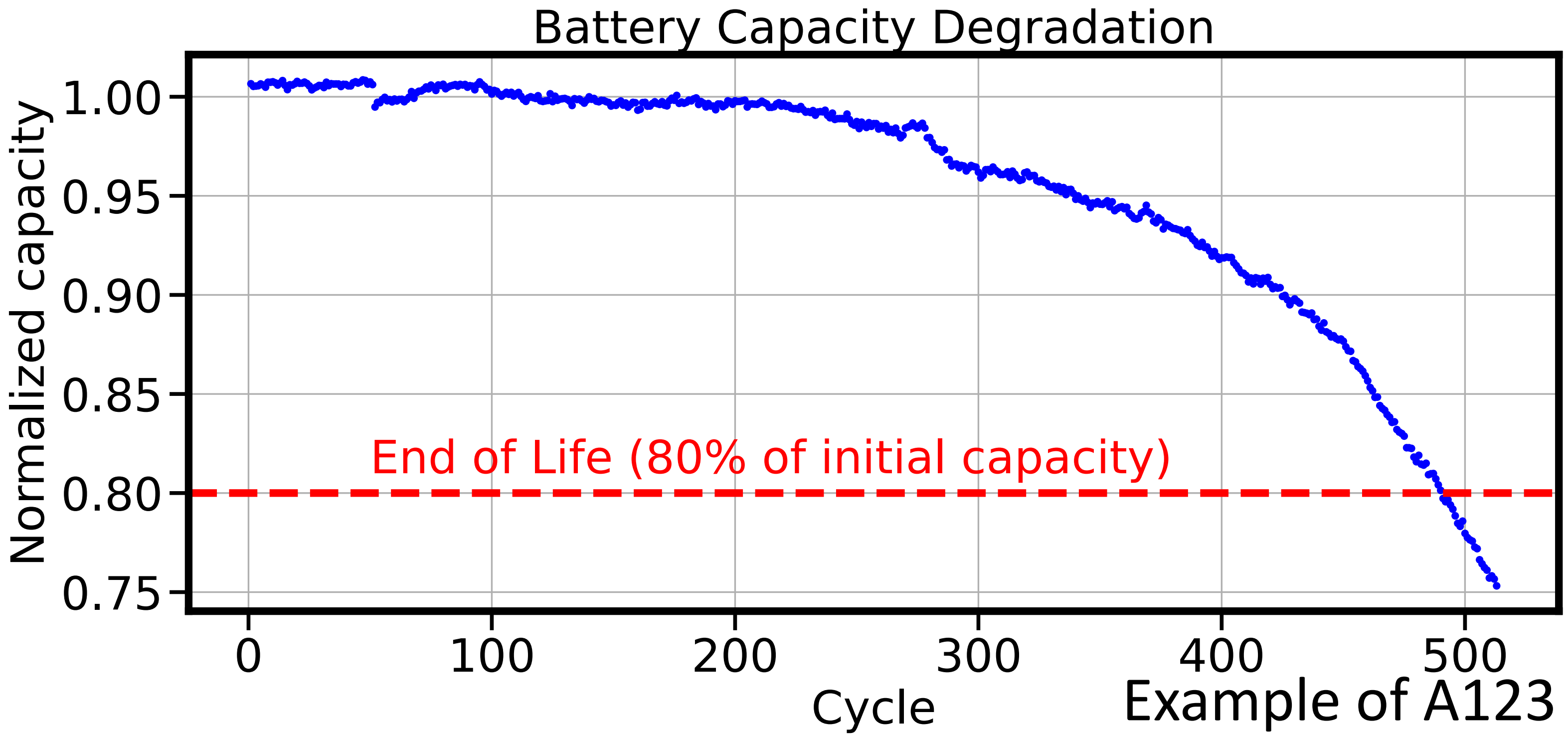
- **Anticipate Knee Points During Early Degradation Stages:** Define and predict knee points in the battery aging trajectory at early stages, considering varying usage and environmental conditions, to enhance reliability assessments.

- **Integrate Microstructural Insights for Enhanced SOH Prediction:** Leverage advanced microstructural data and insights to improve the accuracy of State of Health (SOH) predictions, capturing subtle degradation mechanisms in Li-ion batteries.

Objective 1

Construct ML models to accurately predict the degradation trajectory and estimate the end-of-life (EOL) of Li-ion batteries based on operational and environmental conditions.

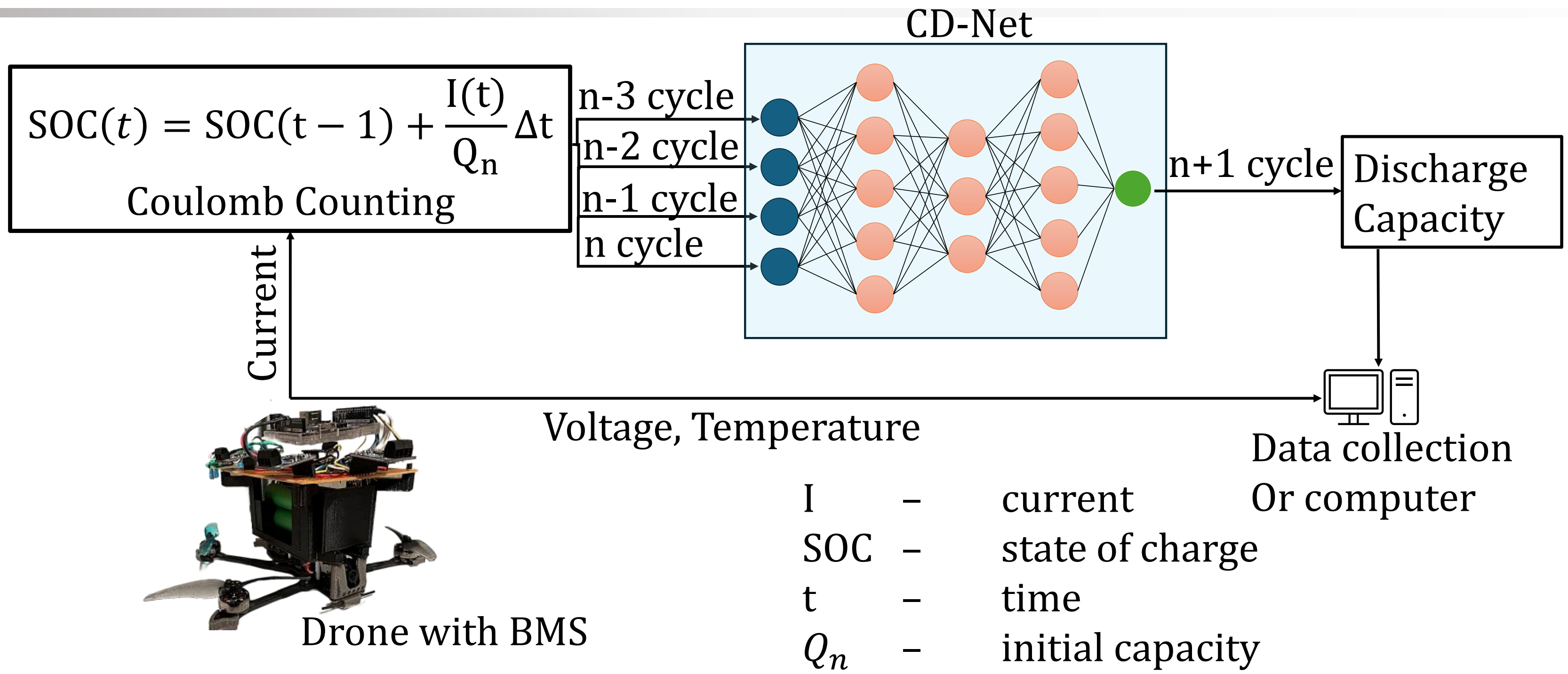
End of life for Li-ion batteries



Example of A123 LFP cell

- Li-ion batteries degrade over time, and their capacity reduces with each cycle.
- The battery is considered to have reached the end of life (EOL) when its capacity drops to 80% of its initial value.

In-operando data collection with ML predictions



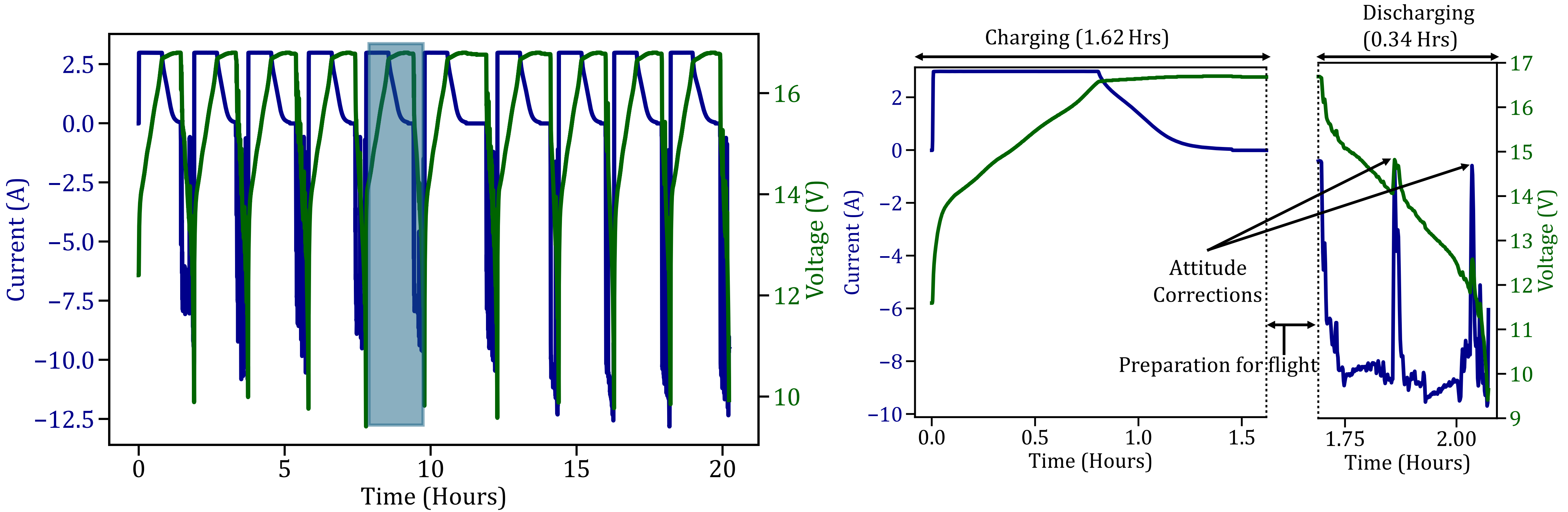
A drone with BMS on top, deep learning which helps to predict the discharge capacity by using CD-Net developed in-house by Sudarshan et al 2024

- Data collected using the BMS is transferred to the computer on the cloud side.
- Current and battery parameters like nominal capacity were used to predict the capacity of the battery pack.

Vajja, J.V.R.; Serov, A.; Sudarshan, M.; Singh, M.; Tomar, V. In Operando Health Monitoring for Lithium-Ion Batteries in Electric Propulsion Using Deep Learning. *Batteries* **2024**, *10*, 355. https://doi.org/10.3390/batteries10100355

Current and Voltage Profiles

In-air

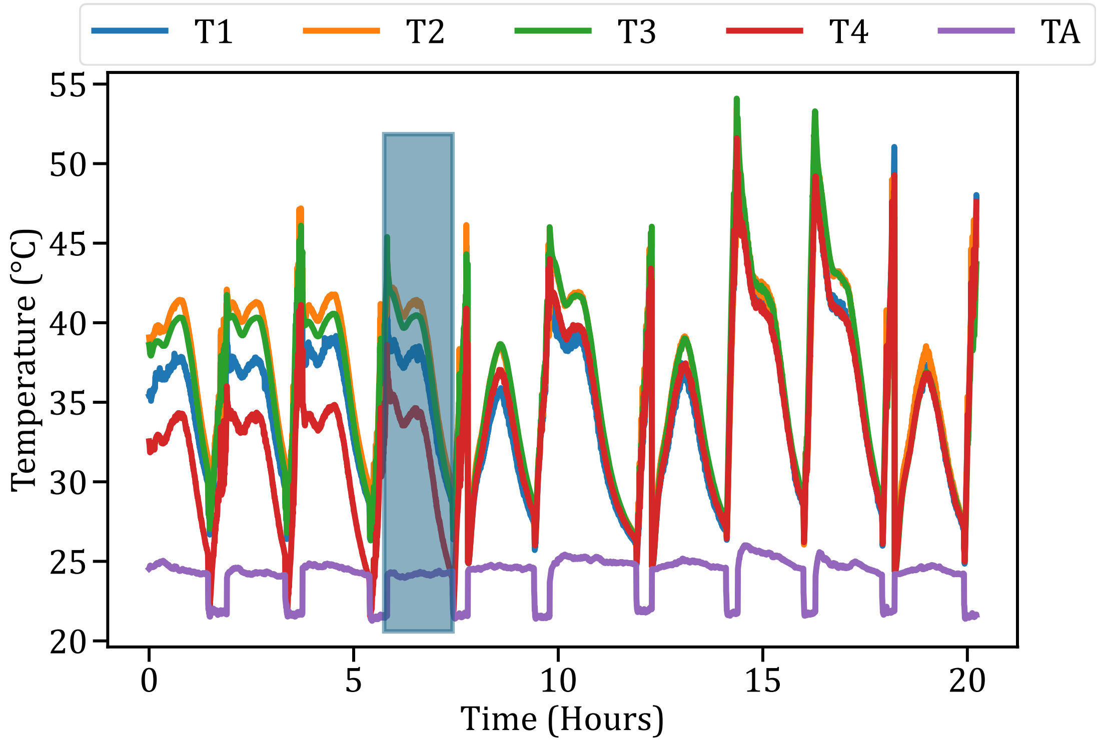


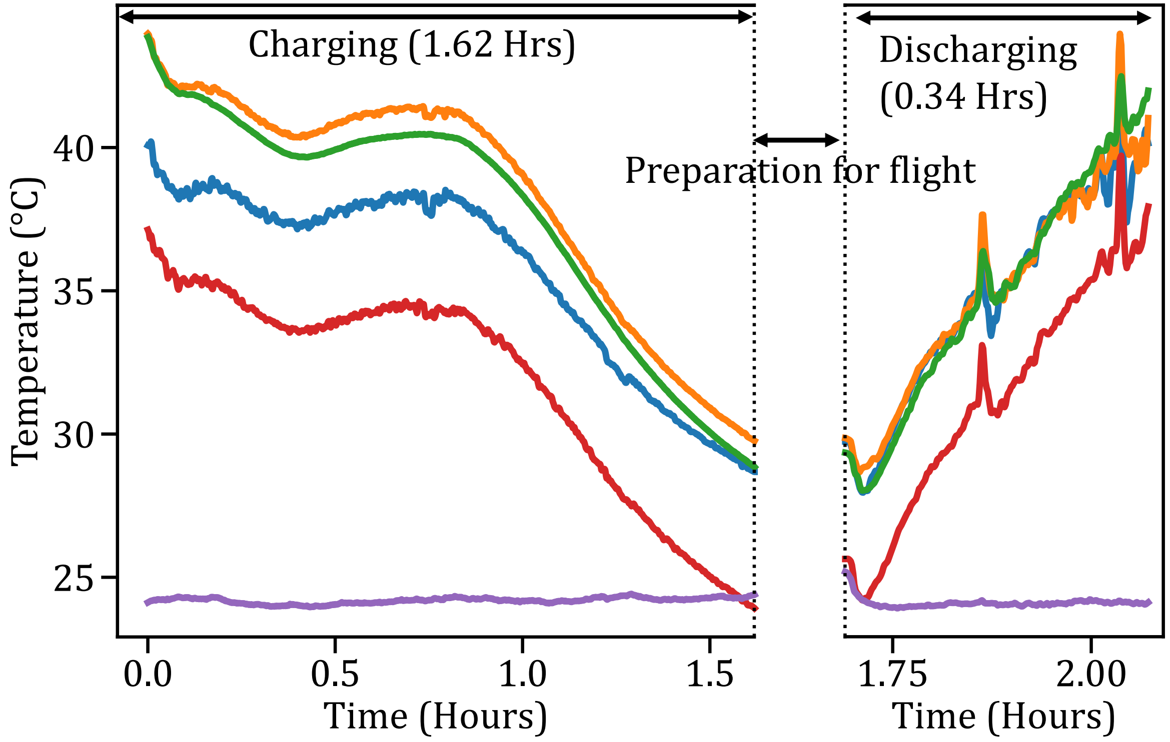
- Discharge of the fully charged NCA battery pack would last 10-30 minutes during operation.
- Discharge of the battery reaches as high as 4 C during operation.

Vajja, J.V.R.; Serov, A.; Sudarshan, M.; Singh, M.; Tomar, V. In Operando Health Monitoring for Lithium-Ion Batteries in Electric Propulsion Using Deep Learning. *Batteries* **2024**, *10*, 355. https://doi.org/10.3390/batteries10100355

Temperature Profile

In-air

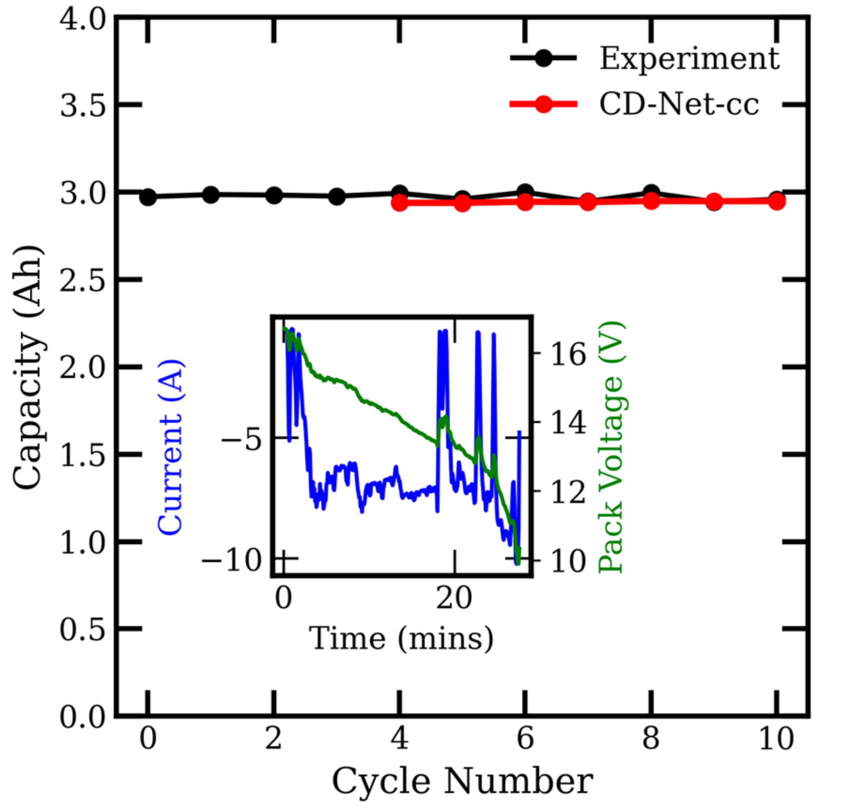




- Each cell on the battery pack showed different temperatures during operation.
- Dip in ambient temperature indicates the airflow during flight.
- Highest temperature was observed in T3 around 55 ° C

Vajja, J.V.R.; Serov, A.; Sudarshan, M.; Singh, M.; Tomar, V. In Operando Health Monitoring for Lithium-Ion Batteries in Electric Propulsion Using Deep Learning. *Batteries* **2024**, *10*, 355. https://doi.org/10.3390/batteries10100355

Discharge Capacity Predictions in-operando



- Deep learning predictions of capacity compared with coulomb counting capacity.
- In-air experiments showed oscillating capacity due to the discharge profile during operation.
- Deep learning was able to predict capacity with that discharge profile.

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Vajja, J.V.R.; Serov, A.; Sudarshan, M.; Singh, M.; Tomar, V. In Operando Health Monitoring for Lithium-Ion Batteries in Electric Propulsion Using Deep Learning. *Batteries* **2024**, *10*, 355. https://doi.org/10.3390/batteries10100355

Interfacial Multiphysics Lab

Objective 2

Define and predict knee points in the battery aging trajectory at early stages, considering varying usage and environmental conditions, to enhance reliability assessments.

Effects of cycling protocol

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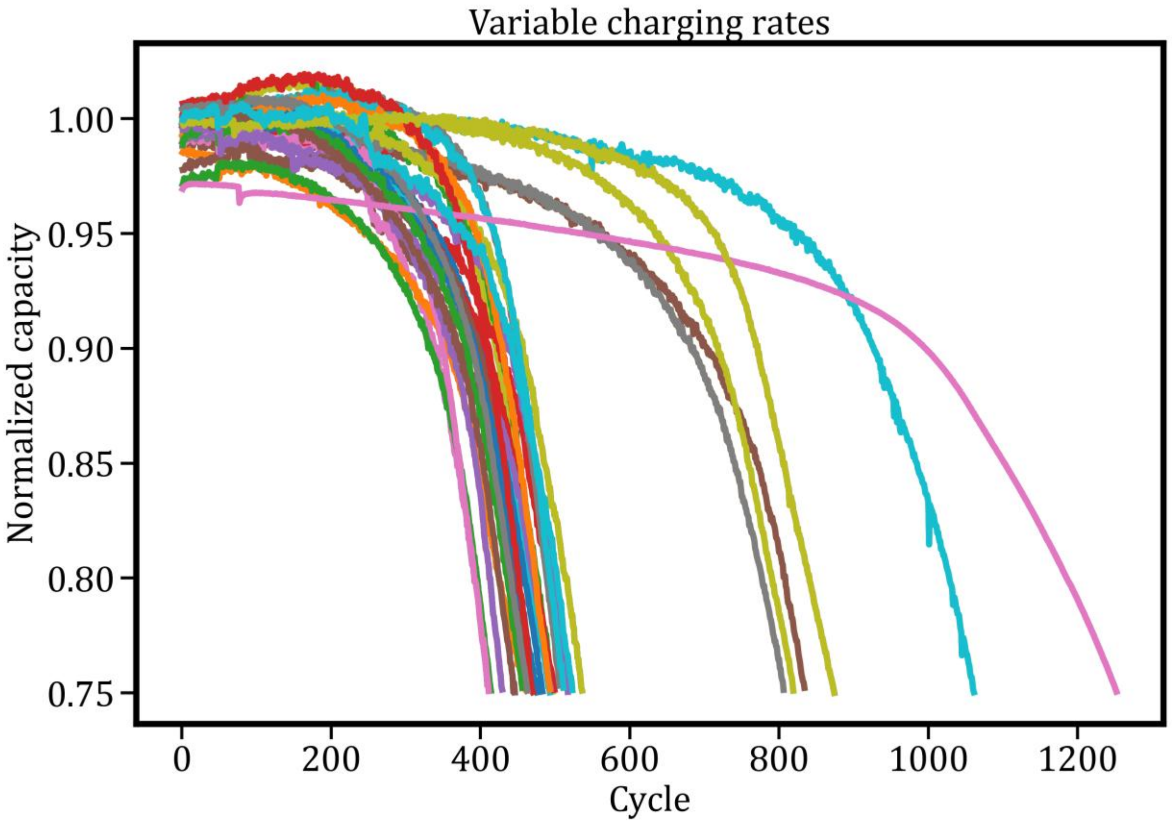


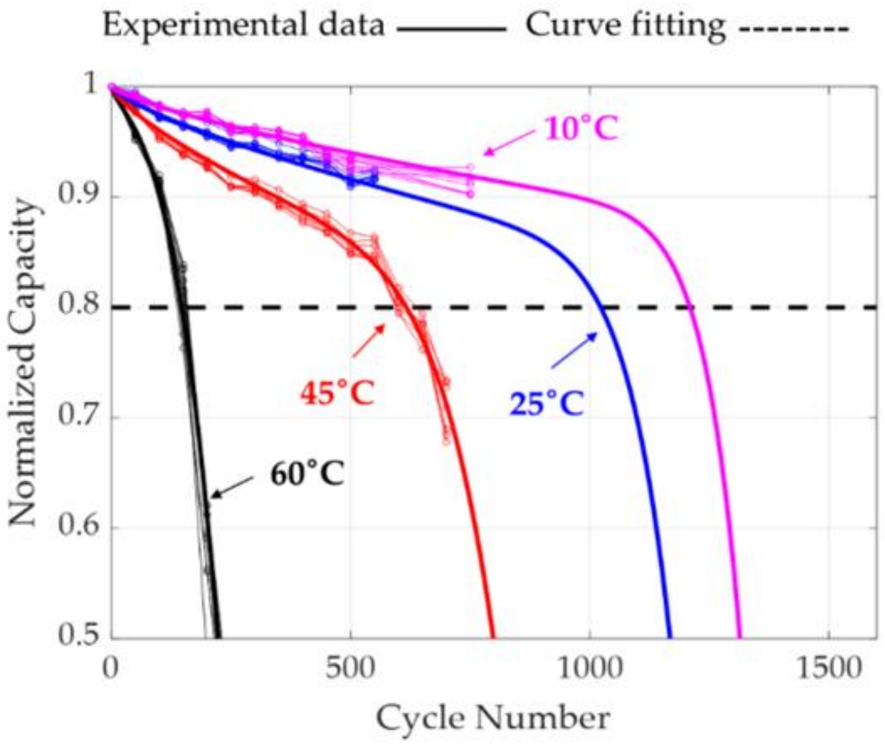
Example of A123 LFP cells Cycled under:

- variable charging current 3C to 8C
- Constant discharge 4C
- Nominal capacity is 1.1 Ah.

- LFP cells were cycled in a temperature-controlled chamber.
- Changing in charging or discharging current on the Li-ion battery causes capacity degrade faster.

Severson, K.A., Attia, P.M., Jin, N. et al. Data-driven prediction of battery cycle life before capacity degradation. Nat Energy 4, 383–391 (2019). https://doi.org/10.1038/s41560-019-0356-8

Effects of ambient temperature



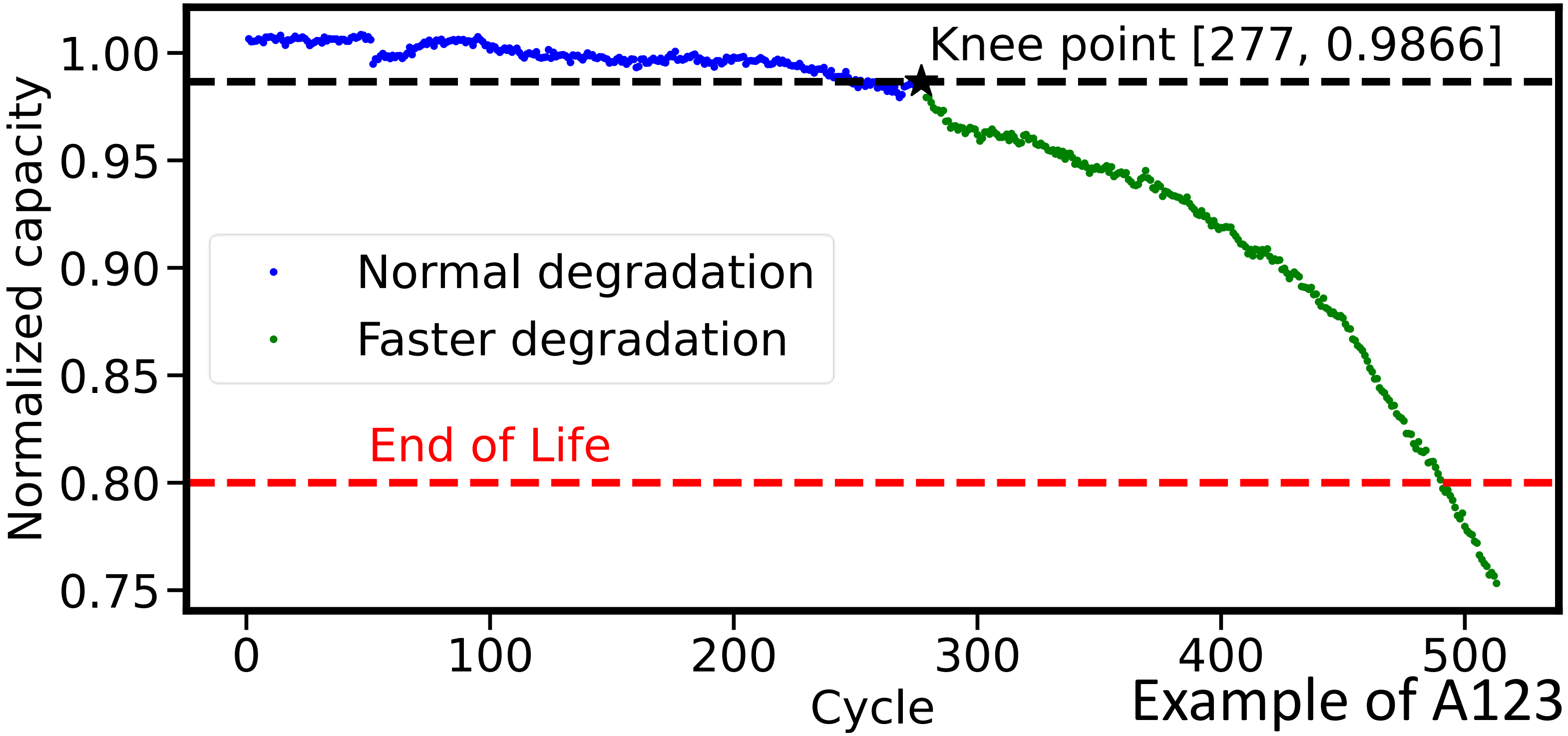
Example of LCO pouch cells Cycled under:

- CCCV charge of 1.5 Ah
- Constant discharge at 0.7C
- Nominal capacity is 3.6 Ah.

- Constant current and constant voltage charge and constant current discharge on the battery and increasing ambient temperature cause faster capacity degradation.

Diao, Weiping, Saurabh Saxena, Bongtae Han, and Michael Pecht. 2019. "Algorithm to Determine the Knee Point on Capacity Fade Curves of Lithium-Ion Cells" *Energies* 12, no. 15: 2910. https://doi.org/10.3390/en12152910.

Two phase degradation of Li-ion Batteries



Example of A123 LFP cell

- Li-ion batteries undergo two-phase degradation, where the rate of capacity loss is initially slow in the first phase and accelerates in the second phase.
- The knee point is defined as the point where there is a significant change in the rate of degradation.

Severson, K.A., Attia, P.M., Jin, N. et al. Data-driven prediction of battery cycle life before capacity degradation. Nat Energy 4, 383–391 (2019). https://doi.org/10.1038/s41560-019-0356-8

Impact of Charging Rate and Ambient Temperature on Battery Degradation

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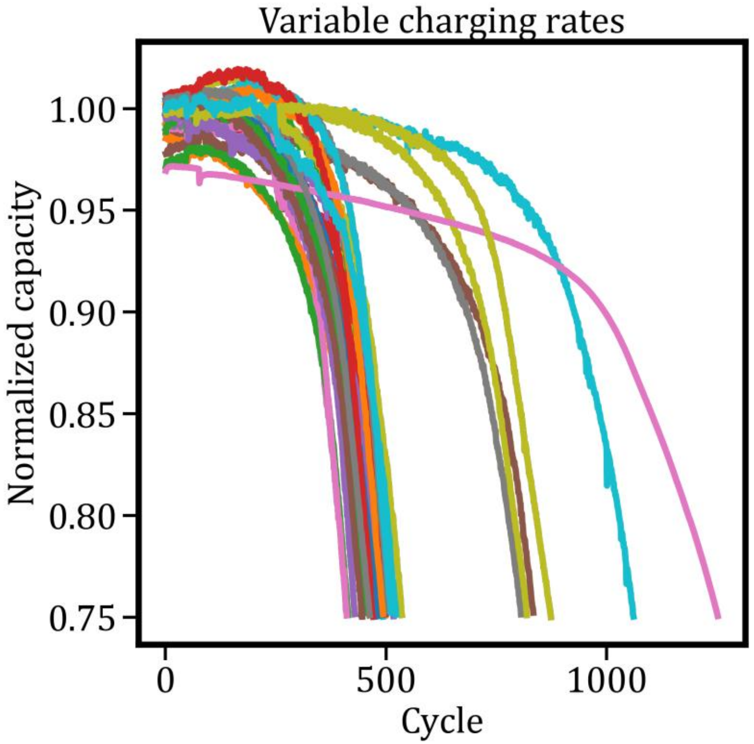
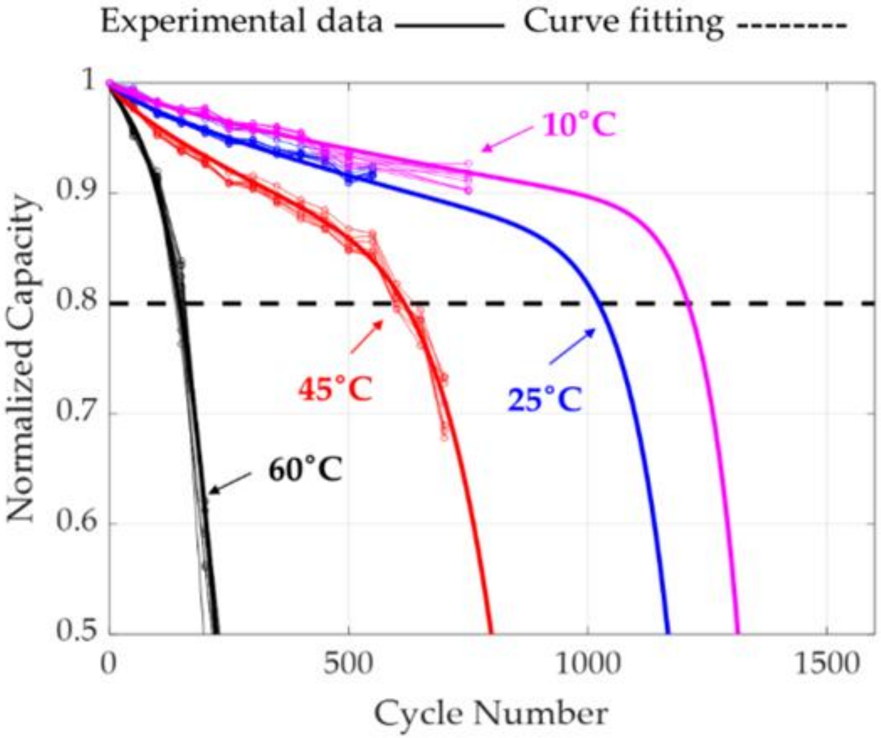
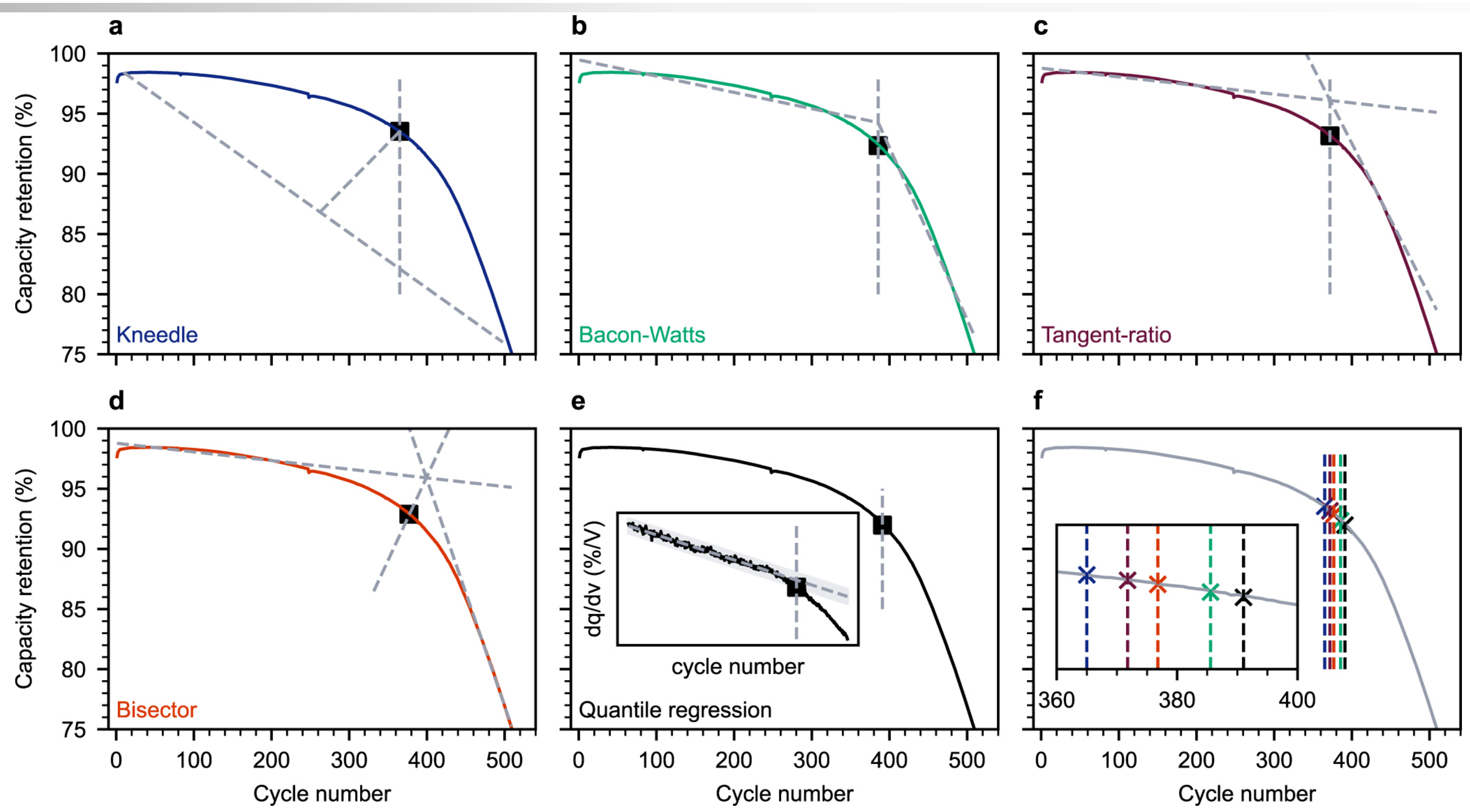




- Delaying knee point implies increase of remaining useful life.

Severson, K.A., Attia, P.M., Jin, N. et al. Data-driven prediction of battery cycle life before capacity degradation. Nat Energy 4, 383–391 (2019). https://doi.org/10.1038/s41560-019-0356-8
Diao, Weiping, Saurabh Saxena, Bongtae Han, and Michael Pecht. 2019. "Algorithm to Determine the Knee Point on Capacity Fade Curves of Lithium-Ion Cells" *Energies* 12, no. 15: 2910. https://doi.org/10.3390/en12152910.

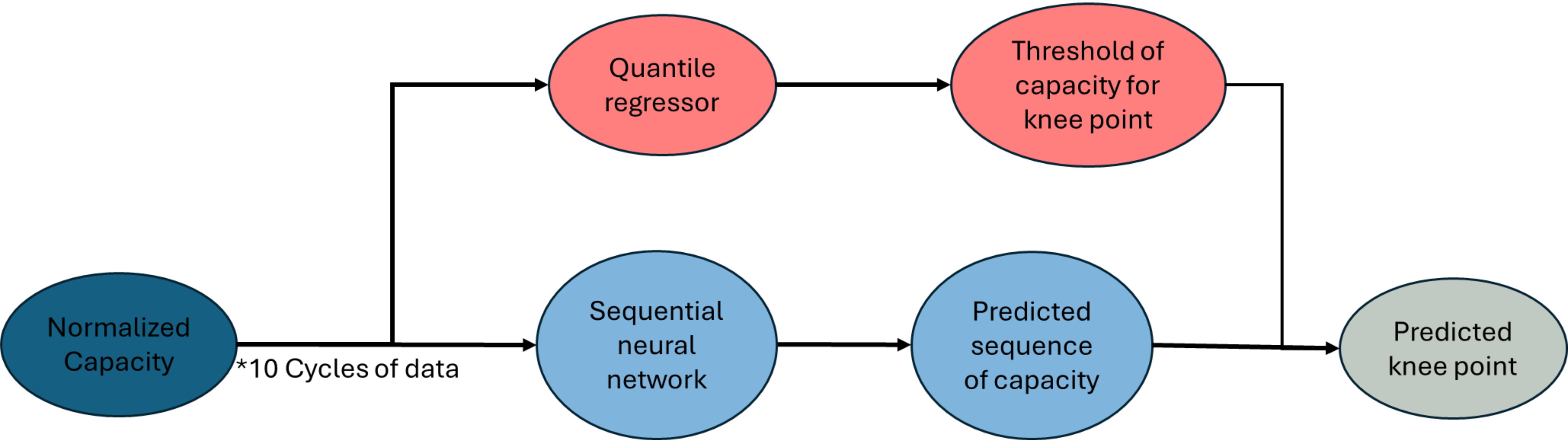
Methods to define knee point in Li-ion batteries



- Kneedle, Bacon-watts, Tangent-ratio and Bisector methods require the entire life cycle data of battery to define the knee point.
- Quantile regression method has an advantage over others by adapting to the incoming cycle data.

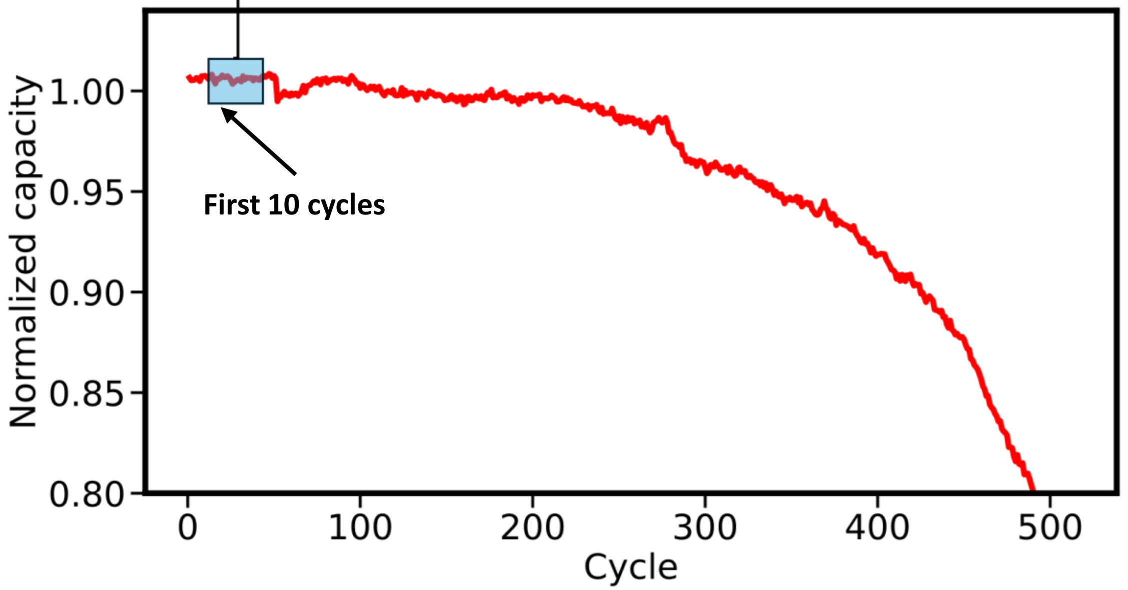
P. M. Attia, A. Bills, F. Brosa Planella, P. Dechent, G. dos Reis, M. Dubarry, P. Gasper, R. Gilchrist, S. Greenbank, D. Howey, O. Liu, E. Khoo, Y. Preger, A. Soni, S. Sripad, A. G. Stefanopoulou, and V. Sulzer, "Review—'Knees' in Lithium-Ion Battery Aging Trajectories," *J. Electrochem. Soc.*, vol. 169, no. 6, p. 060517, Jun. 2022, doi: 10.1149/1945-7111/ac6d13.

Current Methodology for Knee Point Prediction

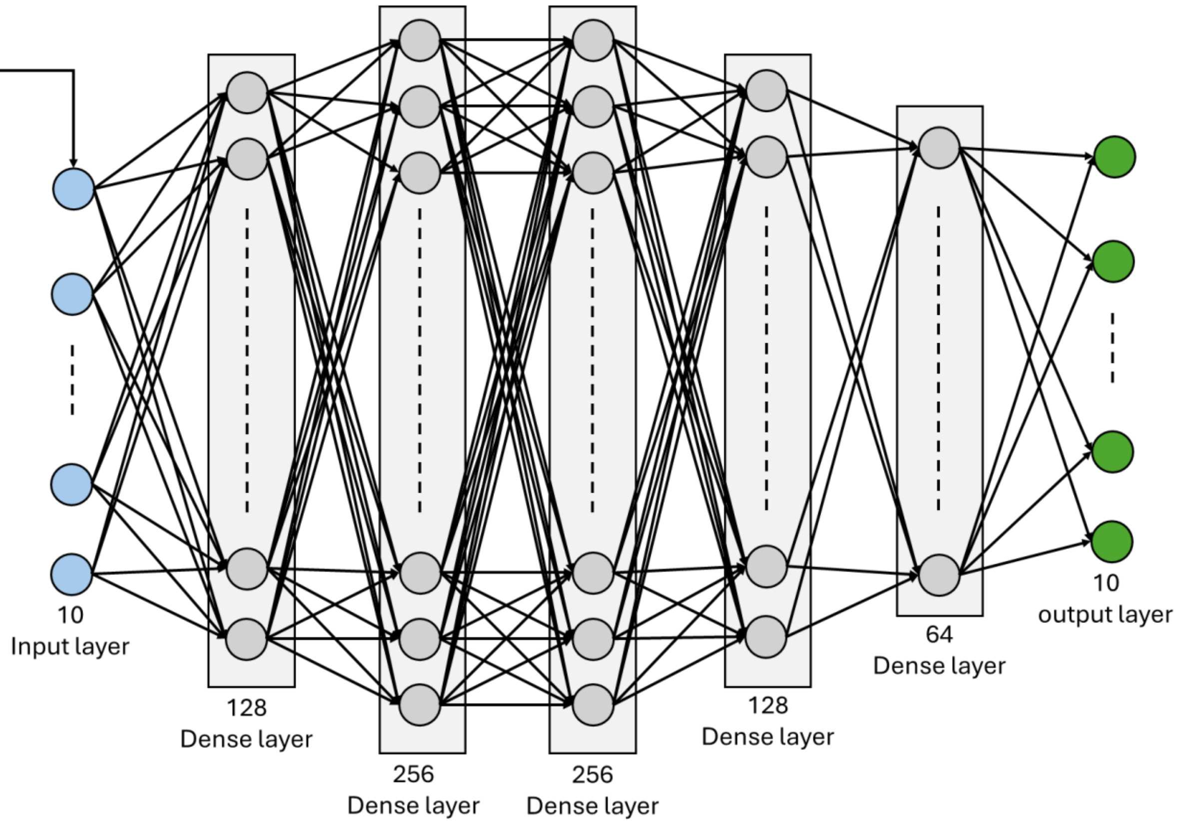


- Using normalized discharge capacity of the battery, knee point was predicted.
- Sequential neural network used to predict sequential capacity of next 10 cycles
- Quantile regression used to find knee point for predicted capacity data.

Inputs for neural network predictions

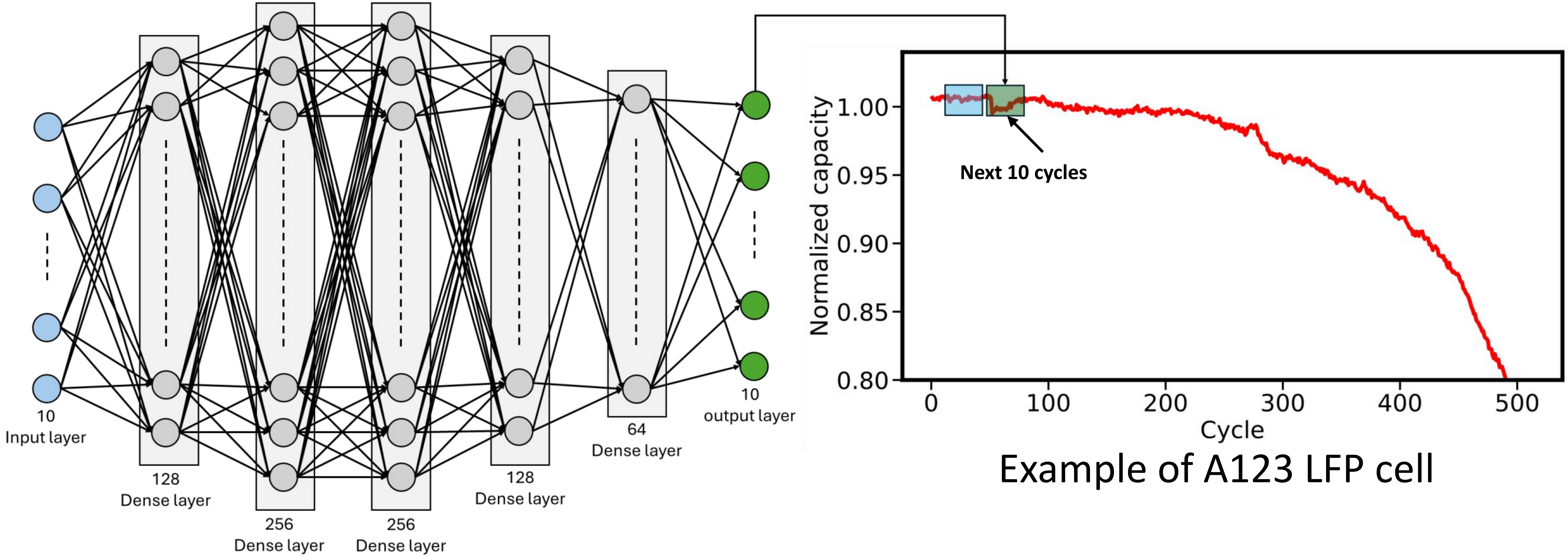


Example of A123 LFP cell



- Normalized capacity as a function of cycle is the input for sequential neural network with relu activation function and adam optimizer.

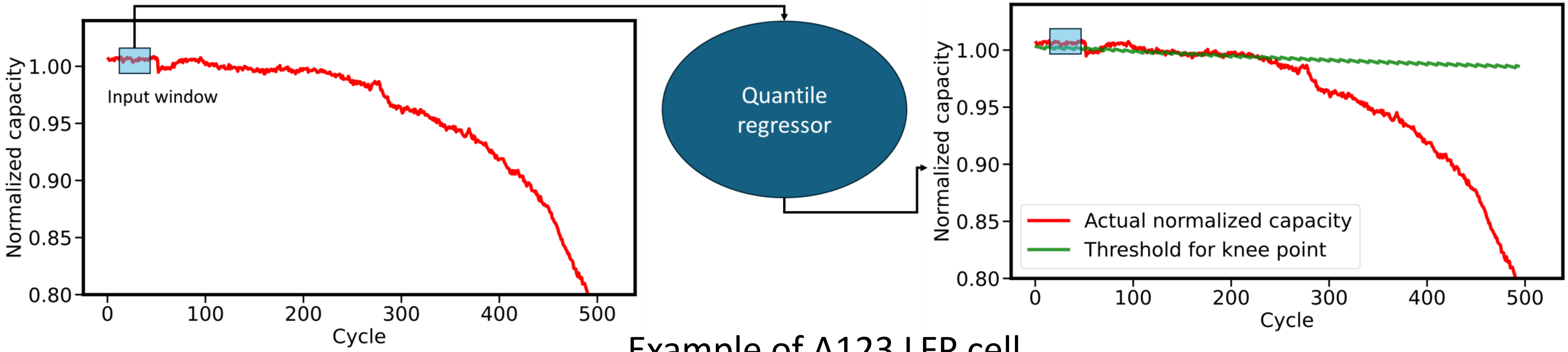
Predicted sequence of capacity data



Example of A123 LFP cell

- Using the neural network and inputs of capacity of 10 cycles, the next 10 cycles capacity of the Li-ion battery is predicted.

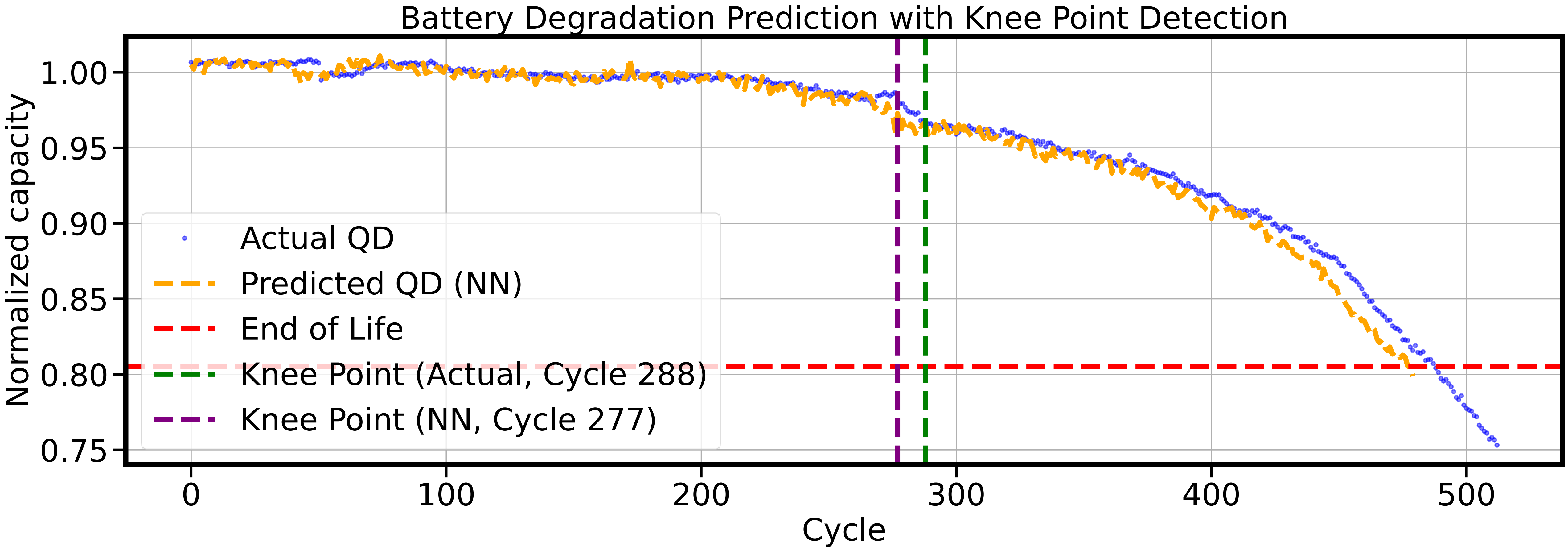
Threshold for knee identification in Capacity data



Example of A123 LFP cell

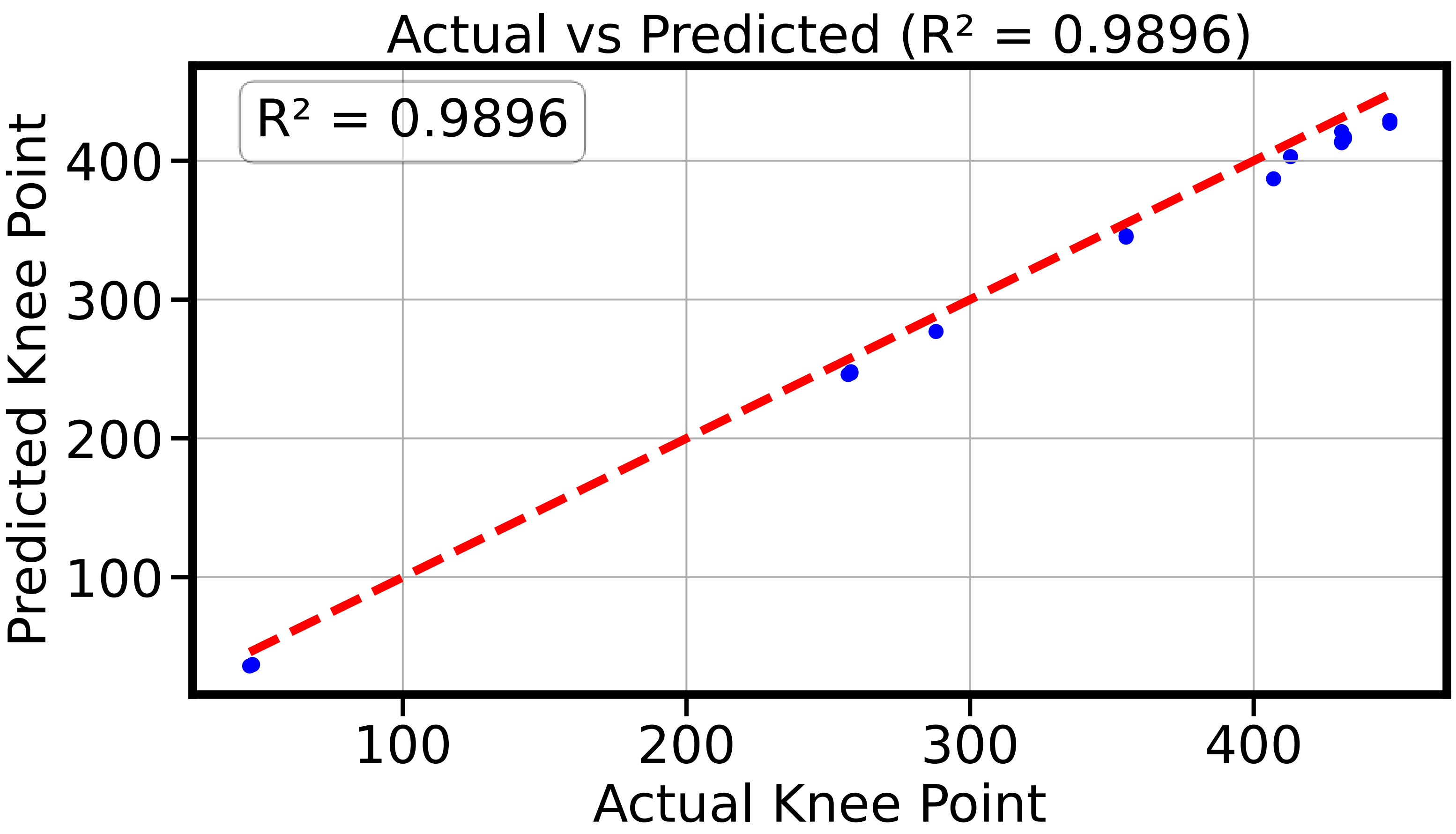
- Using input window of normalized capacity as a function of cycle, quantile regression model was used to find the threshold of capacity.
- Using this threshold of capacity, knee point is defined when the capacity of a cycle dips beyond the threshold.

Operation Driven Change in Knee Point



- Root mean square error of the predicted knee point is 100 cycles
- Root mean absolute error of the predicted knee point is 10 cycles

R squared plot in Knee Point Prediction



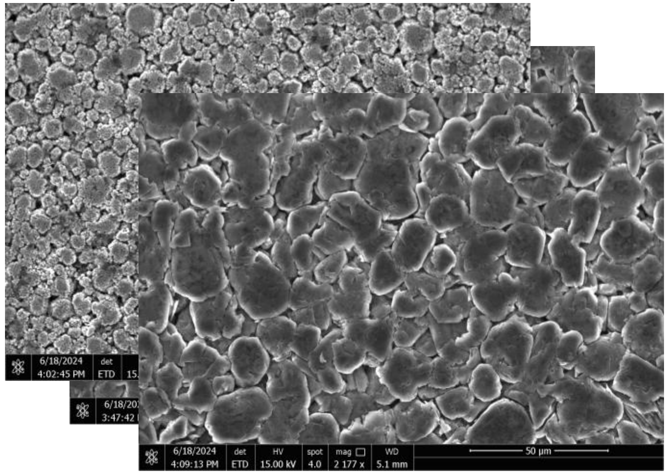
- R squared value of 0.9896 was achieved.

Objective 3

Leveraging advanced microstructural data and insights to improve the accuracy of State of Health (SOH) predictions, capturing subtle degradation mechanisms in Li-ion batteries.

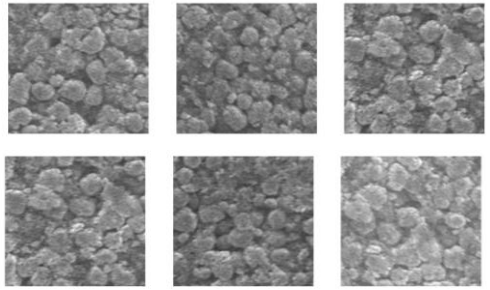
Image augmentation/Rotation Model

Data Acquisition



SEM images of anode and cathode surface

Data Augmentation



Transformation techniques such as rotation, scaling, random cropping helps improve the robustness and invariance of the model

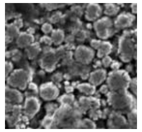
Inputs

Model training using EfficientNet B7 architecture

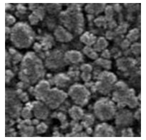
Outputs

Categories:

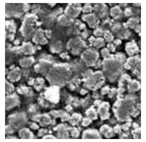
100 cycles



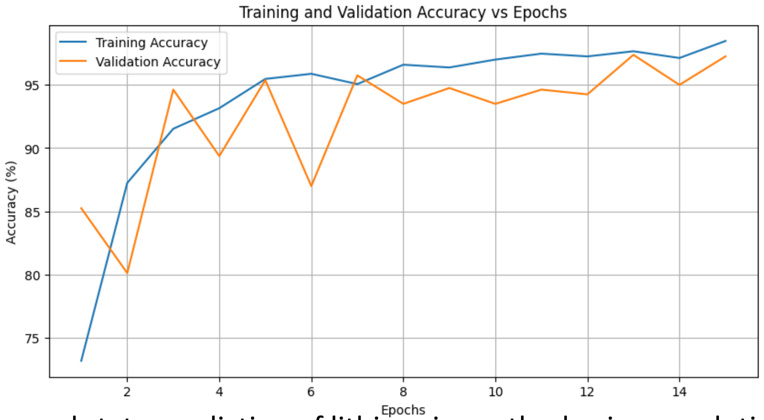
Pristine



Formation cycle only



Initial result:



Oh, J., Yeom, J., Madika, B. et al. Composition and state prediction of lithium-ion cathode via convolutional neural network trained on scanning electron microscopy images. npj Comput Mater 10, 88 (2024). https://doi.org/10.1038/s41524-024-01279-6

Summary

- Machine Learning Predictions:
  - Developed ML models successfully forecast the capacity degradation trajectory of Li-ion batteries with high accuracy across varying conditions.
  - Knee points in the degradation trajectory are effectively detected at early stages, enabling proactive maintenance and performance optimization.

- Microstructural Correlations:
  - Established strong correlations between microstructural degradation mechanisms and State of Health (SOH) predictions.
  - Advanced insights into the underlying microstructural changes improve the understanding of battery aging processes, enhancing SOH prediction accuracy.

Future Work

- The integration of machine learning with microstructural analysis offers a robust framework for accurately predicting Li-ion battery (LIB) degradation.
- This approach enables precise early detection of knee points, facilitating improved end-of-life (EOL) management and optimizing battery performance across diverse operating conditions.

Lab/Contact Information

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Questions?