Lithium-ion battery diagnostics using electrochemical impedance via machine-learning

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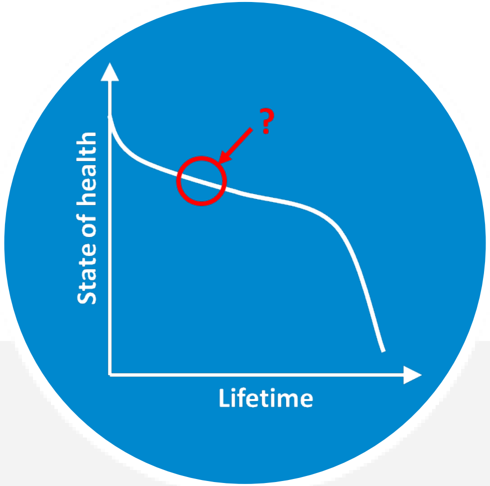
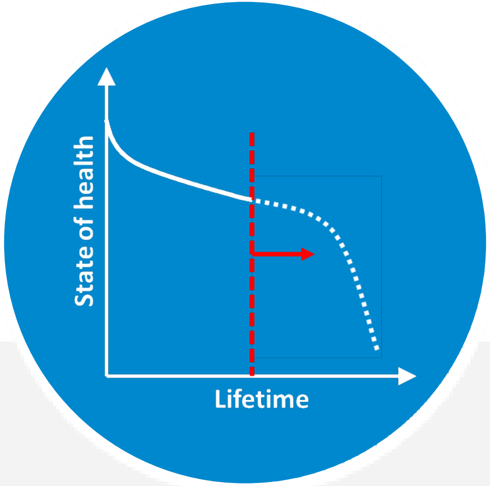
ECS Boston 2023, A01-0397

Challenges for battery monitoring and lifetime



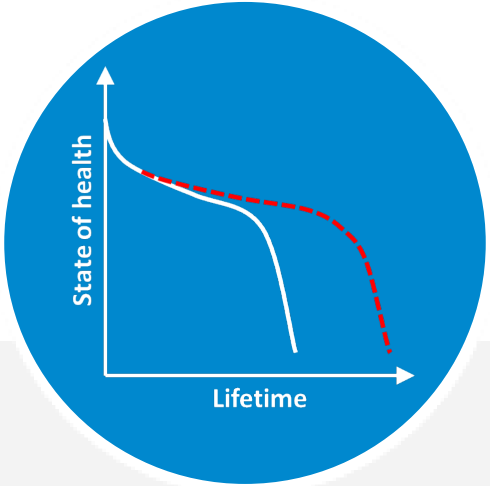
Diagnosis

Detect battery state using available information from cheap, rapid, scalable measurements.



Prediction

Anticipate future battery performance by synergizing lab data and online diagnostics.

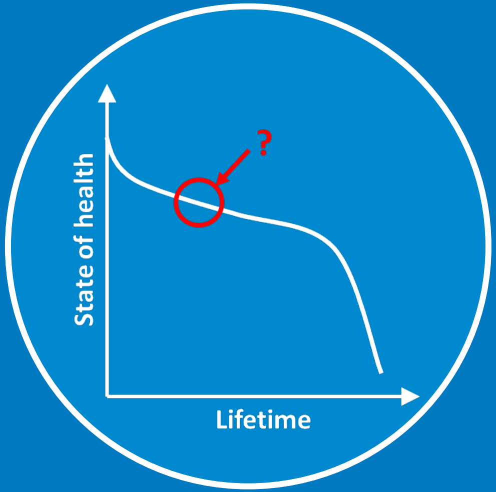


Optimization

Extend battery lifetime or balance system utilization with degradation costs using predictive models.

Battery state diagnosis

P. Gasper, A. Schiek, K. Smith, Y. Shimonishi, S. Yoshida, "Predicting battery capacity from impedance at varying temperature and state of charge using machine-learning." *Cell Reports Physical Science* (2022) 3 101184.



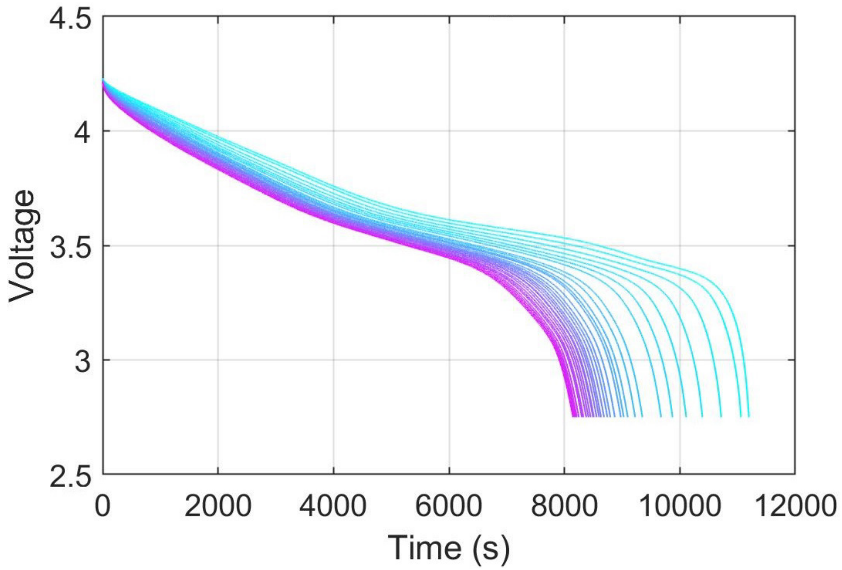
Battery health diagnostics

Lab-based capacity check

+ Accurate

- Slow

- Controlled conditions

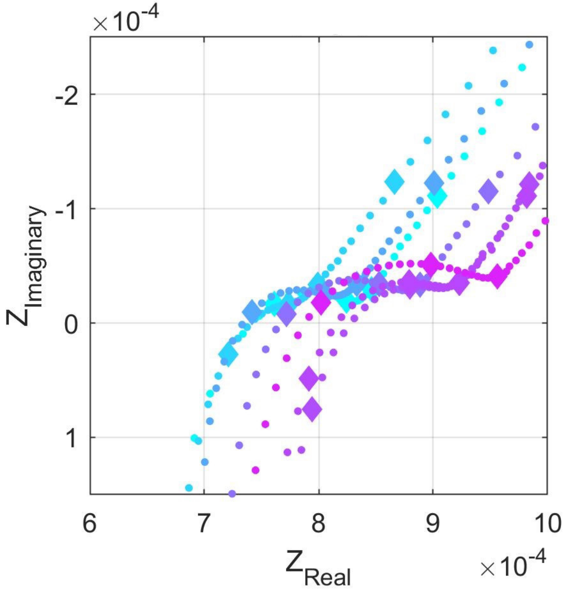


Real-time impedance

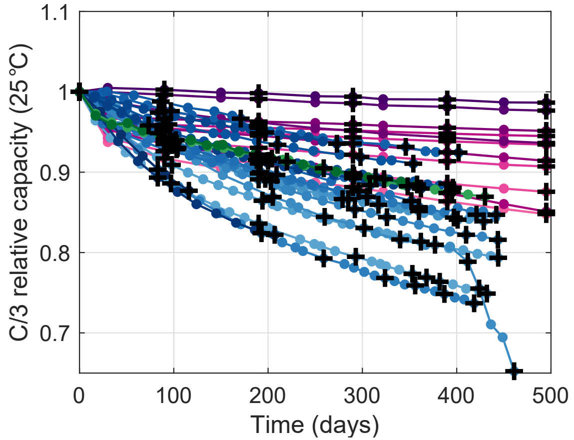
+ Fast

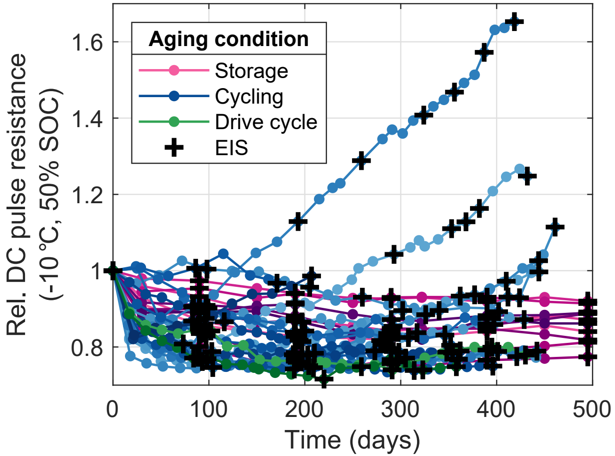
- Uncontrolled conditions

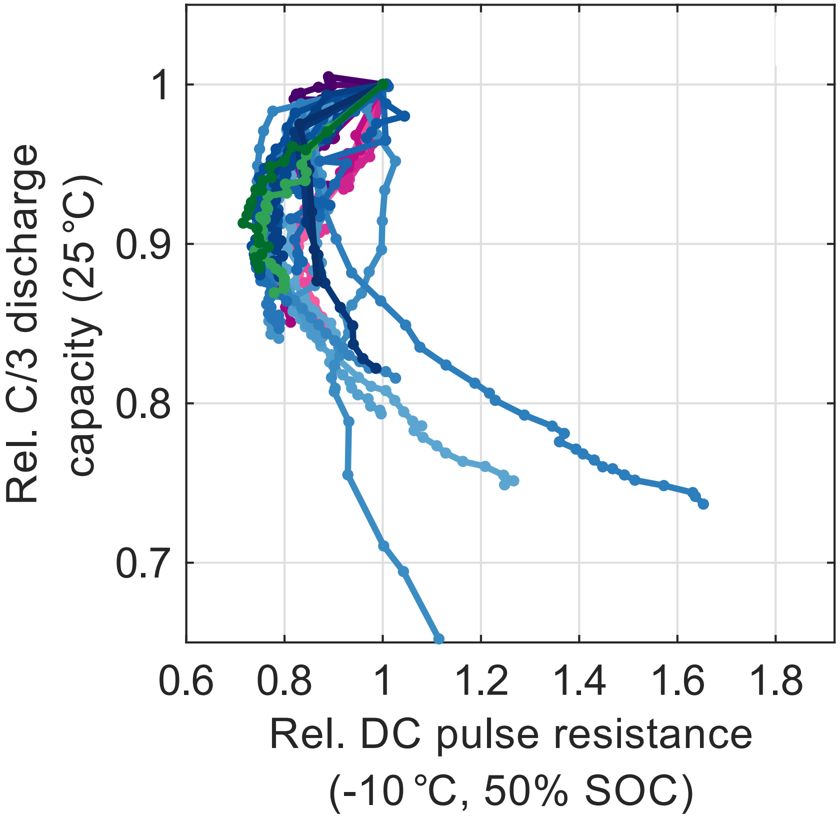
- Measures resistance, not capacity



Challenge: Resistance ≠ Capacity ≠ Health

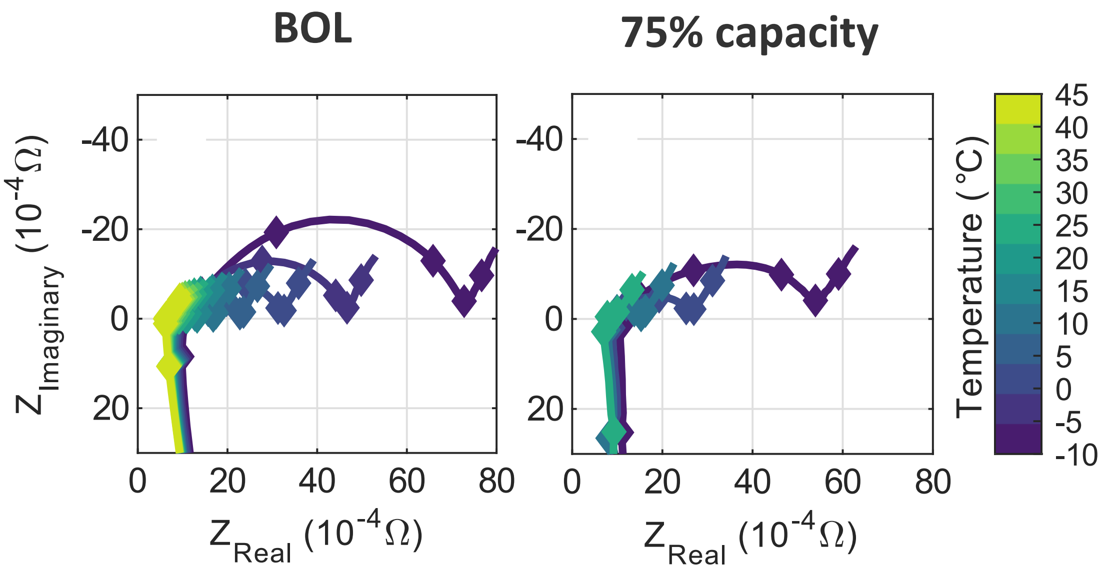






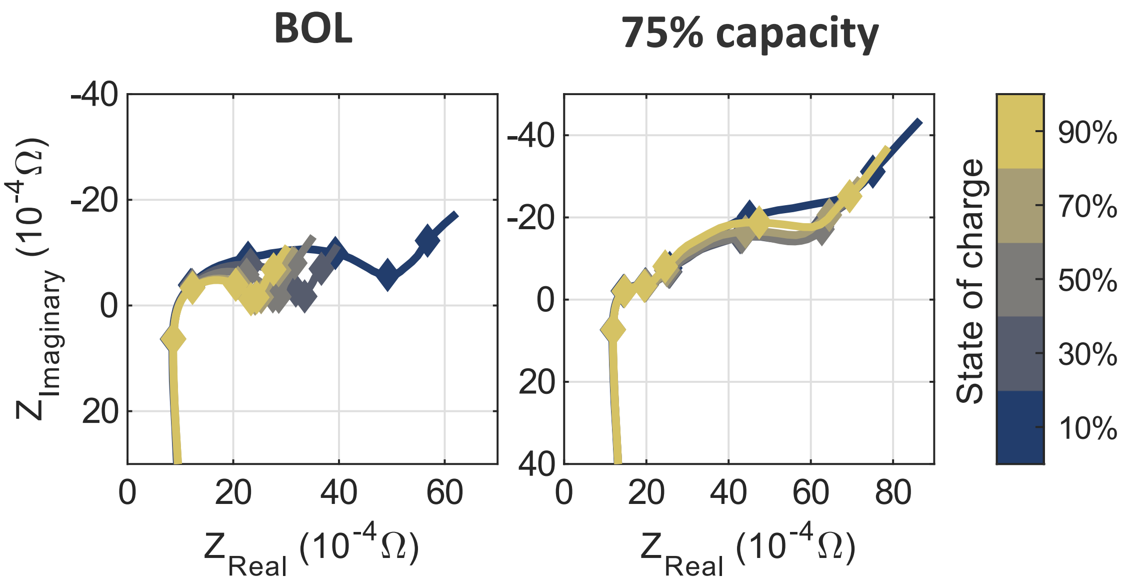
Challenge: Resistance is sensitive to everything

- Temperature



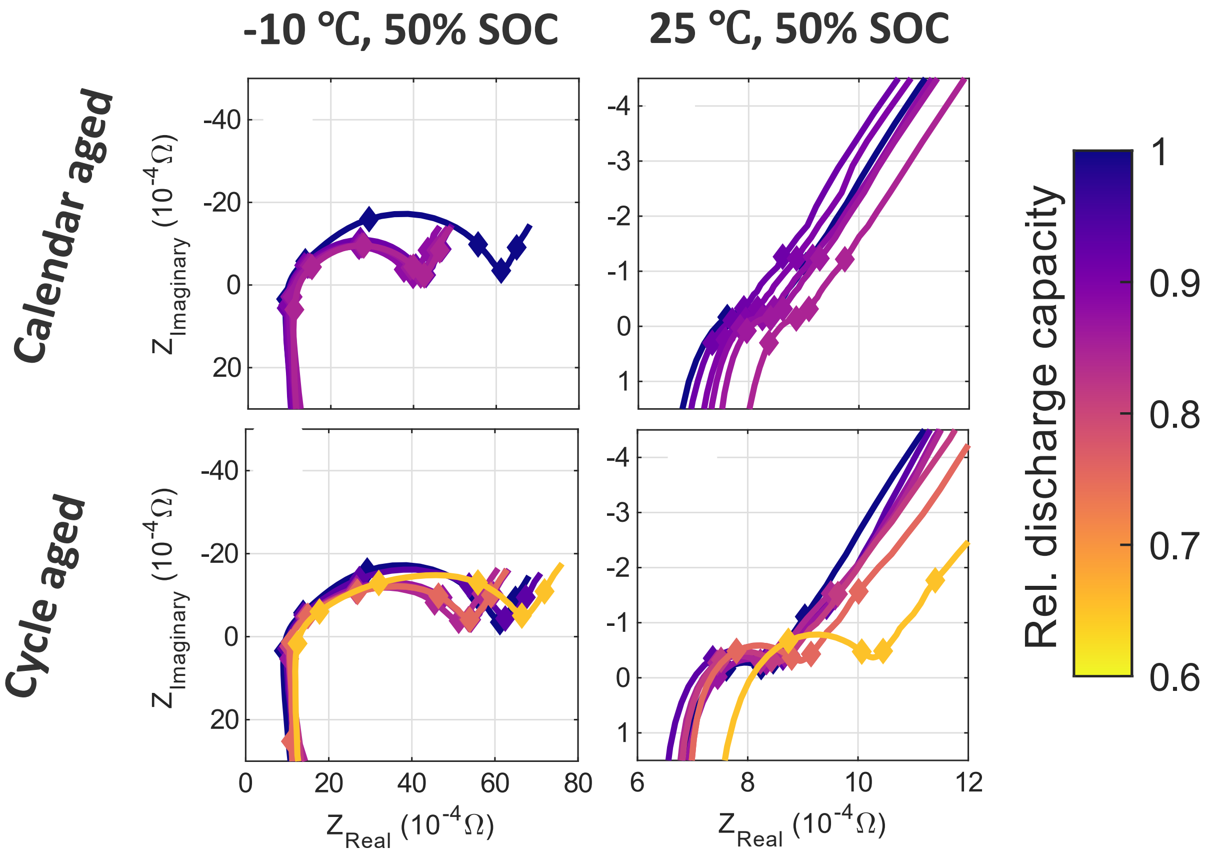
Challenge: Resistance is sensitive to everything

- Temperature
- State-of-charge



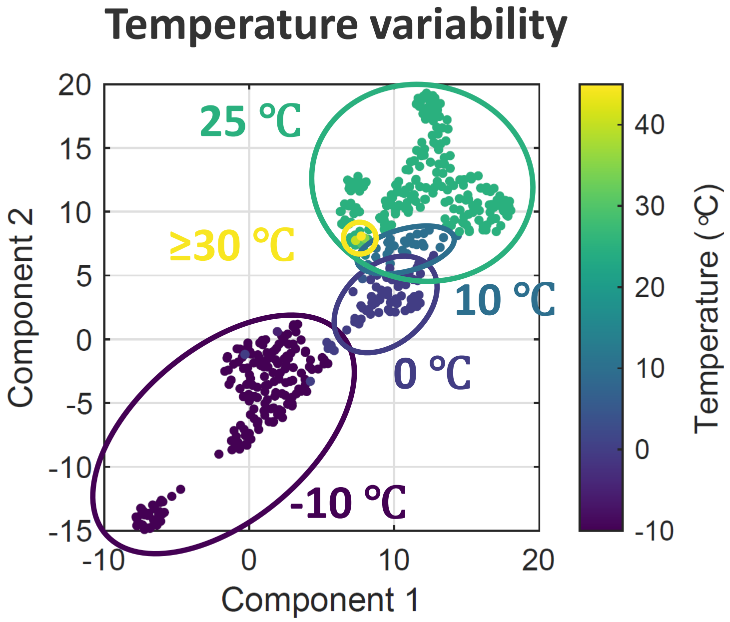
Challenge: Resistance is sensitive to everything

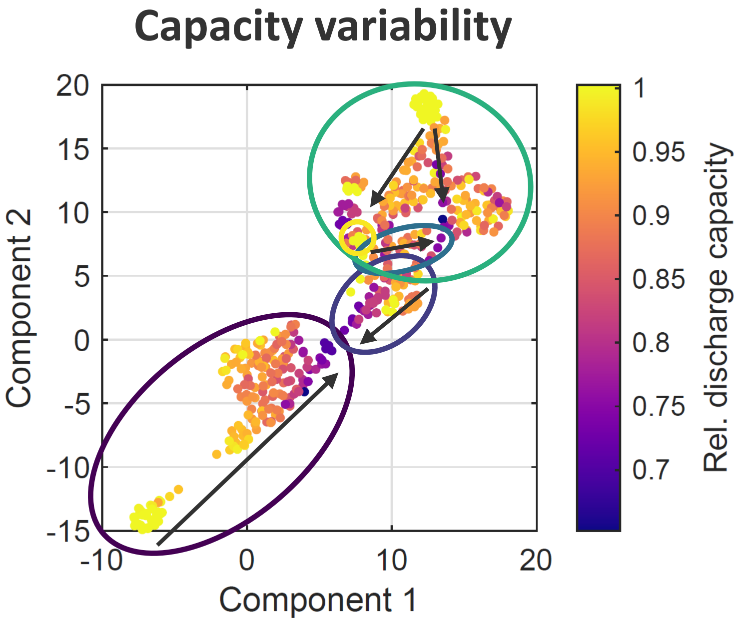
- Temperature
- State-of-charge
- Aging



Visualizing high-dimensional data

ML community has a variety of tools for reducing the dimensionality of data (images, spectra, …) that can help interpret the complexity of any given learning task.



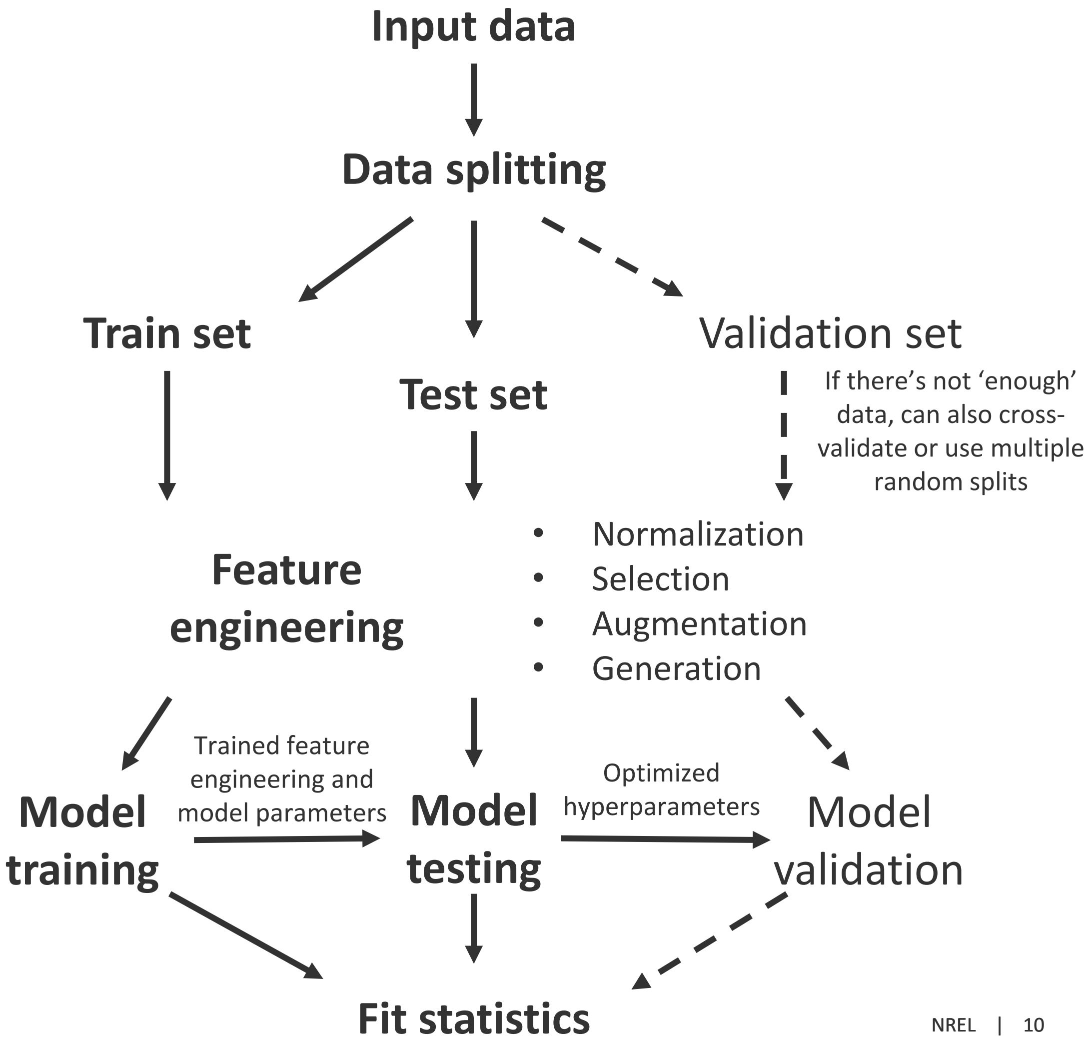


Temperature estimation is likely much easier than capacity estimation.

Constructing a machine-learning pipeline

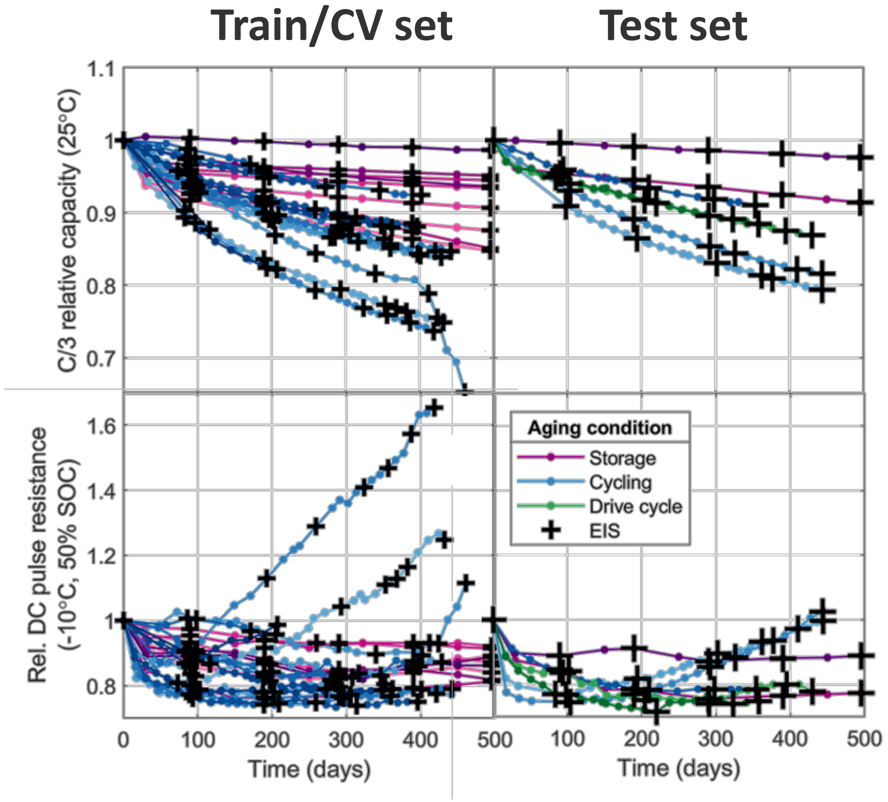
A defined machine-learning pipeline improves replicability and allows for experimentation.

1. Split data according to your hypothesis
2. Engineer features based on real-world constraints, expert knowledge, ...
3. Choose model architecture
4. Evaluate absolute and relative statistical metrics



1. Data splitting

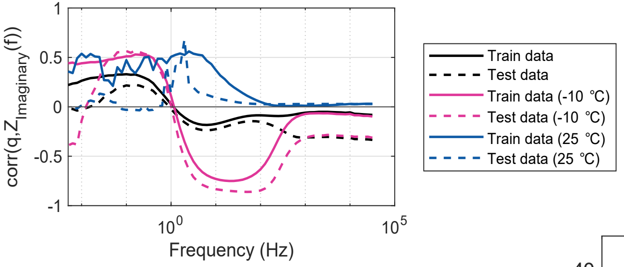
- 6 of 32 cells held out for test set
- Hyperparameter optimization via hold-one-cell-out cross-validation on training set



2. Feature engineering

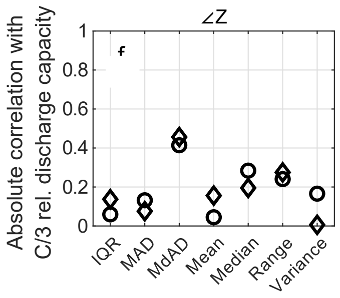
Feature selection

- 1 or 2 frequencies: exhaustive search
- > 3 frequencies: algorithmic search

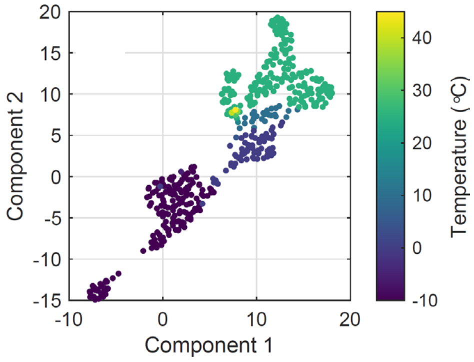


Feature extraction

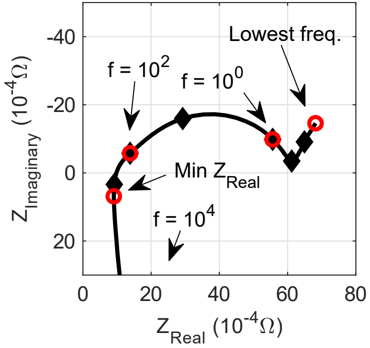
Statistical features

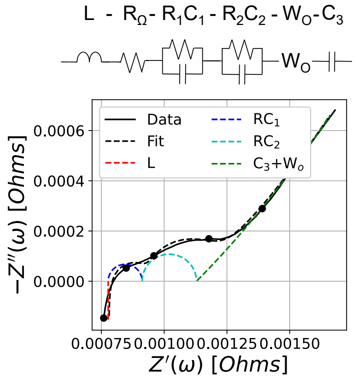


Model-based dimensionality reduction



Domain knowledge



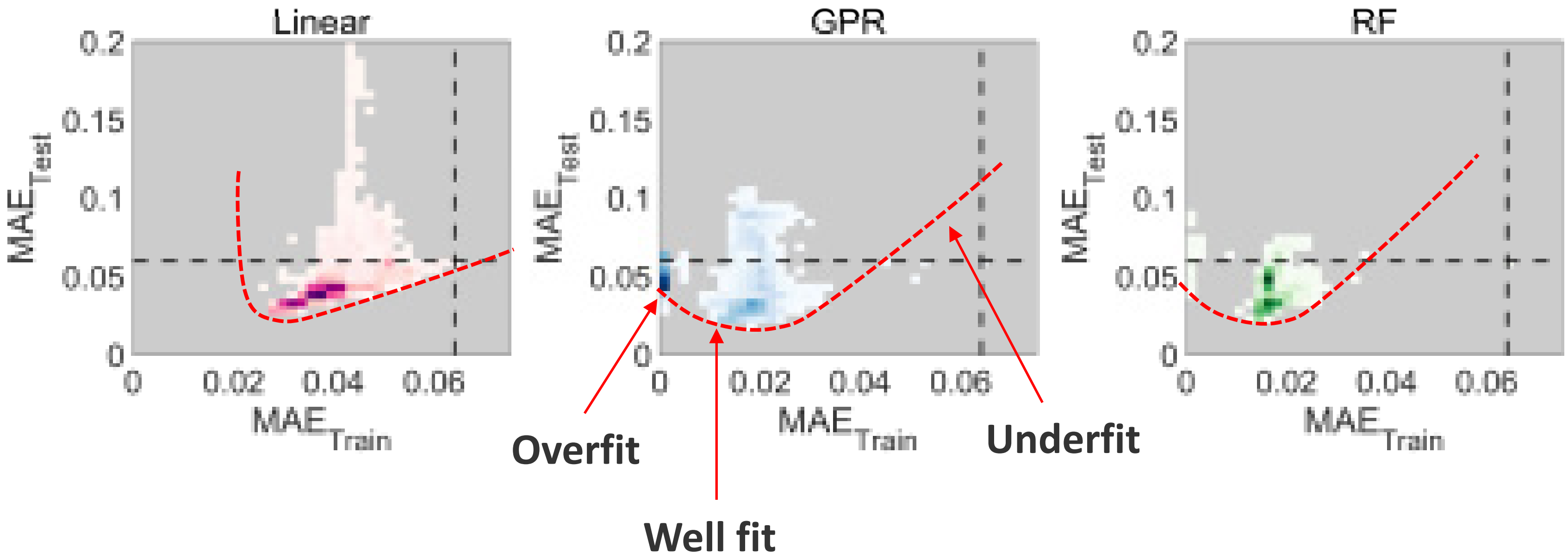


3. Model architectures

Linear	Gaussian process regression	Random forest
$\mathbf{y} = \mathbf{x}^T\boldsymbol{\beta} + \varepsilon$	$\mathbf{y} = h(\mathbf{x})^T\boldsymbol{\beta} + f(\mathbf{x})$ Basis function Covariance function $f(\mathbf{x}) = GP(0, k(x,x'))$	Bagged ensemble of boosted binary decision trees
Minimize MSE loss	Maximize likelihood	Minimize MSE loss
Regularized via L_1 (ridge regression) or L_2 (LASSO regression) norms added to loss	Fairly well self-regulated	Optimize forest size, leaf size, pruning rate via Bayesian hyperparameter optimization

Results – Model architectures

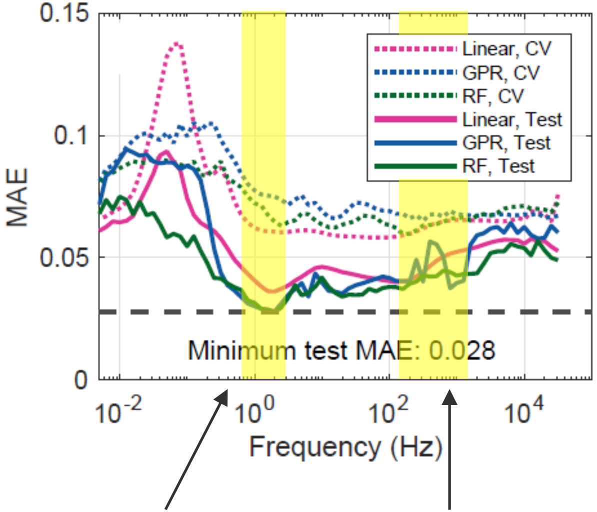
Linear model performance varies widely based on features and regularization. GPR and RF models are better regularized but more likely to overfit.



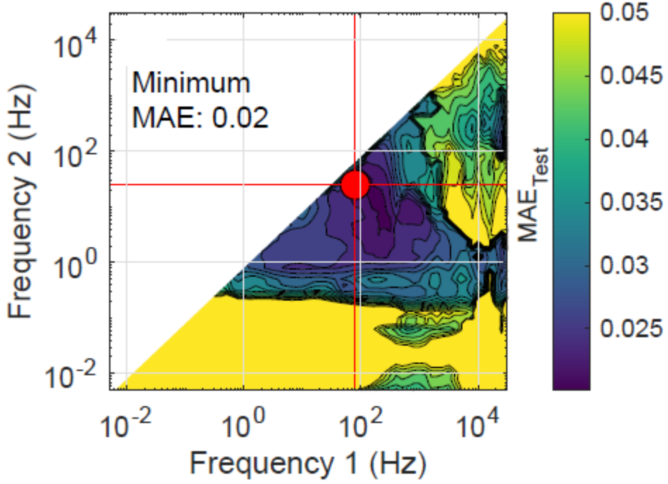
Results - Features

Selecting impedance from two frequencies is the most reliable strategy for predicting capacity from EIS. The frequencies selected matter.

1-frequency models

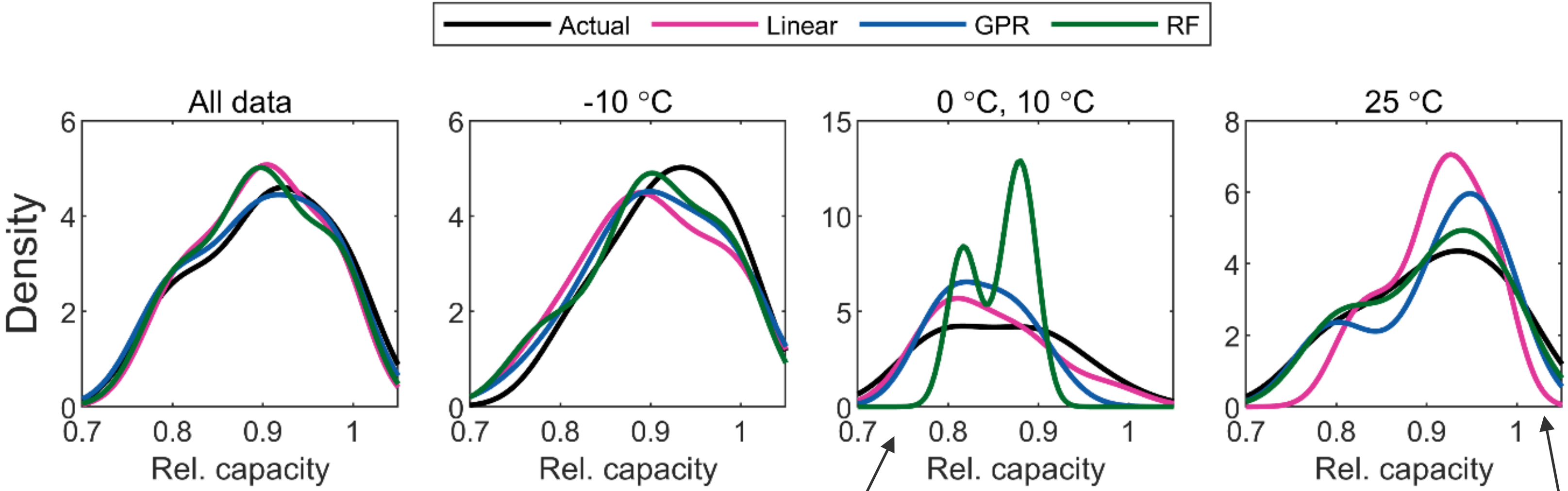


2-frequency models



10^0 Hz **10^2-10^3 Hz** **Low error plateau 10^0-10^2 Hz**

Models have varying systematic errors

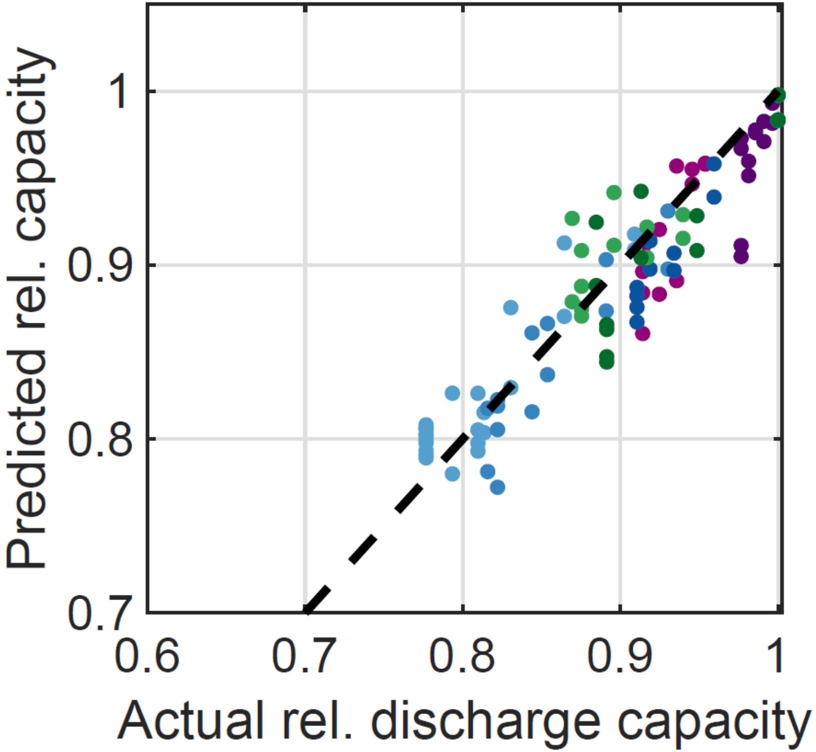


GPR and Linear perform better than RF at middling temperatures

GPR and Linear perform worse than RF at higher temperatures

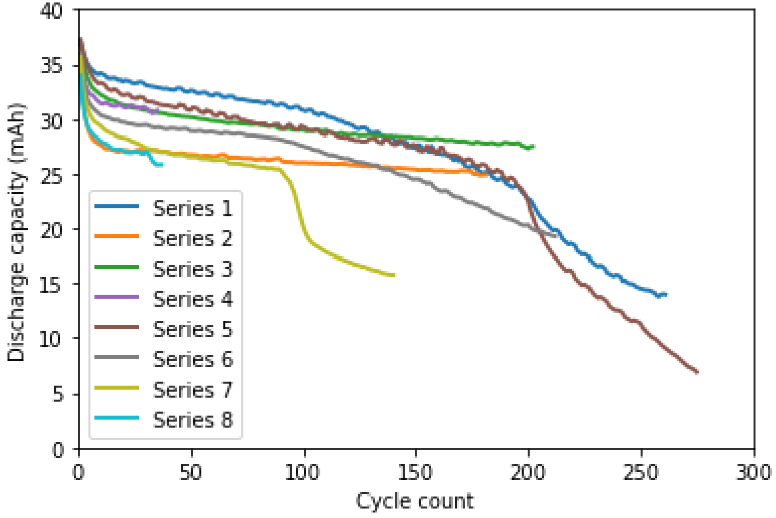
Best model may be an ensemble

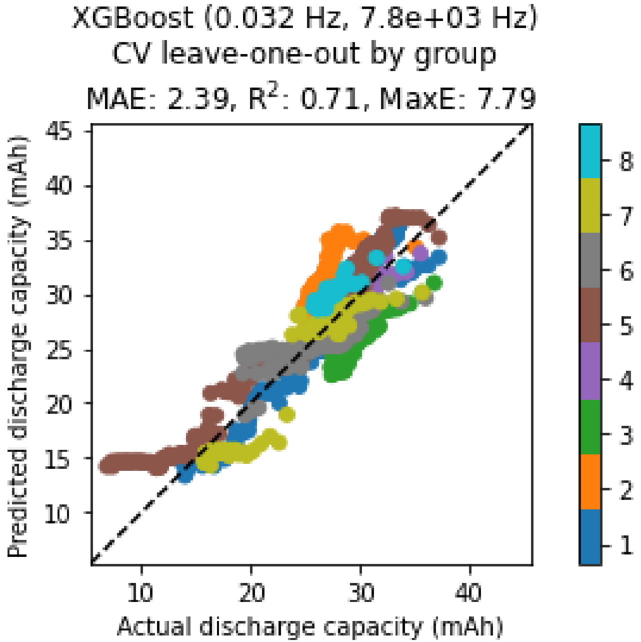
Model	MAE_{Test}	$MaxAE_{Test}$
Baseline	6.1%	12.0%
Linear (ridge)	2.3%	8.2%
GPR (25 Hz, 79 Hz)	2.0%	11.4%
RF (2 Hz, 500 Hz)	2.0%	11.3%
Ensemble	**1.9%**	**7.2%**



Bonus – replication on other data sets

Zhang et al, “Identifying degradation patterns of lithium ion batteries from impedance spectroscopy using machine learning”, *Nature Comms* (2020) 11 1706.





Conclusions

Machine-learning models can be used to predict battery capacity from EIS measurements recorded at unknown temperature and state-of-charge with about 2% average error.

Critical frequency regime **for this cell** is 10^0-10^2 Hz.

www.github.com/NREL/battery_capacity_from_eis

www.github.com/battery-data-commons/mrs-sp22-tutorial/tree/main/predict_capacity_from_eis

Thank you!

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