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

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

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

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

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
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

Domain knowledge

Model-based dimensionality reduction
# 3. Model architectures

<table>
<thead>
<tr>
<th>Linear</th>
<th>Gaussian process regression</th>
<th>Random forest</th>
</tr>
</thead>
<tbody>
<tr>
<td>$y = x^T \beta + \epsilon$</td>
<td>$y = h(x)^T \beta + f(x)$</td>
<td>Bagged ensemble of boosted binary decision trees</td>
</tr>
<tr>
<td>Minimize MSE loss</td>
<td>Maximize likelihood</td>
<td>Minimize MSE loss</td>
</tr>
<tr>
<td>Regularized via $L_1$ (ridge regression) or $L_2$ (LASSO regression) norms added to loss</td>
<td>Fairly well self-regulated</td>
<td>Optimize forest size, leaf size, pruning rate via Bayesian hyperparameter optimization</td>
</tr>
</tbody>
</table>
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.
Selecting impedance from two frequencies is the most reliable strategy for predicting capacity from EIS. The frequencies selected matter.
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

<table>
<thead>
<tr>
<th>Model</th>
<th>$\text{MAE}_{\text{Test}}$</th>
<th>$\text{MaxAE}_{\text{Test}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Baseline</td>
<td>6.1%</td>
<td>12.0%</td>
</tr>
<tr>
<td>Linear (ridge)</td>
<td>2.3%</td>
<td>8.2%</td>
</tr>
<tr>
<td>GPR (25 Hz, 79 Hz)</td>
<td>2.0%</td>
<td>11.4%</td>
</tr>
<tr>
<td>RF (2 Hz, 500 Hz)</td>
<td>2.0%</td>
<td>11.3%</td>
</tr>
<tr>
<td>Ensemble</td>
<td>1.9%</td>
<td>7.2%</td>
</tr>
</tbody>
</table>
Bonus – replication on other data sets

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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www.nrel.gov

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