239th ECS Meeting
with the 18th International Meeting on Chemical Sensors (IMCS)
DIGITAL MEETING • May 30-June 3, 2021

A01-0002

# Big Data for Li-Ion Diagnosis and Prognosis

**M. Dubarry and D. Beck**

matthieu@hawaii.edu

School of Ocean and Earth Science and Technology, University of Hawai'i at Mānoa

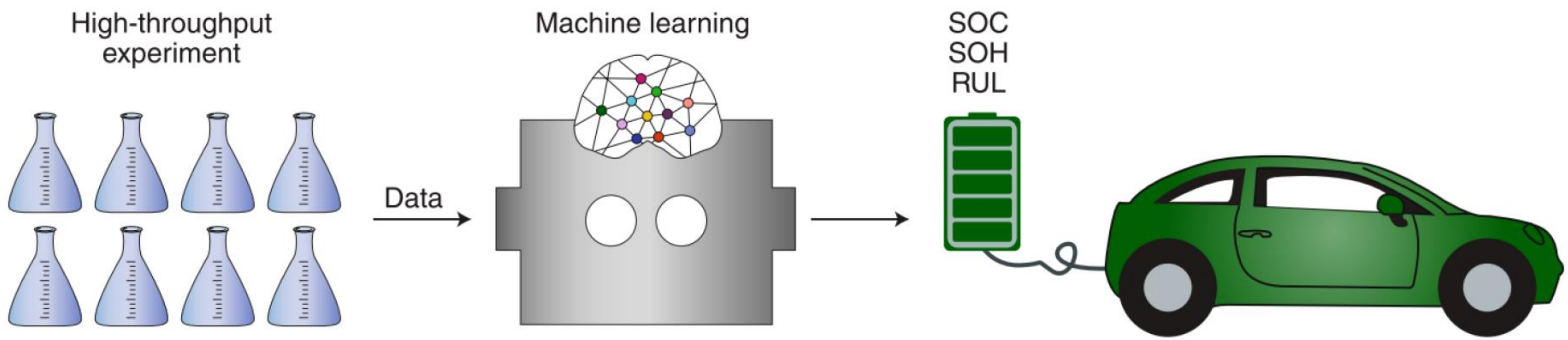
HNEI Hawai'i Natural Energy Institute, University of Hawai'i at Mānoa

1680 East West Road, POST 109,
Honolulu, HI 96822
Ph: (808) 956-2349 ● Fax: (808) 956-2336

-PakaLi+ Battery Laboratory

# Artificial Intelligence

## Objective/Significance



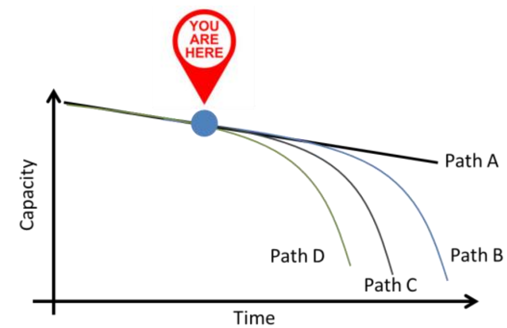

Little to no effort

Lot of effort

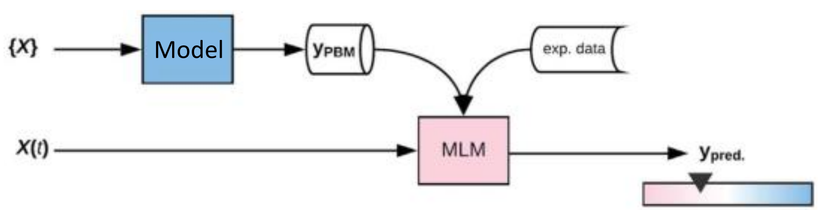
Man-Fai Ng et al., Nature Machine Intelligence, 2(3) p. 161-170 (2020)

Experimental data is costly and time consuming,
Most studies only test a couple batteries,
Biggest dataset: 124 batteries with only charge varying

Problematic because of path dependence.




**Current state of the art is far from the big data needed to make AI work**




Aylol et al., Journal of The Electrochemical Society, 2021 168 030525

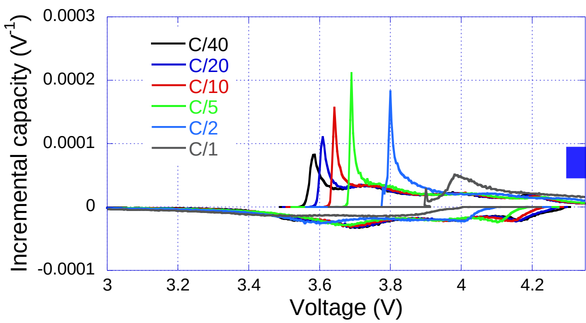
**Solution: Transfer Learning**
**Create synthetic training datasets**

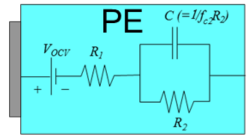
Dubarry M. et al., Journal of Power Sources 479 (2020) 228806

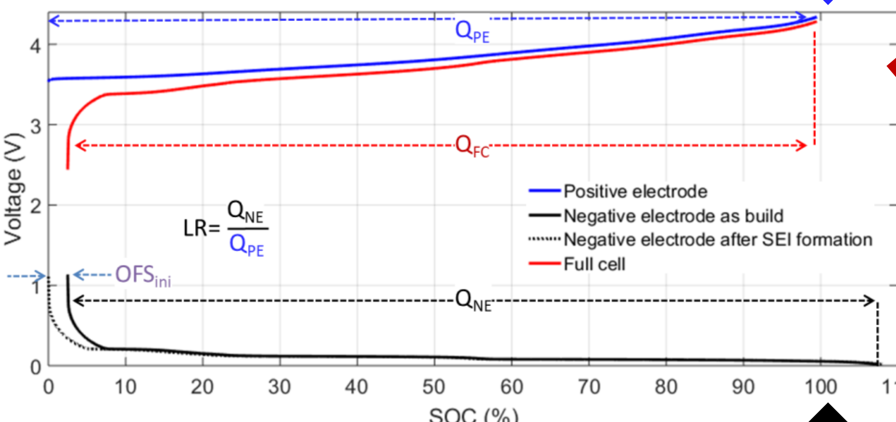
Big Data for Li-Ion Diagnosis and Prognosis

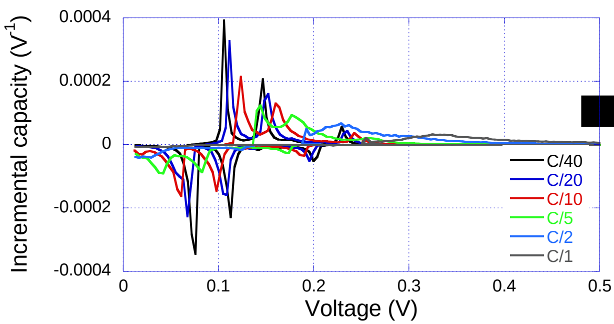
# Mechanistic modeling

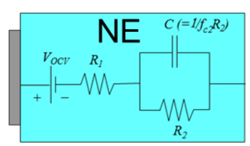
## General Approach

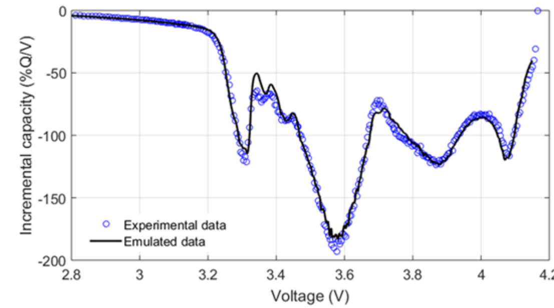


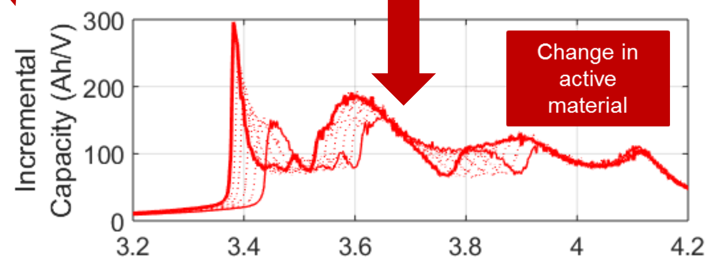



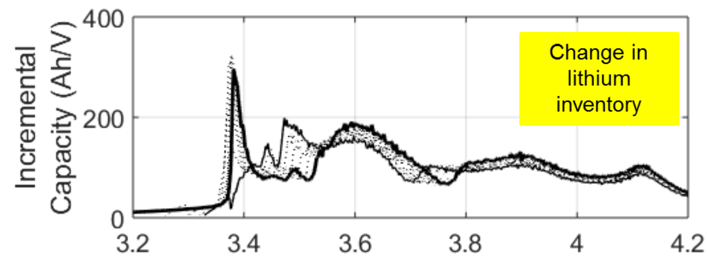



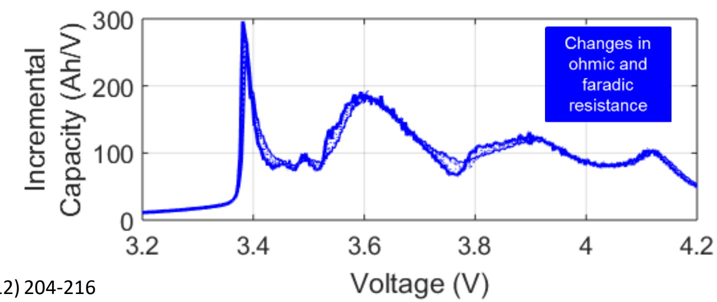



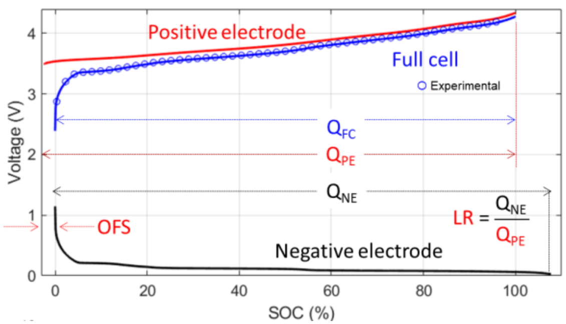




https://www.soest.hawaii.edu/HNEI/alawa/

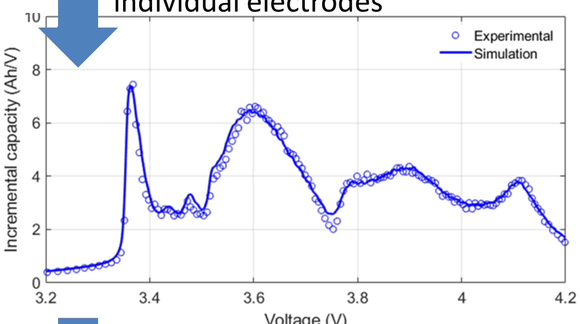
Dubarry M. et al. Journal of Power Sources 219 (2012) 204-216

# Mechanistic modeling

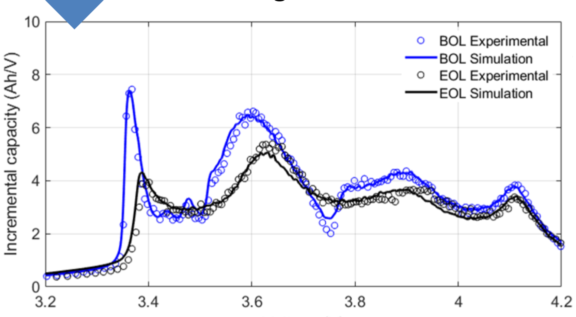
## Simulation of duty cycles and prognosis

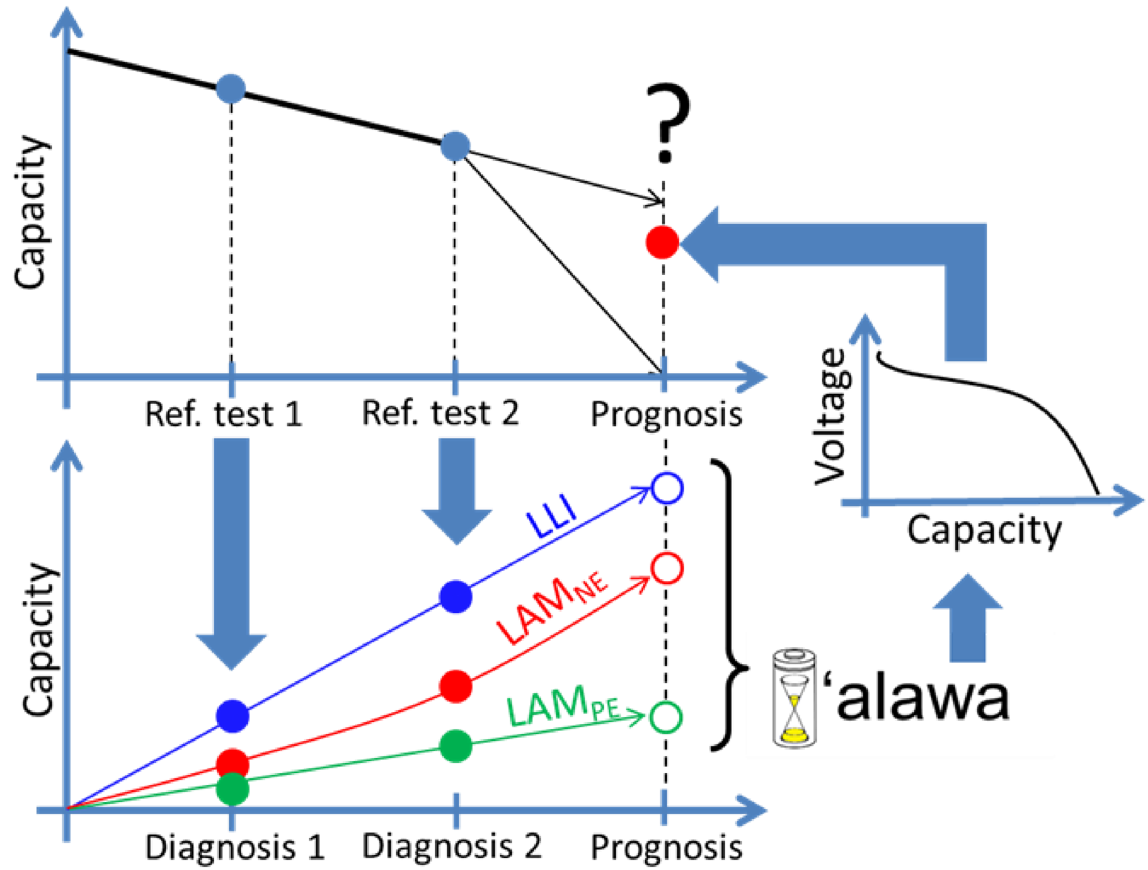



Match experimental cell based on individual electrodes




Vary matching parameters to emulate degradation



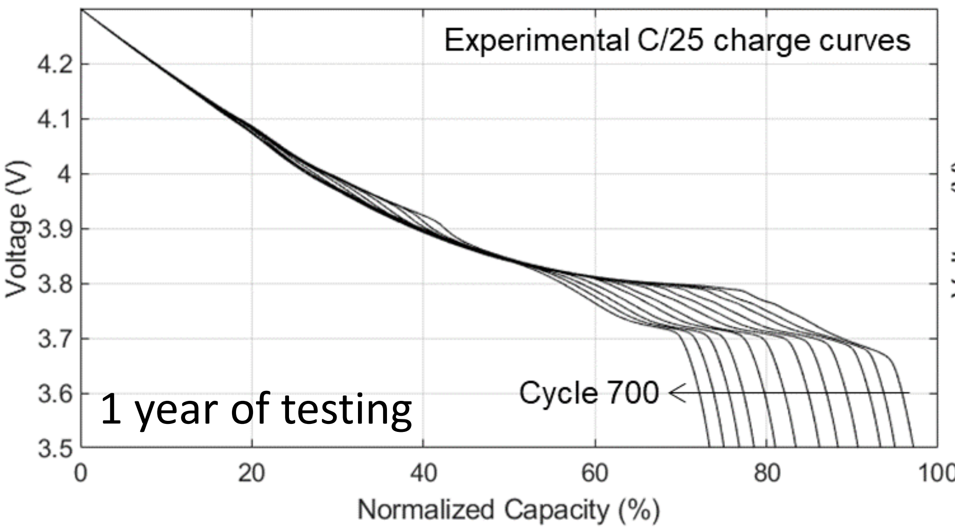

Dubarry M. et al., Journal of Energy Storage, 29, 101391 (2020); doi: 10.1016/j.est.2020.101391

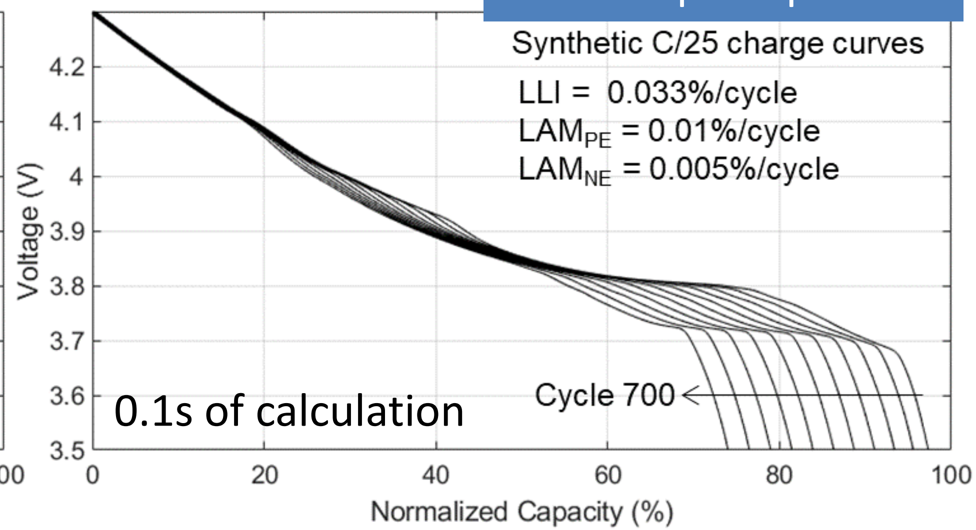
# Big Data for Li-Ion Diagnosis and Prognosis

# Mechanistic modeling

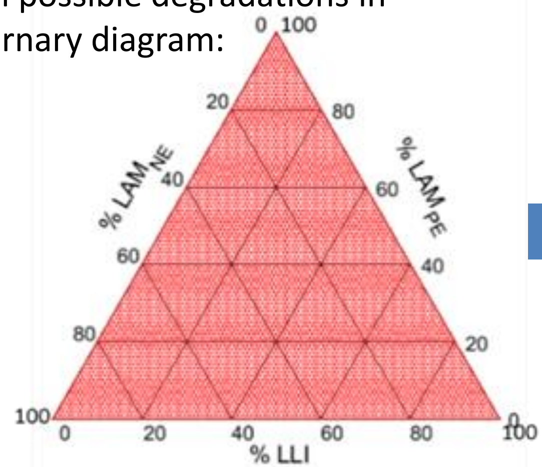
## Emulation of battery electrochemical response

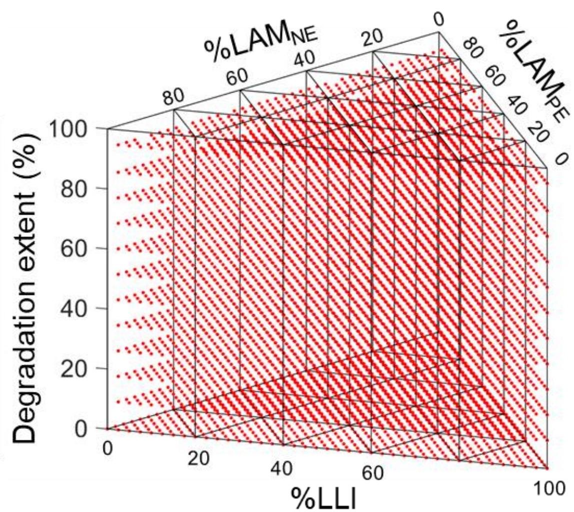
Aging reconstructed from simple equations




All possible degradations in ternary diagram:




Infinite training data for diagnosis AI algorithms

Dubarry M. et al., Journal of Power Sources 479 (2020) 228806

Dubarry, M., et al. (2017)., Journal of Power Sources **360**: 59-69.

# Computed datasets: Replicate complexity of real scenarios

## Open access synthetic datasets : LFP, NCA, NMC811 vs. Graphite

### V vs. Q datasets

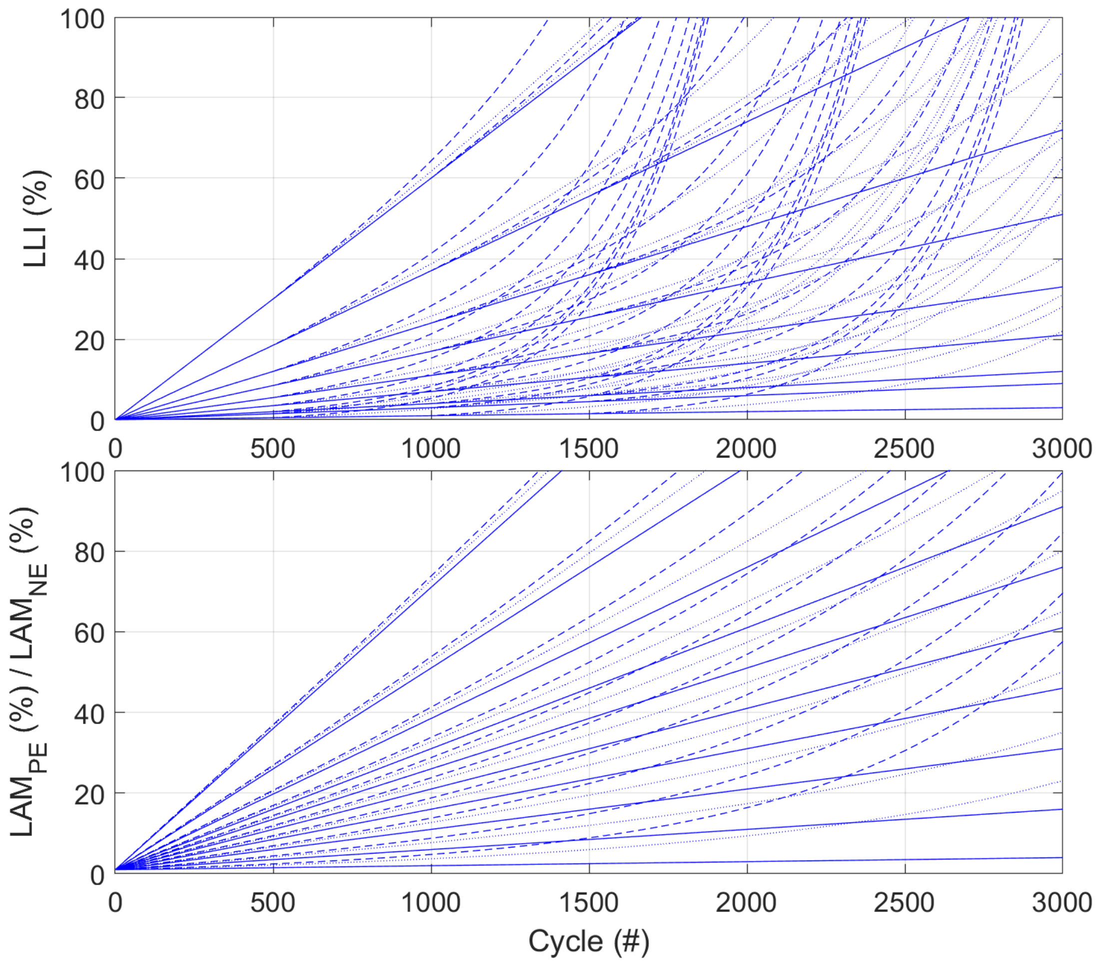
- >5,000 {LLI,$LAM_{PE}$,$LAM_{NE}$}
- At least 0.85% resolution
- > 700,000 V vs. Q curves

### Duty cycle datasets

- > 125,000 unique LLI/LAM evolution
- > 3,000,000 V vs. Q curves
- 8 parameters varied

  $\%deg = a \times cycle + e^{(b \times cycle)-1)}$

  for LLI, $LAM_{NE}$, & $LAM_{PE}$ plus delay and plating rev.





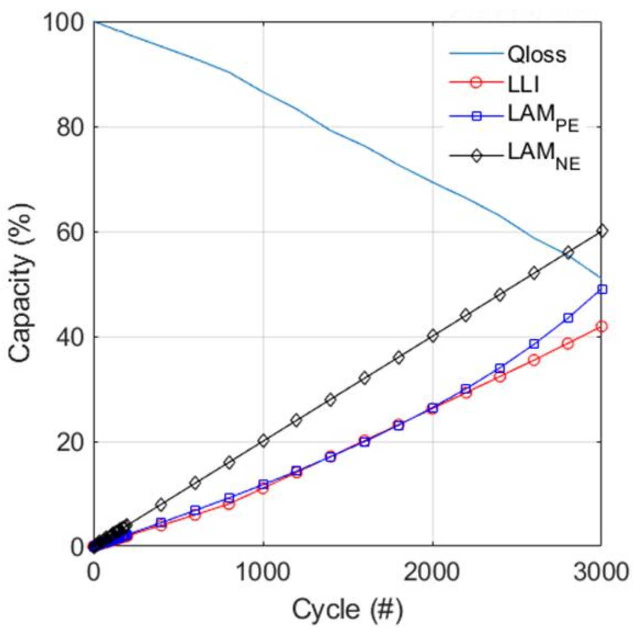
Mendeley Data, 2020; Vol. 2021, 10.17632/6s6ph9n8zg.3
Mendeley Data, 2020; Vol. 2021, 10.17632/bs2j56pn7y.3
Mendeley Data, 2021, 10.17632/2h8cpszy26.1
Mendeley Data, 2021, 10.17632/pb5xpv8z5r.1

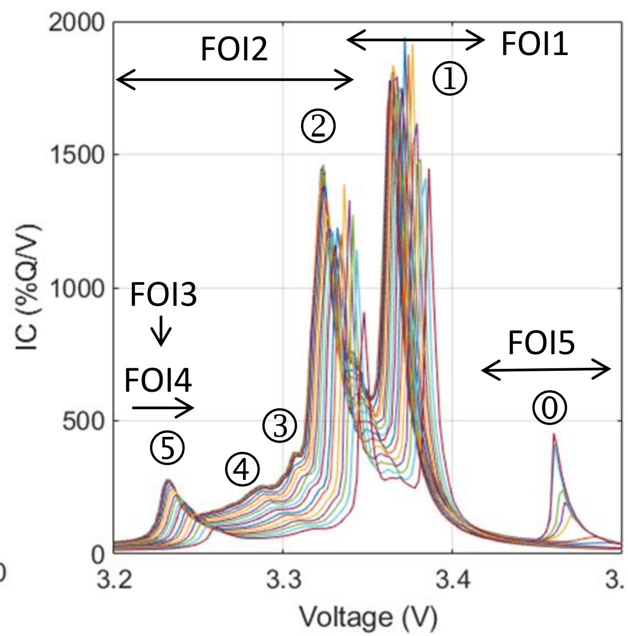
Dubarry M. et al., Journal of Power Sources 479 (2020) 228806
Dubarry M. et al., *Energies,* 2021, 14(9), 2371

# Diagnosis

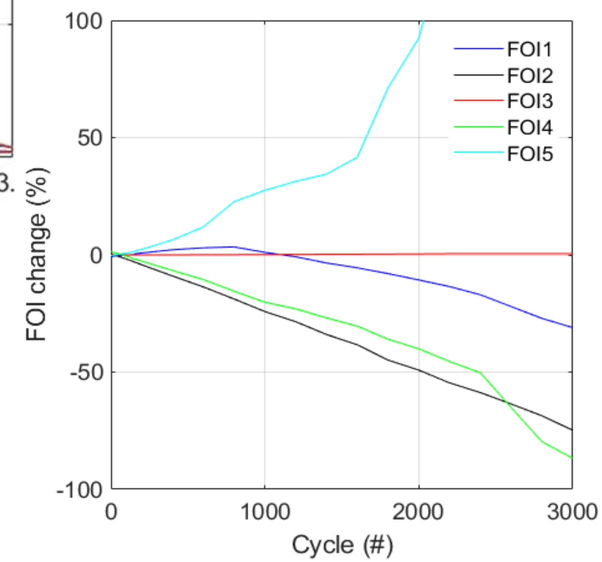
## Analyze the >125,000 duty cycle

### Example of a randomly selected duty cycle




Track FOI evolution



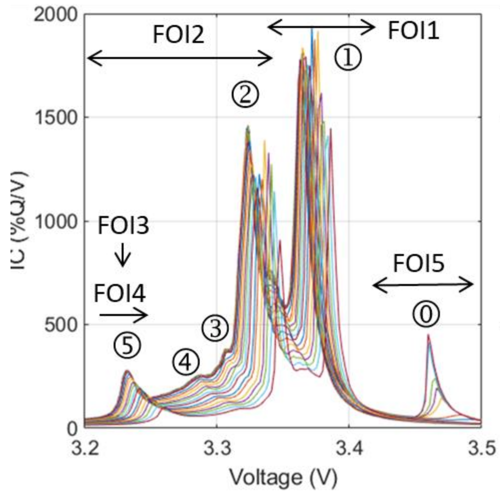

Use that information
to quantify LLI and LAMs
→ Diagnosis

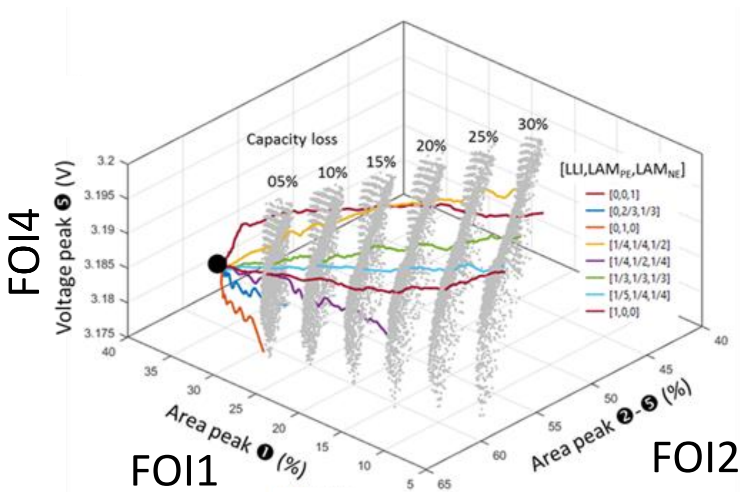
Dubarry M. et al., *Energies,* 2021, 14(9), 2371

# Diagnosis

## Apply to entire dataset: example at cycle 100

| | LLI | $LAM_{PE}$ | $LAM_{NE}$ | Capacity loss |
|---|---|---|---|---|
| FOI1 | -0.74 | -0.03 | 0.62 | -0.72 |
| FOI2 | -0.03 | 0.09 | -0.99 | -0.06 |
| FOI3 | 0.04 | -0.36 | 0.73 | 0.07 |
| FOI4 | 0.38 | -0.17 | -0.79 | 0.36 |
| FOI5 | -0.51 | -0.26 | 0.78 | -0.47 |



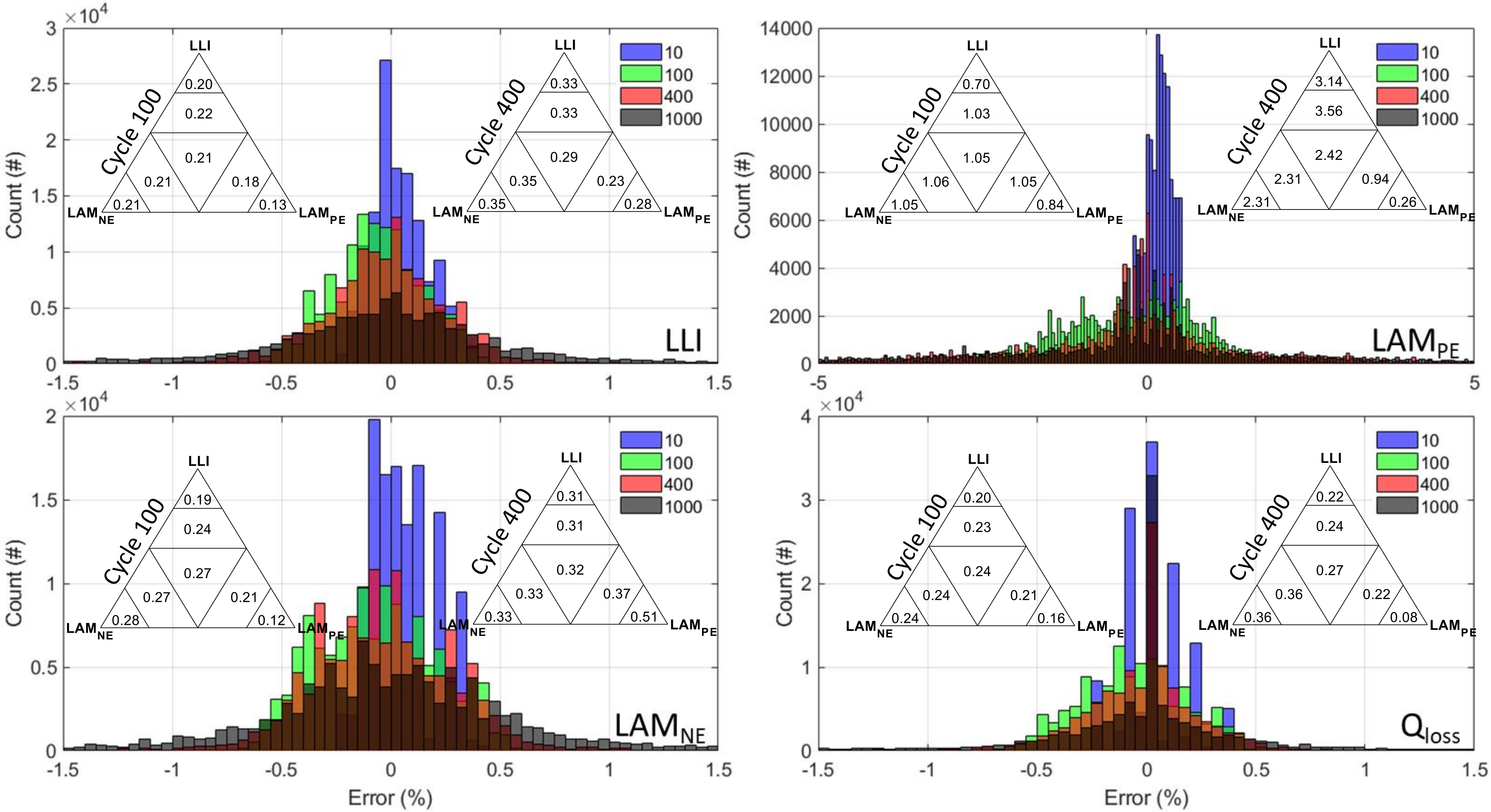

Single FOI determination will never allow a universal diagnosis.

Solution: Consider FOIs together

Dubarry M. et al., *Energies*, 2021, 14(9), 2371
Dubarry M. et al., *J. Power Sources*, **360** (2017), 59.

# Diagnosis

## Apply to entire dataset



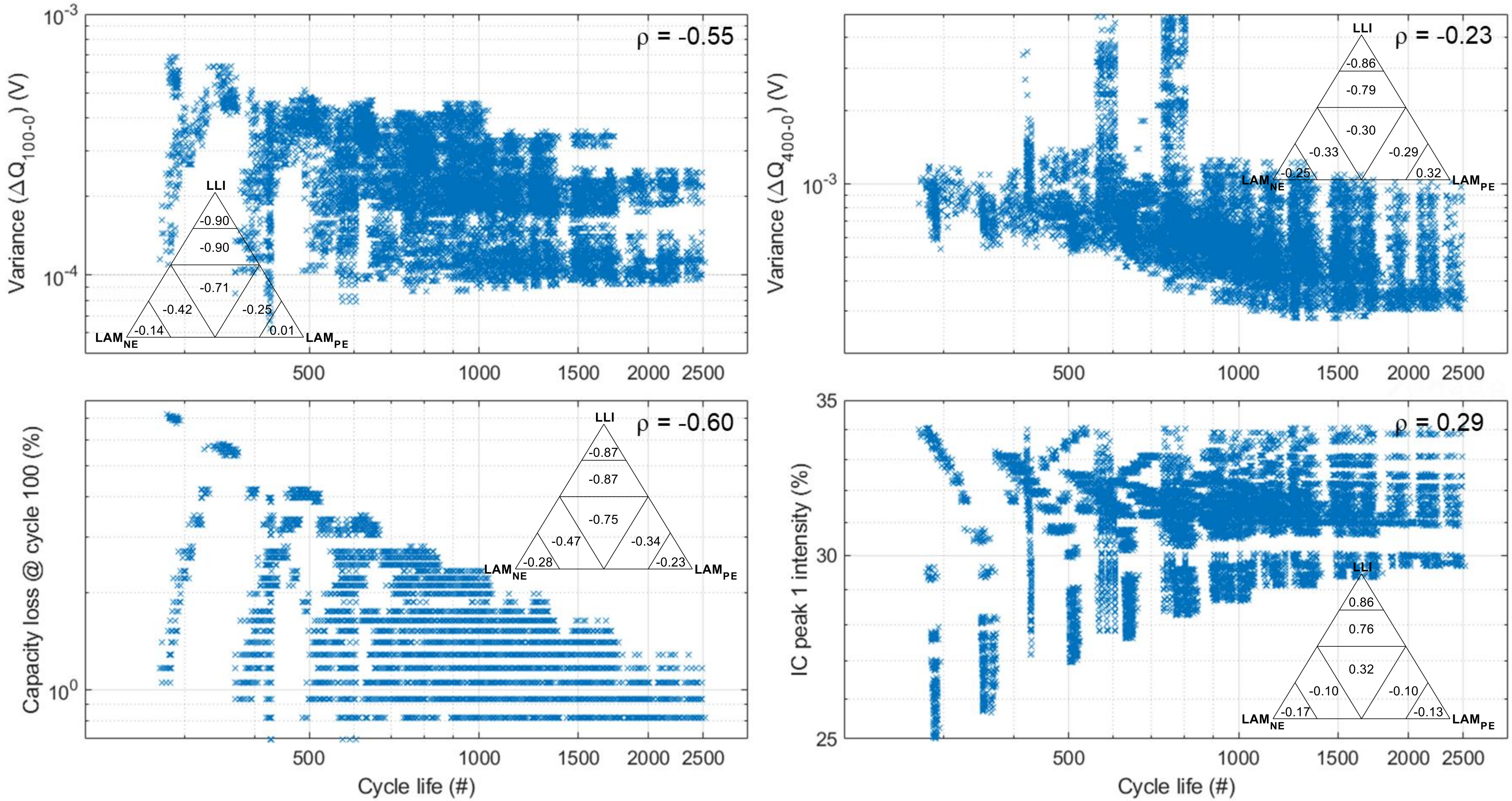

|Diagnosis error| < 1% @ 4 cycles and for > 125,000 duty cycles

Dubarry M. et al., *Energies,* 2021, 14(9), 2371

# Prognosis

## Datasets can be used for training or for sensibility analysis.

### What parameters can be used for early prognosis?

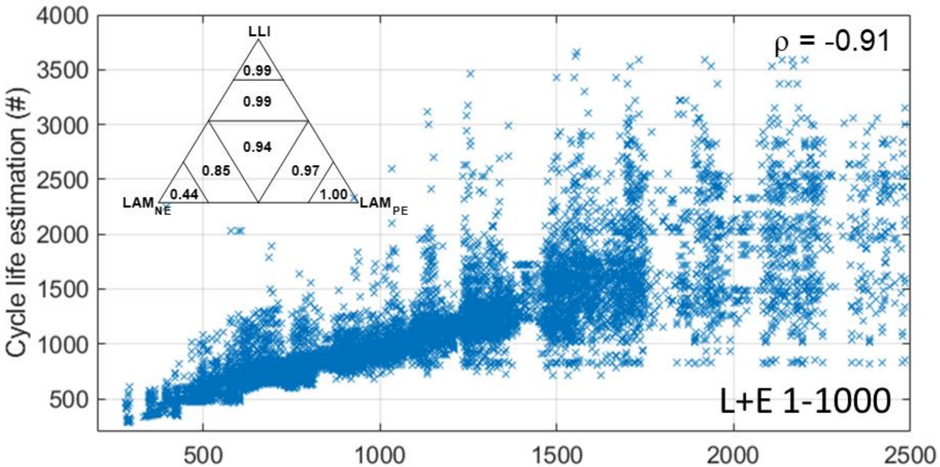


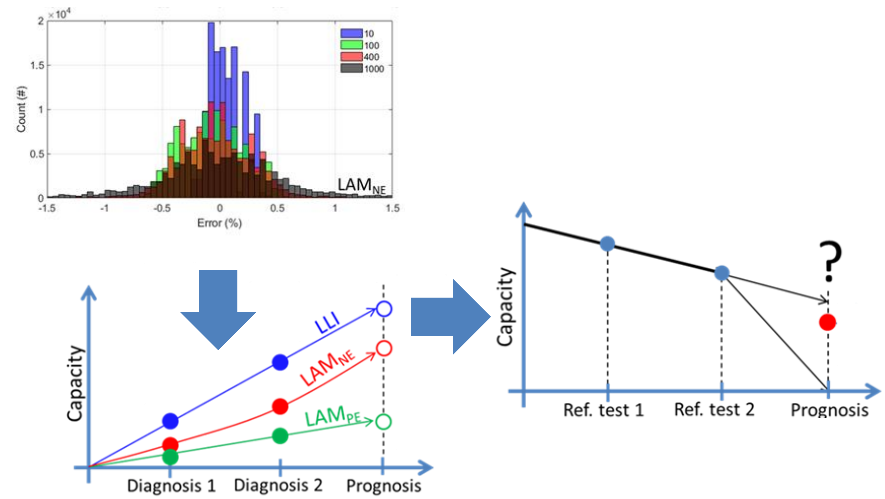

**Single parameter early prognosis might be hard to get for complex degradations**

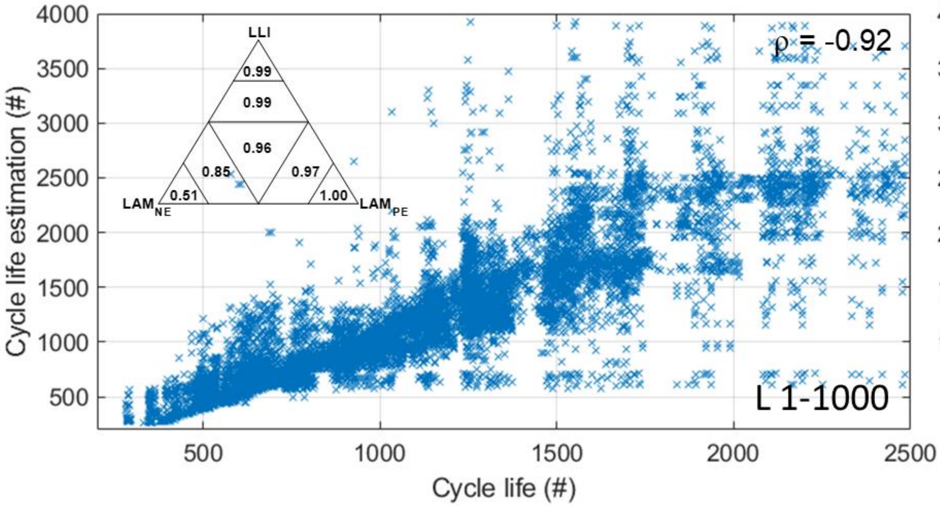
Dubarry M. et al., *Energies*, 2021, 14(9), 2371

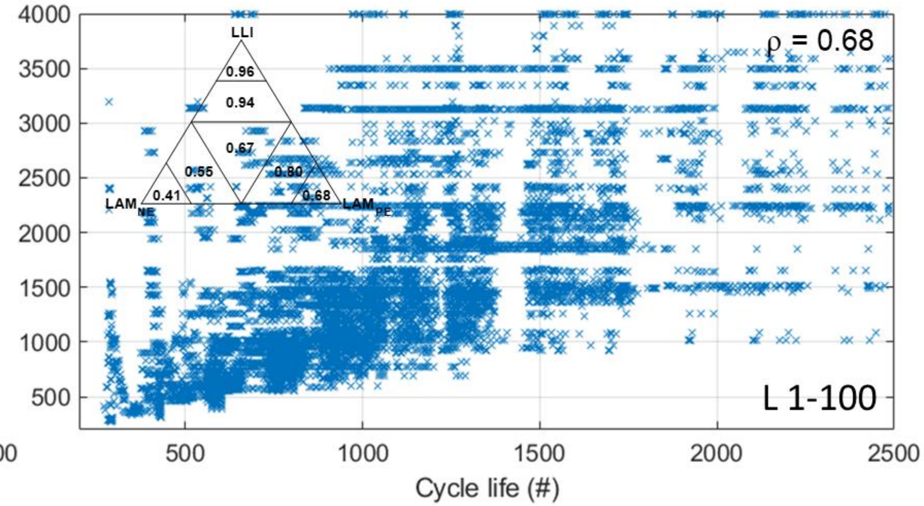
# Prognosis

## Early Prognosis




Better prognosability than single parameter determination
On par with ML multi feature for some degradation paths

Dubarry M. et al., *Energies*, 2021, 14(9), 2371

# Conclusions

Proof-of-concept methodology to generate **big data training datasets**

Universal tool for creation of data indistinguishable from real one

**Broad applicability**: cell chemistries, designs, and operating modes

Methodology could be **applied to different conditions** such as rate and temperature

Can handle **lithium plating with adjustable reversibility**

Ideal to **test validity** of different approaches for diagnosis or prognosis

The approach **do not remove the need for experimental testing**

It is still essential, and the only way, to decipher which conditions cater to specific degradation.

More details: Dubarry M. et al., Journal of Power Sources 479 (2020) 228806
Dubarry M. et al., Energies, 2021, 14(9), 2371

# Acknowledgments

This work was supported by the Office of Naval Research (ONR)
Asia Pacific Research Initiative for Sustainable Energy Systems (APRISES)

*Thank you for tuning in!*

Other presentation on blended electrodes: A01-0044


A01-0002

[matthieu@hawaii.edu](mailto:matthieu@hawaii.edu)