Machine-learning for battery health diagnosis

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Machine-Learning for Batteries Tutorial
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National Renewable Energy Laboratory

Image credit: Nicholas Brunhart-Lupo

Role of machine-learning in science and engineering

Machine-learning is a powerful set of techniques for mapping between experimental data and values you want to predict.

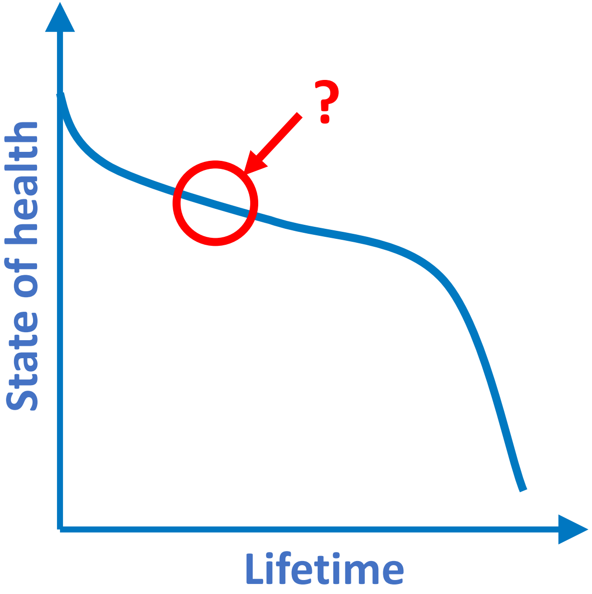
Measurement A → Measurement B
Composition → Structure
Processing → Performance

Machine-learning is most useful when first-principles or numerical modeling approaches fail, due to complexity or computation cost (image classification, physics informed neural networks).

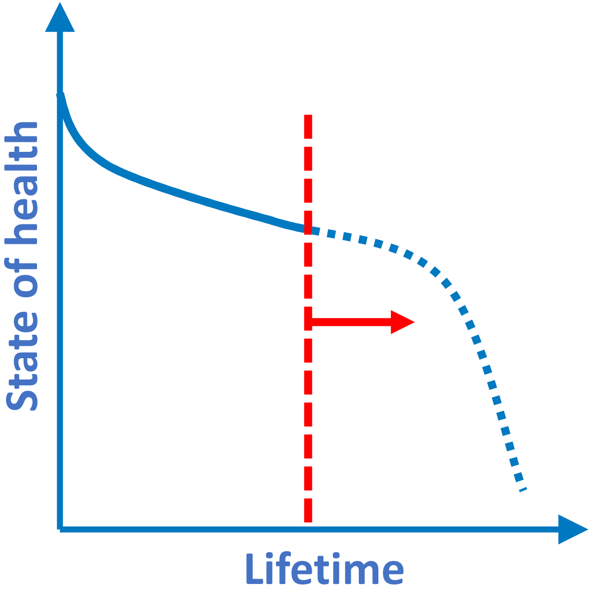
Data science tools/frameworks can help extract quantitative or qualitative information from previously unmanageable data sets.

Opportunities for ML in battery degradation

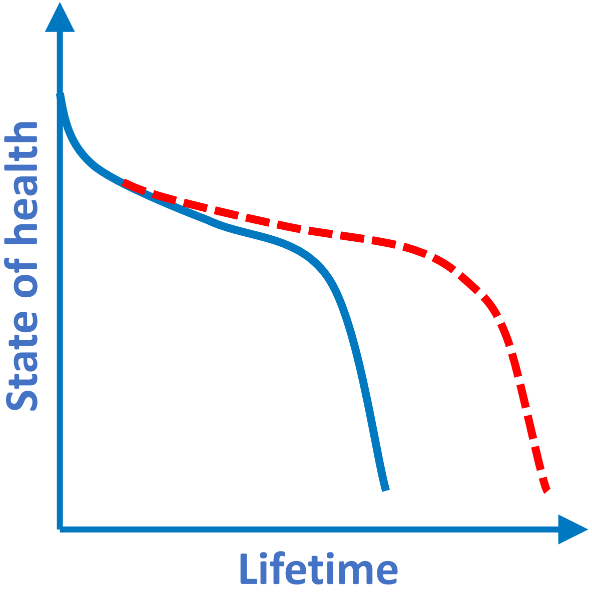
Diagnosis



Prediction



Optimization



Machine-learning (ML) for health diagnosis

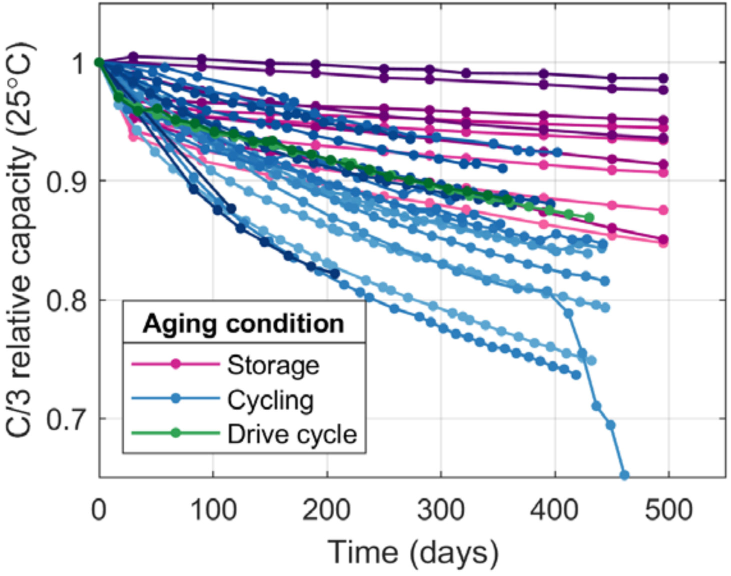
K. Smith, P. Gasper, A. Colclasure, Y. Shimonishi, S. Yoshida. 2021. Lithium-ion battery life model with electrode cracking and early-life break-in process. *Journal of the Electrochemical Society*, in press, https://doi.org/10.1149/1945-7111/ac2ebd.

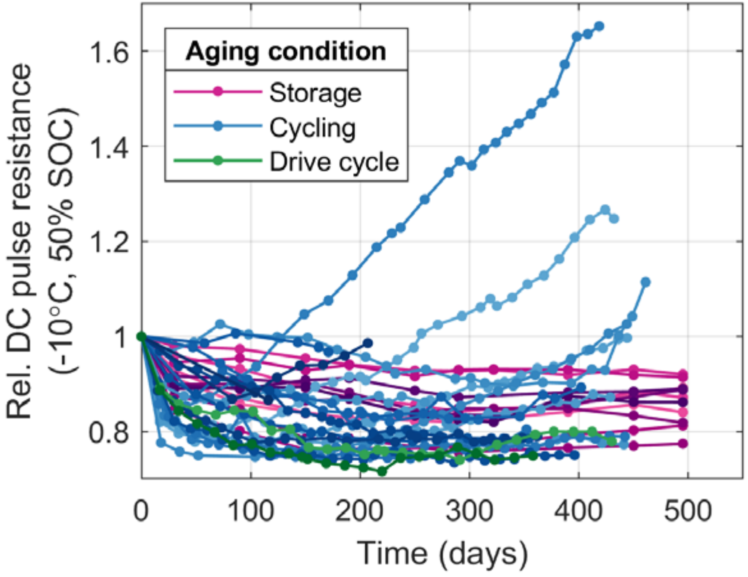
P. Gasper, A. Schiek, K. Smith, Y. Shimonishi, S. Yoshida. 2021. Predicting battery capacity from impedance at varying conditions using machine-learning. *In preparation*.

Metrics for battery health

Data recorded at DENSO Corporation

Cell performance can be limited by both capacity and resistance, so it's important to monitor both.



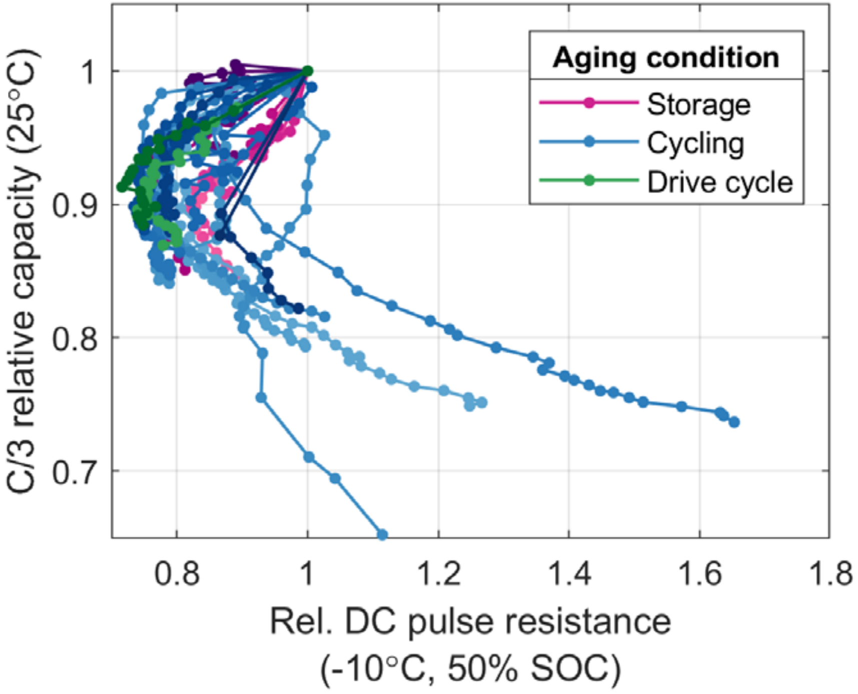


While capacity and resistance seem related, there is a complex relationship between them.

Metrics for battery health

Data recorded at DENSO Corporation

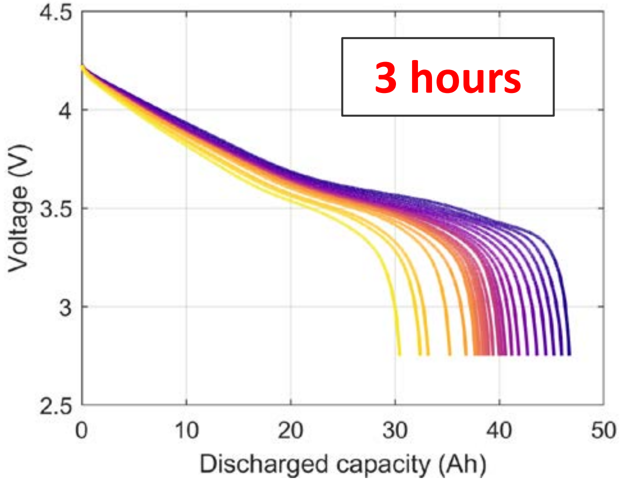
Capacity and resistance are clearly related, but the relationship is non-linear.



Measuring battery health metrics

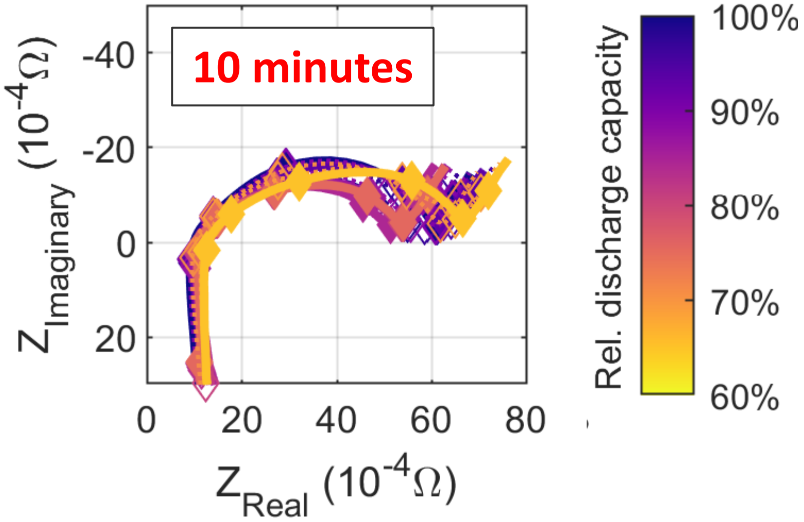
Data recorded at DENSO Corporation

To monitor vehicle battery capacity, we could simply fully discharge the battery periodically during its life, like we do in the lab.



However, these measurements must be recorded under controlled conditions, and take a long time.

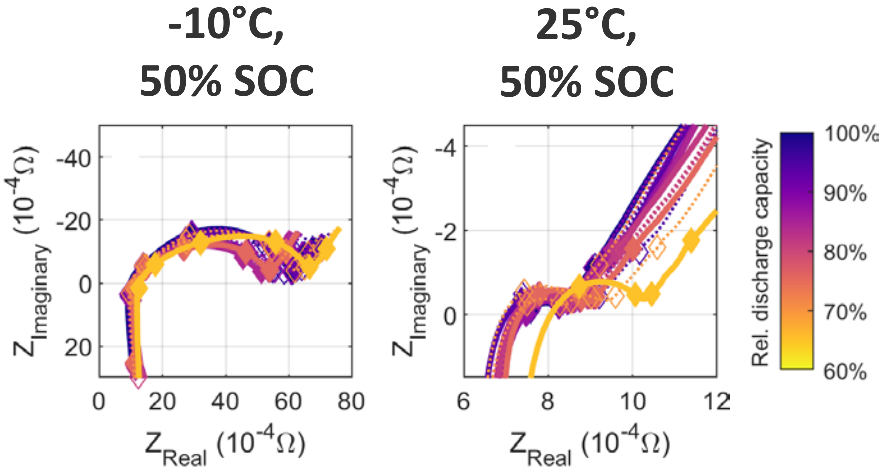
We could instead use a faster measurement, requiring less energy and time, and utilize machine-learning to map to capacity.

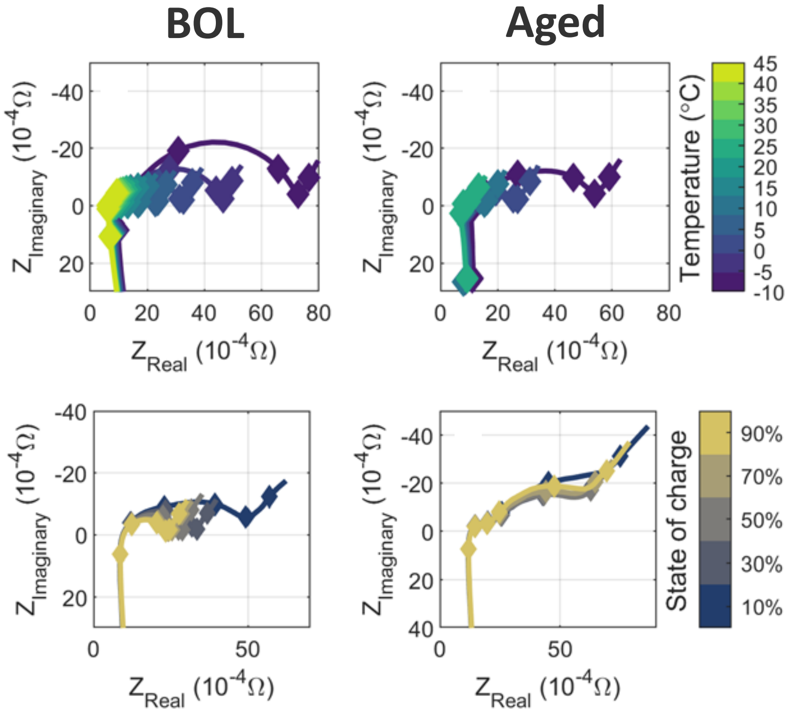


Visualizing high dimensional data

Data recorded at DENSO Corporation

To reflect real-world variation in battery state, EIS was recorded not only versus SOH, but also at varying temperature and SOC.





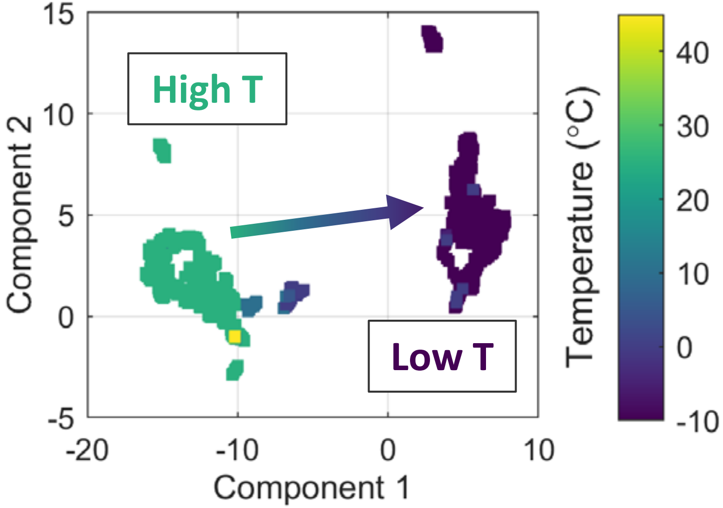
This is data for 1 cell. There are 31 cells!

Visualizing high dimensional data

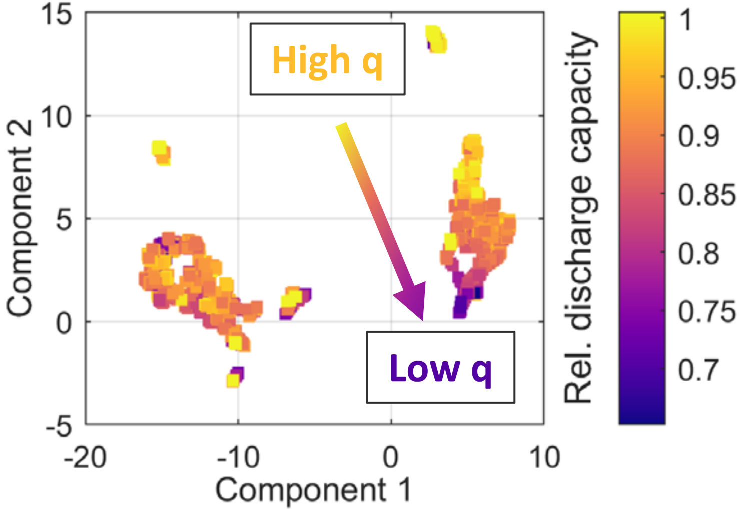
Data recorded at DENSO Corporation

However, visualizing raw values of high dimensional data (3D EIS x Capacity x Temperature x SOC) for all measurements is not possible (interpretable). To visualize high dimensional data, there are several ML techniques. Here we are using UMAP.

Temperature has huge impact on EIS measurements.



Capacity trend more obvious at low temperature than high.



Modeling goals

Goal 1:

Predict capacity (at a specific temperature and rate), which is slow to measure, using EIS (at varying temperature and SOC).

$$q = f(EIS)$$

Goal 2:

Train a model on lab data and use it onboard electric vehicles.

e.g.,

Train a model that works well on cells it hasn't seen before.

Define relationships between variables

Use expert-knowledge and judgement to propose relationships between variables.

Experimental variables $\quad$ **T_{EIS}** $\quad$ **SOC_{EIS}**

Measured variables $\quad$ **EIS** $\longrightarrow$ **Capacity**

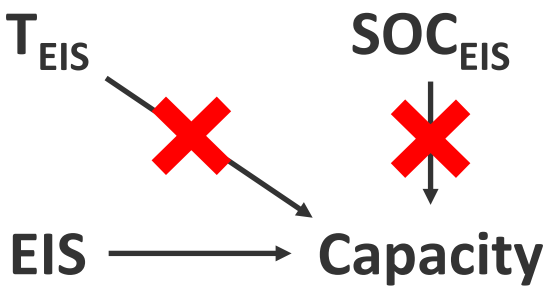
Simplest approach is to ignore experimental variables.

Define relationships between variables

Use expert-knowledge and judgement to propose relationships between variables.

Experimental variables

Measured variables



T_{EIS} and SOC_{EIS} should not be used as model inputs, unless we can prove they do not impact the capacity prediction.

Define relationships between variables

Use expert-knowledge and judgement to propose relationships between variables.

Experimental variables

Measured variables

$$\begin{tikzcd} \mathbf{T_{EIS}} \arrow[d] & \mathbf{SOC_{EIS}} \arrow[dl] \\ \mathbf{EIS} \arrow[r] & \mathbf{Capacity} \end{tikzcd}$$

T_{EIS} and SOC_{EIS} interact with the EIS, which is then somehow related to cell capacity. We could attempt to remove this interaction using a model (resistance versus temperature, for instance), or hope the ML can handle it.

Training a model

Model training

Start with a simple case, predicting capacity using impedance only at -10°C at 50% SOC with a linear model.

Input data needs to be arranged into a matrix for training.

Z_{Real}	$Z_{Imaginary}$	$\|Z\|$	$\angle Z$
$f_{high} \rightarrow f_{low}$	$f_{high} \rightarrow f_{low}$	$f_{high} \rightarrow f_{low}$	$f_{high} \rightarrow f_{low}$

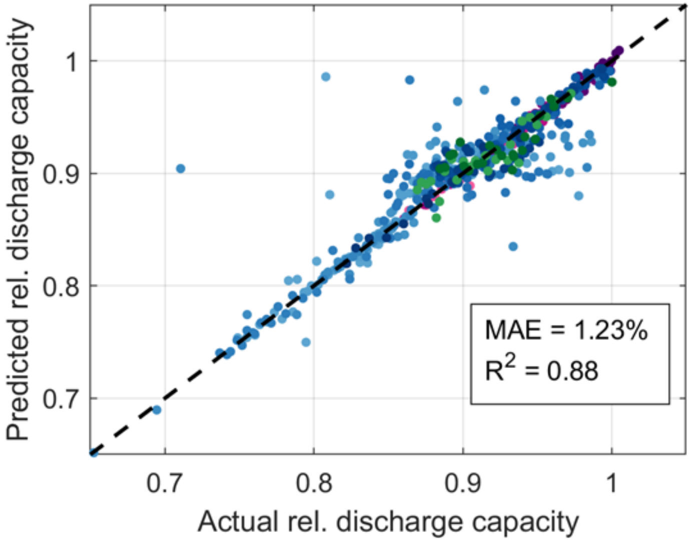
X

10x16 table

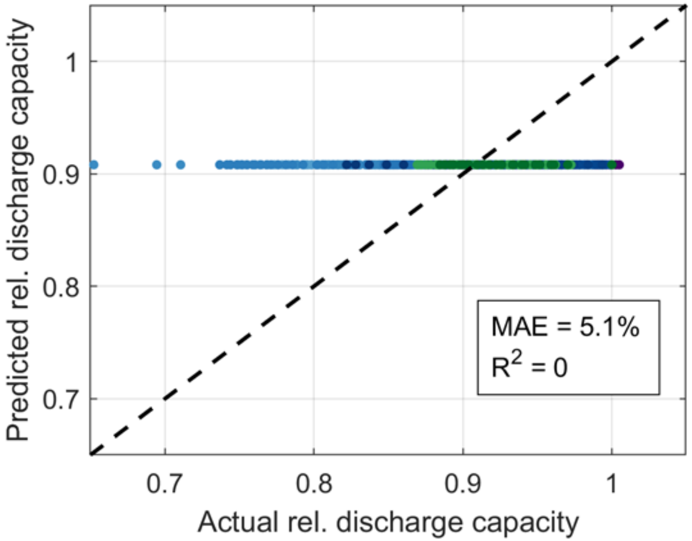
	1 Zreal_1e+02Hz	2 Zreal_79Hz	3 Zreal_63Hz	4 Zreal_50Hz	5 Zimag_1e+02Hz	6 Zimag_79Hz	7 Zimag_63Hz	8 Zimag_50Hz	9 Zmag_1e+02Hz	10 Zmag_79Hz	11 Zmag_63Hz	12 Zmag_50Hz	13 Zphz_1e+02Hz	14 Zphz_79Hz	15 Zphz_63Hz	16 Zphz_50Hz
1	0.0014	0.0015	0.0016	0.0017	-5.7475e-04	-6.4875e-04	-7.2832e-04	-8.1478e-04	0.0015	0.0016	0.0017	0.0018	-22.5654	-23.8694	-25.0787	-26.2158
2	0.0015	0.0016	0.0017	0.0018	-4.3955e-04	-5.0439e-04	-5.7096e-04	-6.3897e-04	0.0016	0.0017	0.0018	0.0019	-15.9462	-17.3864	-18.6560	-19.7276
3	0.0014	0.0014	0.0015	0.0016	-4.7451e-04	-5.4207e-04	-6.1128e-04	-6.8310e-04	0.0014	0.0015	0.0016	0.0018	-19.2709	-20.7165	-21.9353	-22.9755
4	0.0014	0.0014	0.0015	0.0016	-4.5725e-04	-5.2068e-04	-5.8563e-04	-6.6148e-04	0.0014	0.0015	0.0016	0.0017	-18.8791	-20.3135	-21.5151	-22.5439
5	0.0014	0.0015	0.0015	0.0016	-4.5120e-04	-5.1318e-04	-5.7663e-04	-6.4284e-04	0.0015	0.0015	0.0016	0.0017	-18.1104	-19.4649	-20.6123	-21.6052
6	0.0014	0.0014	0.0015	0.0016	-4.5199e-04	-5.1416e-04	-5.7780e-04	-6.4902e-04	0.0014	0.0015	0.0016	0.0017	-18.4249	-19.8156	-20.9864	-21.9948
7	0.0014	0.0015	0.0016	0.0017	-4.6509e-04	-5.2192e-04	-5.8092e-04	-6.4219e-04	0.0015	0.0016	0.0017	0.0018	-17.8761	-19.0159	-20.0146	-20.8709
8	0.0014	0.0014	0.0015	0.0016	-4.5754e-04	-5.2104e-04	-5.8606e-04	-6.6198e-04	0.0014	0.0015	0.0016	0.0017	-18.8932	-20.3287	-21.5312	-22.5605
9	0.0015	0.0016	0.0016	0.0017	-4.6932e-04	-5.2726e-04	-5.8789e-04	-6.5060e-04	0.0016	0.0017	0.0017	0.0019	-17.4570	-18.6246	-19.6692	-20.5575
10	0.0015	0.0016	0.0017	0.0018	-4.4754e-04	-5.0671e-04	-5.7027e-04	-6.3588e-04	0.0016	0.0017	0.0018	0.0019	-16.1314	-17.4859	-18.6904	-19.7078

Model results

The model appears extremely accurate.



These results seem good. But relative to what? What is our baseline?
This is the purpose of dummy models.

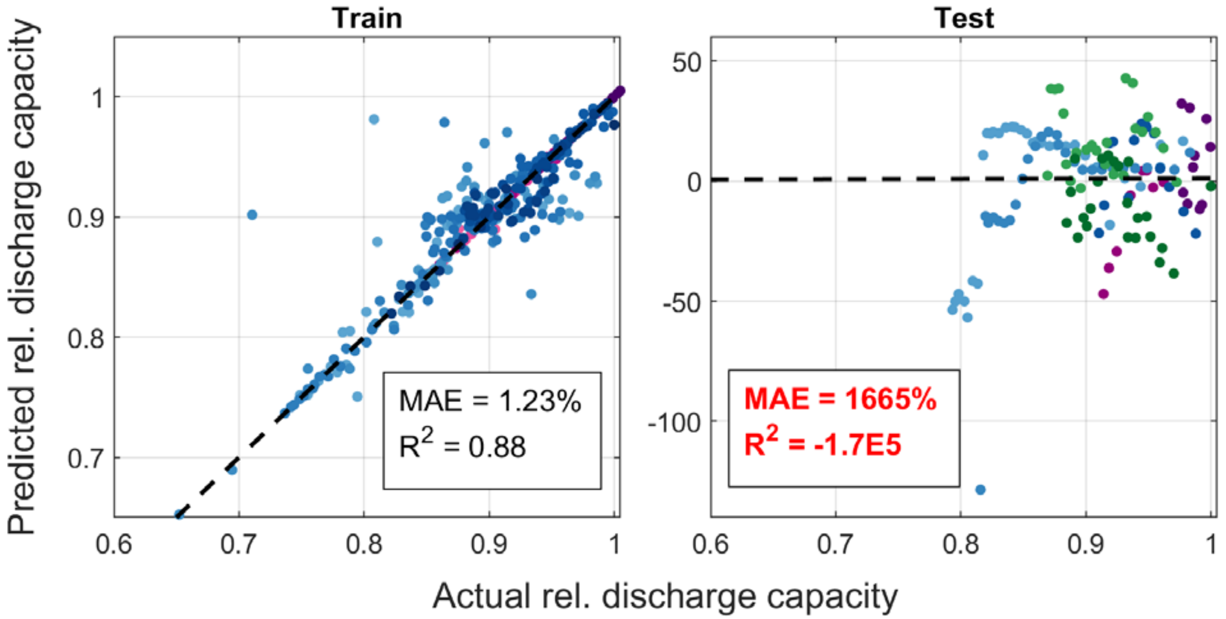


Can we really be sure this will work in a real-world device?

Testing a model

Train/test splits

How can we check to see if we've met our second goal?
This is the purpose of train/test splits. We can train on ~70% of our data, and test on the other third. Note we're splitting *by cell*, not by data point. Thus, we are testing if our model performs well on unseen cells, not unseen EIS measurements.



Overfitting

This is an example of overfitting. One way to understand model fitness is the concept of bias/variance tradeoff. For example, in a linear model:

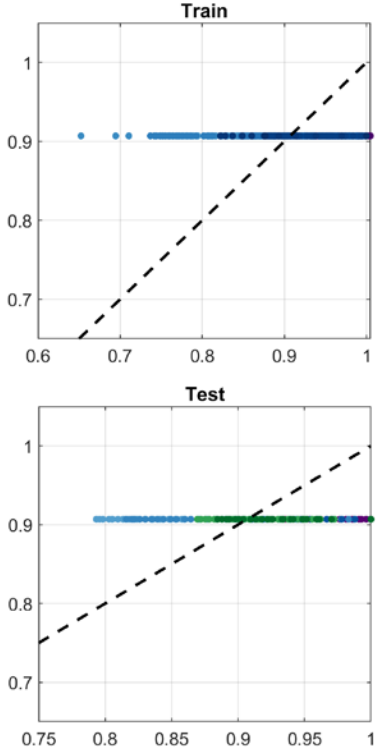
$$\underbrace{\boldsymbol{Y}}_{N \times 1} = \overbrace{\boldsymbol{X}}^{N \times M} \times \underbrace{\boldsymbol{A}}_{M \times 1} + B$$

We train ‘M’ slopes but only 1 bias, B. Thus, if we have many features M, our model will be very sensitive to variance in M but not to the bias. Our dummy model, on the other hand, is all bias, with no variance:

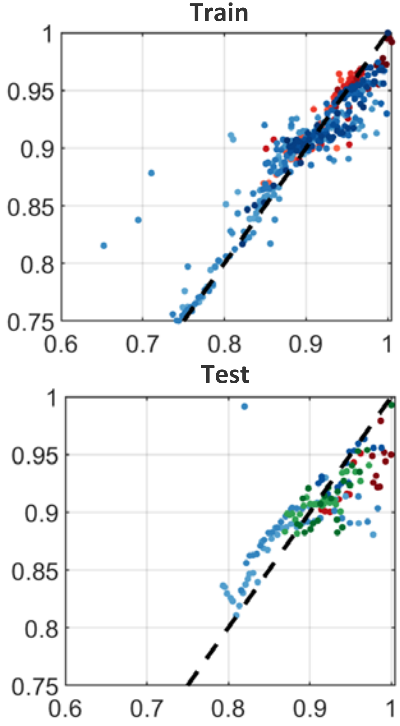
$$\boldsymbol{Y} = B$$

Overfitting

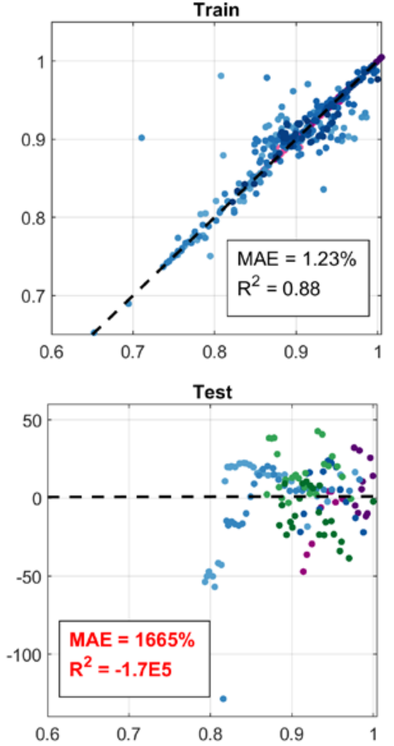
Too much bias



Balanced

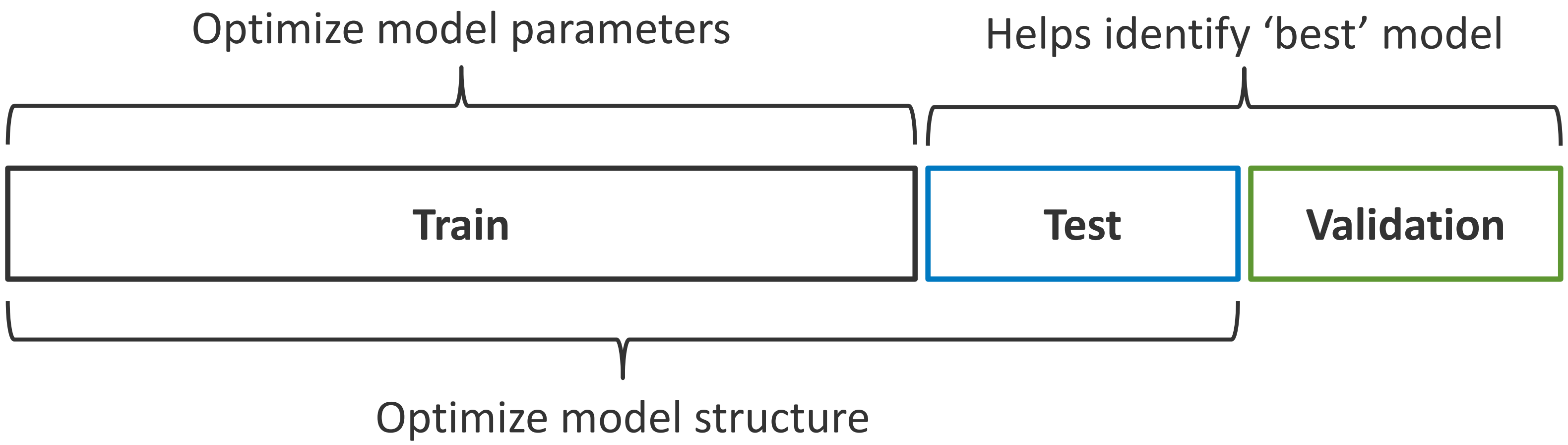


Too much variance



Train/Test/Validation

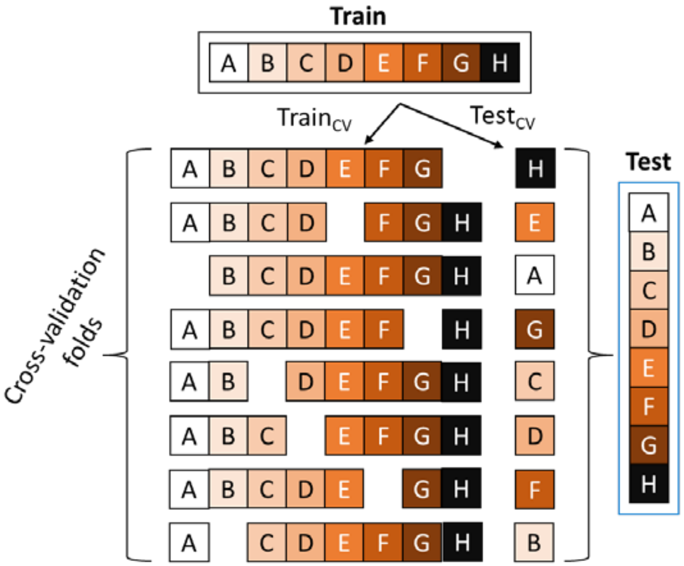
It is best practice to examine how our model performs on multiple sets of unseen data. This helps prevent systematic errors, for example, maybe just the single test set is an 'easy' test. This can also help avoiding issues with data collection, for instance, where train/test/validation data is recorded using different instruments or with varied protocols. Two sets of unseen data also helps to evaluate model 'fitness' with more rigor.



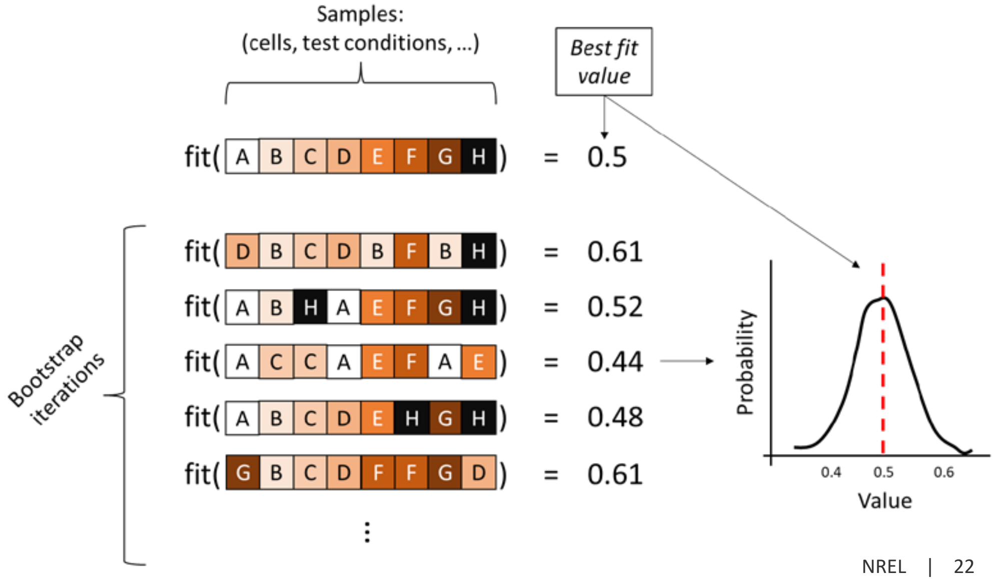
Cross-validation and bootstrapping

However, we may not have a huge amount of available data to create reasonably sized test/validations splits. We can use other approaches, such as cross-validation and bootstrapping, to run multiple train/test splits on different subsets of the data.

Cross-validation



Bootstrapping



Feature engineering:
Selecting and extracting useful features

Feature engineering

Feature engineering is a general term referring to:

- Combining existing features to create new ones **Feature Generation**

$$X_{new} = X_1 * X_2 \qquad X_{new} = X_1^2 \qquad X_{new} = exp(X_1)$$

- Extracting features from data **Feature Extraction**

$$X_{new} = mean(X) \qquad X_{new} = \text{coefficients of } 4^{th} \text{ order polynomial fit to } X$$

- Selecting a subset of useful features **Feature Selection**

These terms are general, and distinctions b/w these terms are sometimes hard to make.

Data is also usually normalized or rescaled prior to making predictions.

Feature generation

If we want to incorporate temperature into our model, we can make interaction terms.

$$\begin{tikzcd}[row sep=small] \mathbf{T_{EIS}} \arrow[dr] & & \\ & \mathbf{T_{EIS} \cdot EIS} \arrow[r] & \mathbf{Capacity} \\ \mathbf{EIS} \arrow[ur] & & \end{tikzcd}$$

Expert knowledge tells us resistance is exponentially related to temperature. We could also propose some activation energies.

$$\mathbf{T_{EIS}} \left\{ \begin{array}{l} \mathbf{\exp(E_{a,1} \cdot T_{EIS})} \longrightarrow \\ \mathbf{\exp(E_{a,2} \cdot T_{EIS})} \longrightarrow \\ \quad \mathbf{\dots} \end{array} \right. \quad \begin{pmatrix} \mathbf{\exp(E_{a} \cdot T_{EIS}) \cdot EIS} \\ \mathbf{\exp(E_{a} \cdot T_{EIS}) \cdot EIS} \\ \mathbf{\dots} \end{pmatrix} \longrightarrow \mathbf{Capacity}$$

$$\mathbf{EIS} \longrightarrow \begin{pmatrix} \dots \end{pmatrix}$$

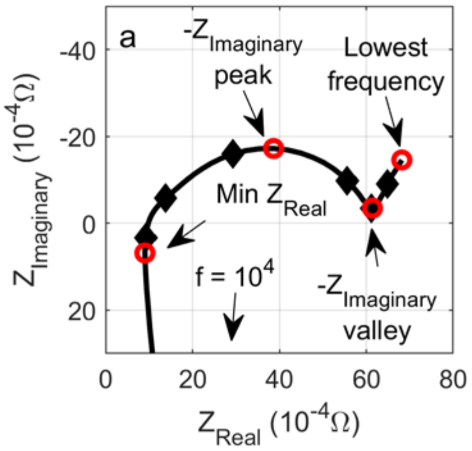
Feature extraction

There are an infinite number of ways to extract features. Some use background knowledge or intuition. There are also algorithms to reduce the dimensionality of a signal, like PCA or UMAP).

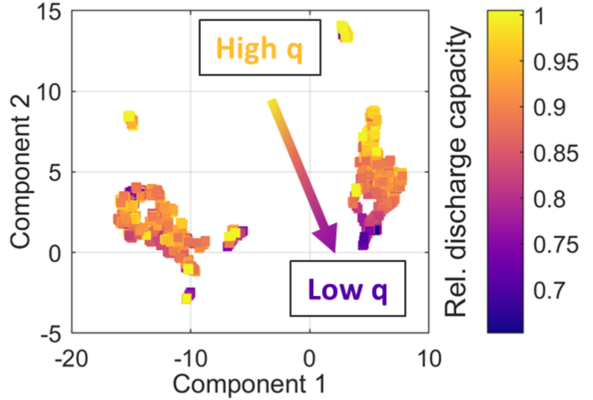
Statistics:

mean	std. dev.
median	variance
range	MAD
IQR	MdAD
skew	kurtosis

Graphical:



Dimensionality reduction:



Feature selection

Feature selection methods are usually classified into three categories:

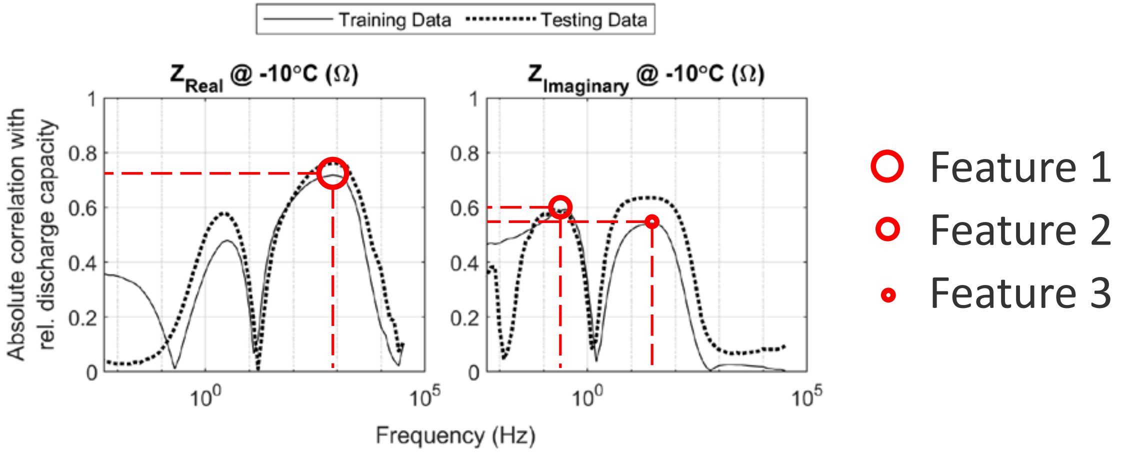
1. Filter (select features before passing to model)
2. Wrappers (use model performance to select features)
3. Embedded (model selects features)

Feature selection

Filter example:

Pick features that are highly correlated to the target, but avoid redundancy

This requires defining a few hyperparameters: the number of features we want, and the threshold for similarity that we use to define redundancy.



Feature selection

Wrapper example:

Exhaustively search through all possible combinations of two frequencies (here, 2346 combinations).

Embedded example:

LASSO (linear models)

ARD (GPR models)

Feature transformation pipelines

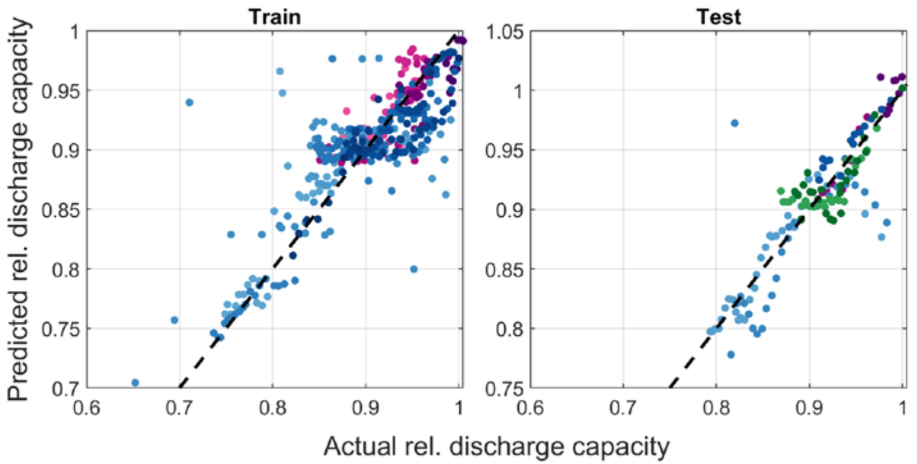
Combining multiple steps of feature normalization, generation, extraction, and selection can result in a complex sequence of steps prior to model training, some of which may have various hyperparameters or have different behaviors during training and testing.

Feature transformation pipelines make combining multiple feature transformations simple.

Model performance with feature engineering

Model results

The model performance on the training set is not as good as before, but cross-validation and testing errors are dramatically better.



Model	MAE_{Train}	MAE_{Test}
Linear, all features	1.23%	1665%
GPR, 2 freq.	2.44%	1.65%

Model interrogation

Model interrogation

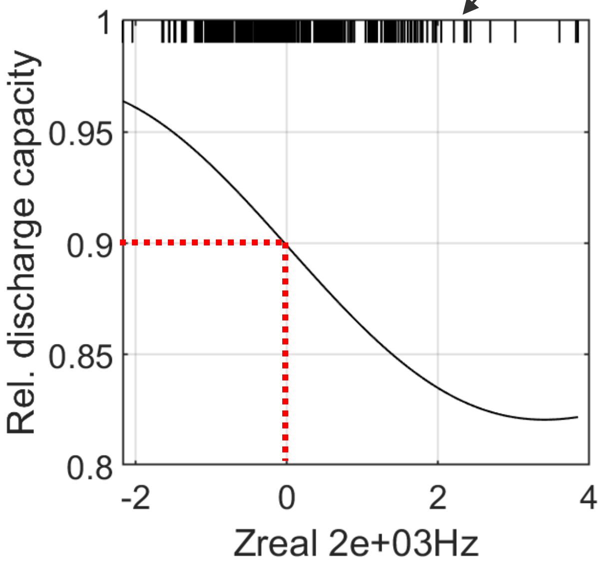
Many ML models are black boxes. We can’t look inside (at least in any way that makes sense to humans), but we can poke them, and see how they wiggle.

- Carefully analyze your predictions
- Partial dependence
- SHAP
- ….

Partial dependence

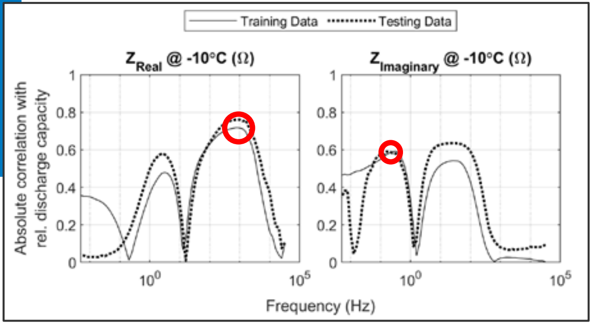
Values for this feature in the training data

Average value of y from the entire data set when all values for this given feature are set to x

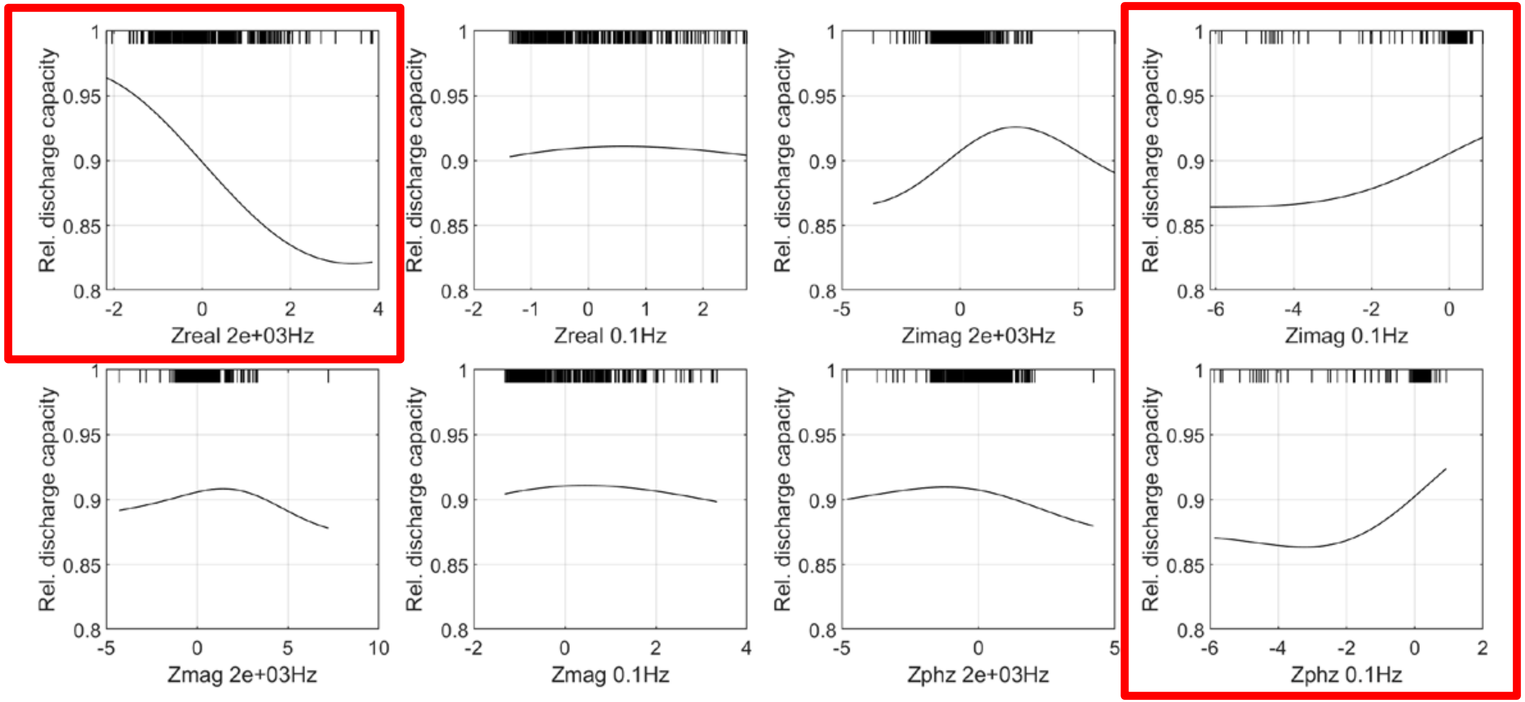


Only one or two features are varied at a time. All other model features use values from the training data.

Partial dependence



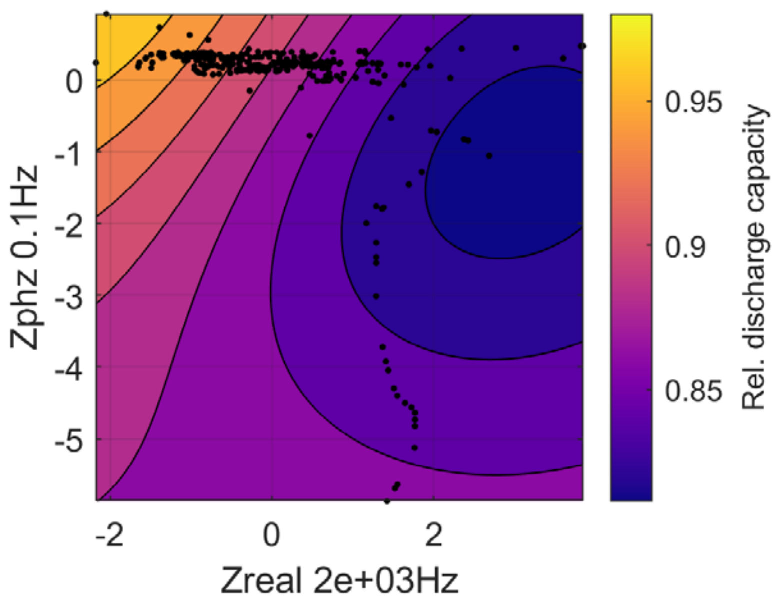
High freq. resistance (Ohmic) strongly predicts capacity

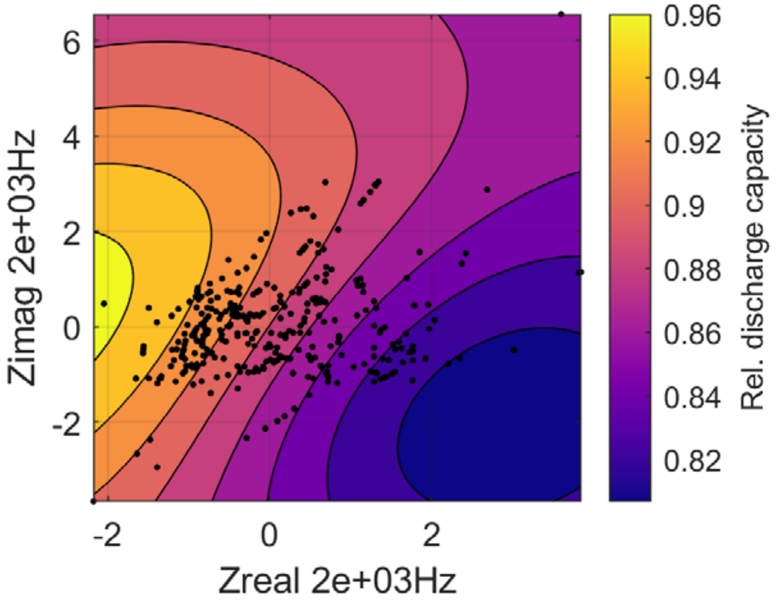


Phase at low freq. helps predict capacity near beginning of life.

Partial dependence

2D partial dependence performs a grid-search on all combinations of 2 features within the measured range of those features in the training data.





Takeaways

Takeaways

Rich, multi-dimensional data is full of information, but can lead to overfitting.

Holding out test data lets us experiment how models behave on unseen data.

Extracting features from raw data can improve modeling results and may help us gain insight into the data.

Interrogate models to get better understanding of model behavior.

Hands-on example

Hands-on example

Develop a regression model to predict battery capacity from EIS using data from Zhang et al. *Nature Communications* **11** 2706 (2020)

Stretch goal(s):

- Use random train/test splits to rigorously determine what the ‘best’ frequency is, independent of your selection of a specific train/test split

Questions?

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