Accelerating battery development by early prediction of cell lifetime

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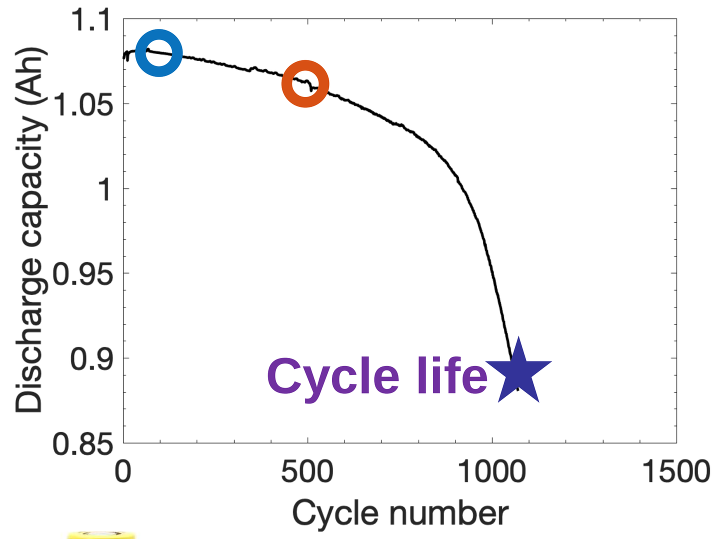
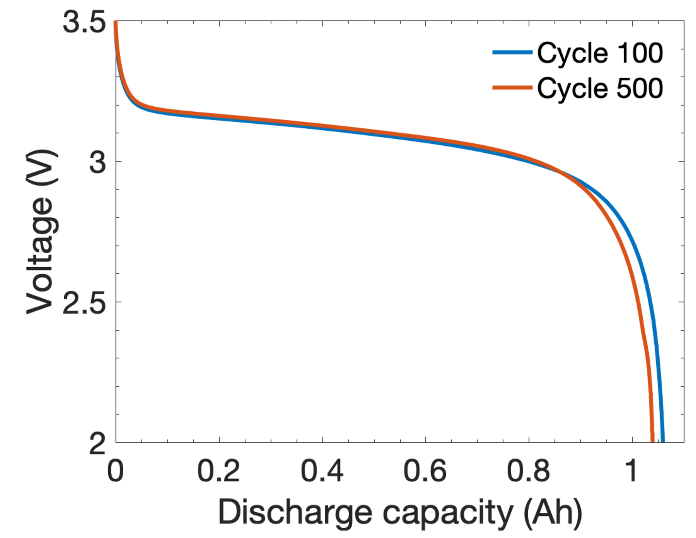
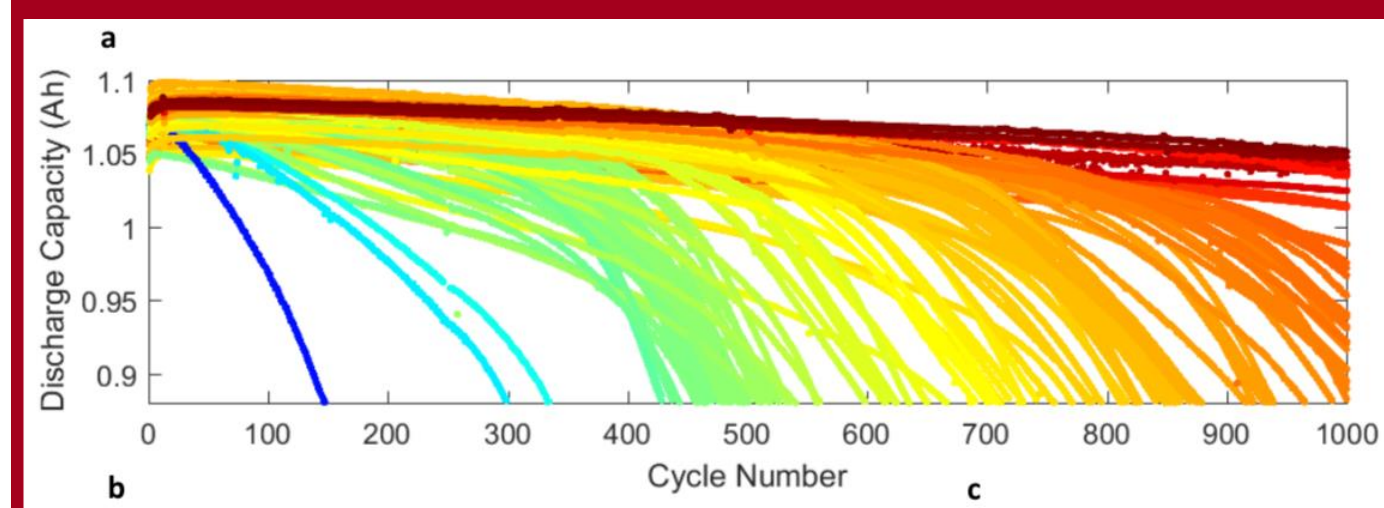
Motivation & objective

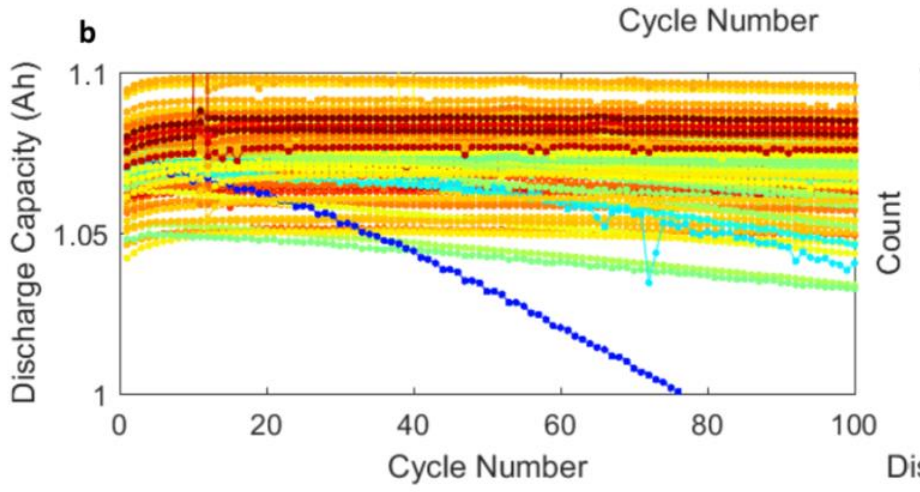
- **Battery testing** typically takes months to years
- Electrochemical models fail to capture dynamics during fast charging
- **Early prediction of cycle life** would accelerate R&D, manufacturing, and optimization
- **Goal:** Predict final cycle life (~1000s of cycles) using <100 cycles

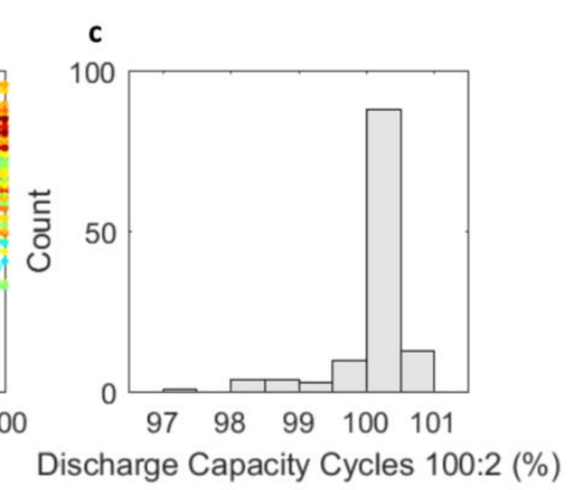




Dataset

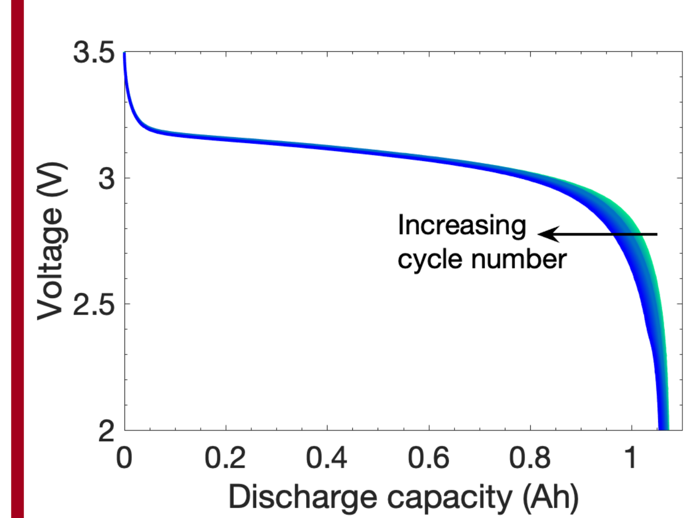


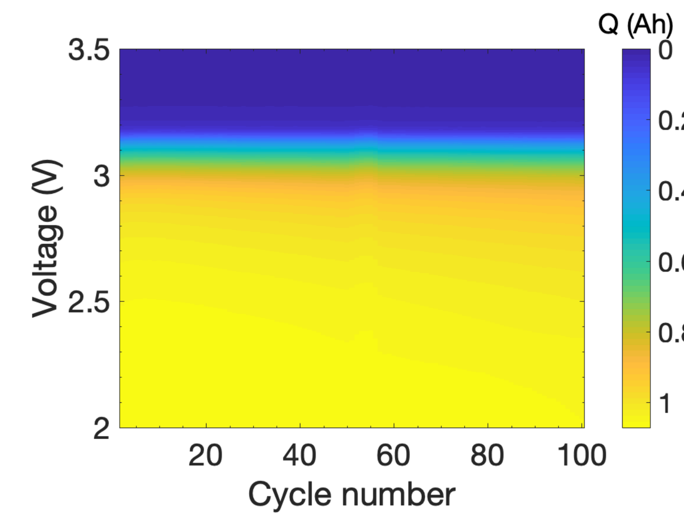


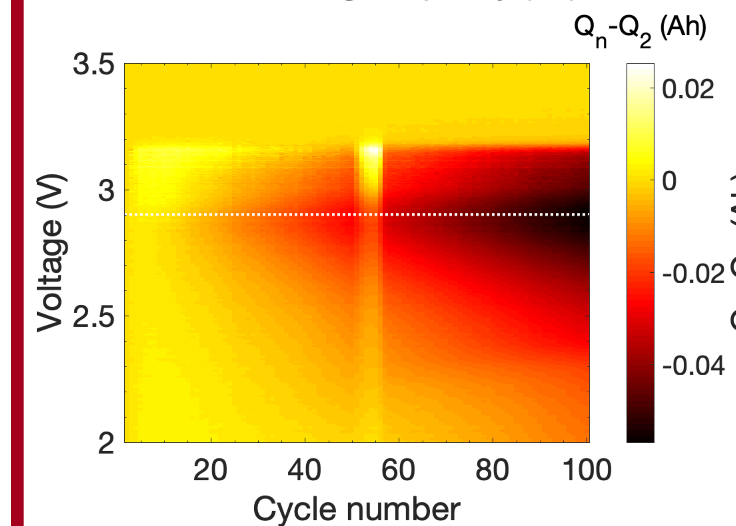


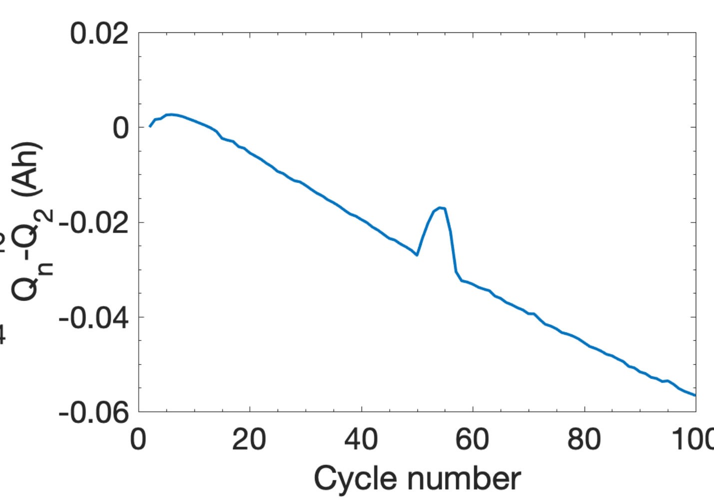
(a) Capacity vs cycle number (red = higher cycle life)
(b) Capacity vs cycle number for first 100 cycles
Initial capacity has weak correlation with cycle life
(c) Capacities initially rise (challenging prediction?)
Dataset: n=124; Cycle lives range from 150 to 2300

Features









Most information-rich data source: **voltage curves**
Develop voltage visualizations for feature extraction
Slices show **linear trend** → good for prediction!
Other features: capacity, temperature, resistance

Techniques

1. Elastic net
Regularized linear regression

$$\theta = \mathrm{argmin}_\theta\left(\|y - X\theta\| + \alpha\left((1-\lambda)||\theta||^2 + \lambda||\theta||_1\right)\right)$$

Simultaneously performs feature selection (via $||\theta||_1$) and regularized coefficient fitting

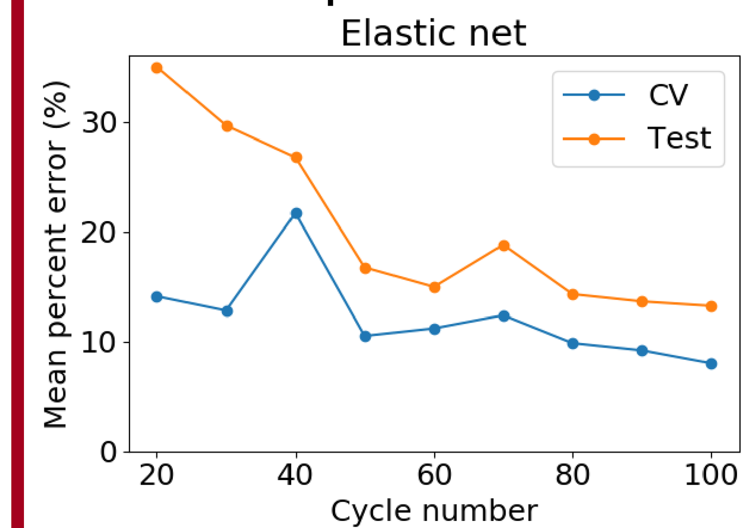
2. Random forest regression
Bagging of decision trees, with subset of features selected ($\sqrt{p}$) to decorrelate trees
Optimize over number of trees (B) & max depth (d)

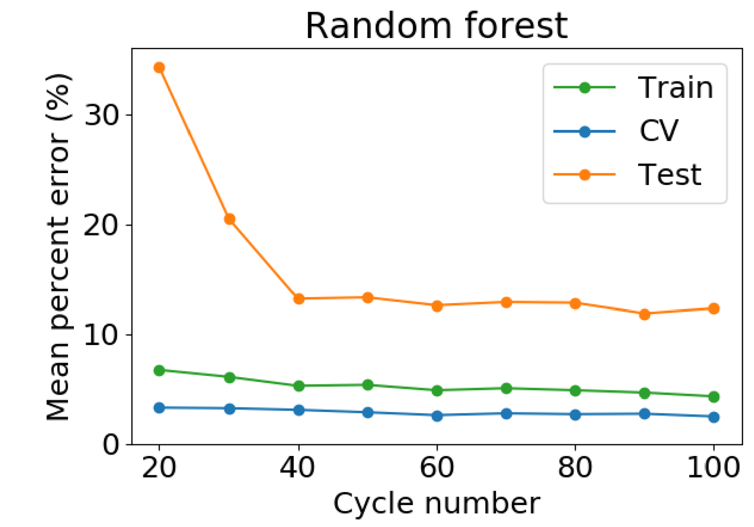
3. Adaboost regression
Sequential tree growing; learns slowly using information from previously grown trees
Optimize over number of trees (B) & learning rate (λ)

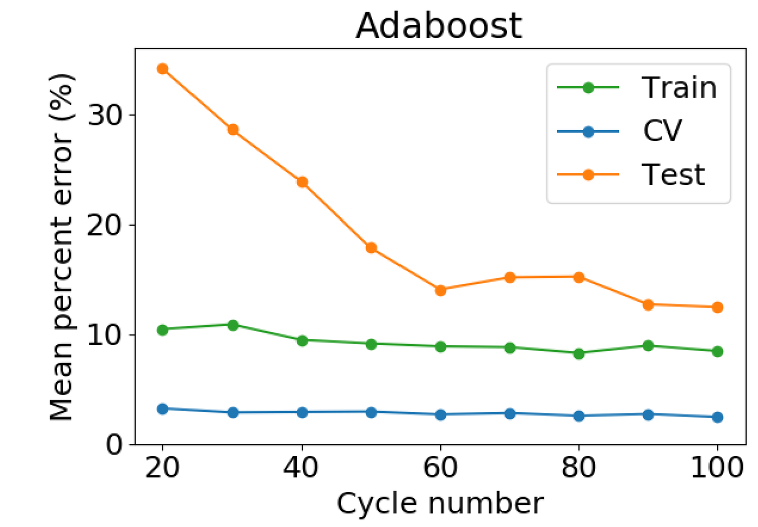
We use **5-fold cross validation** given small dataset
Training set = 84 cells, test set = 40 cells

Results and Discussion

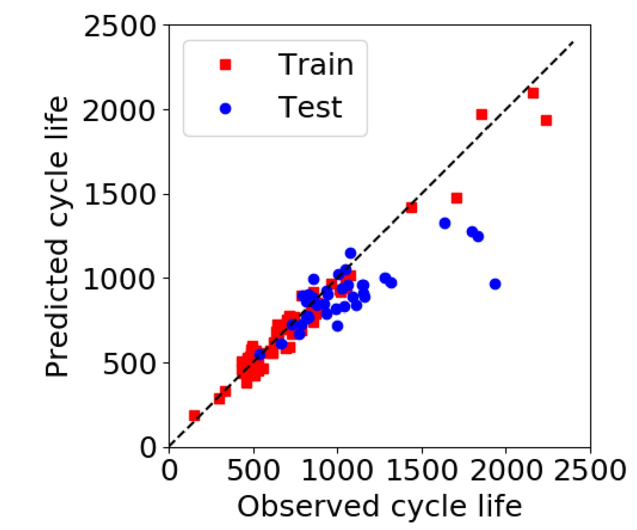
We developed models for 20 – 100 cycles, in increments of 10 cycles:

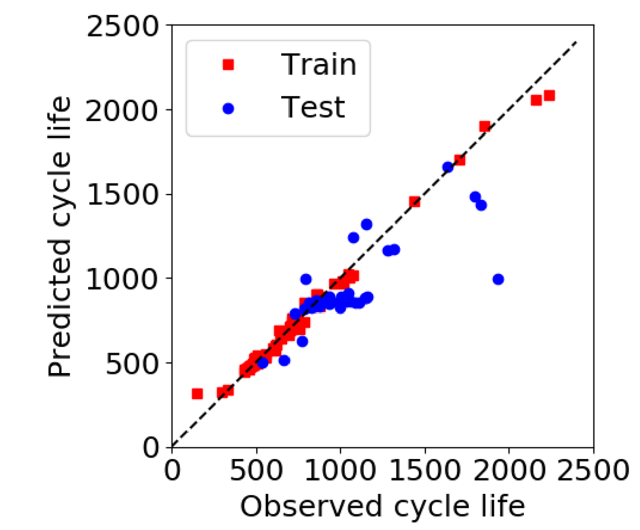


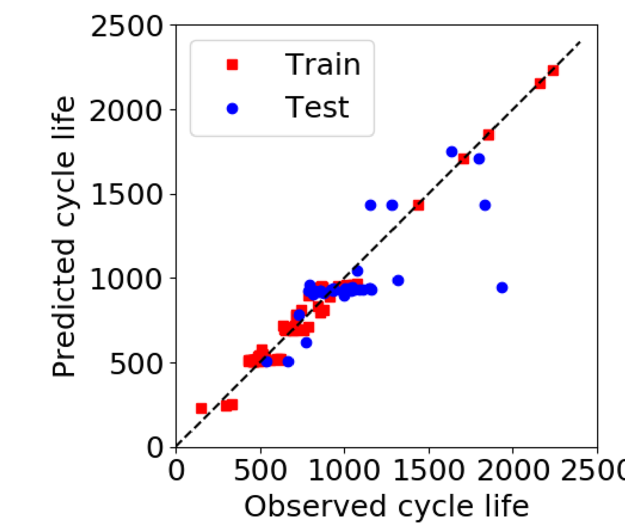




At cycle 100:







Feature selection for elastic net

Feature	20	30	40	50	60	70	80	90	100
SurfFit_p1	1.6	2.3		2.6	1.5	2.0	2.0	1.8	1.9
SurfFit_p2	4.2	3.8	1.4	1.8	1.9	1.9	1.7	1.6	1.2
SurfFit_p3	4.8	3.0		0.2	0.2	0.9	0.5	0.1	
Q_cycle2	0.5			1.6	1.2	1.1	1.4	1.7	1.2
Q_lastcycle	3.9	4.3		1.9	1.7	1.6	1.6	1.8	2.3
chargetime	7.9	7.4	3.8	2.8	1.9	2.2	2.2	2.7	2.4
Tmax	2.1	2.5		1.8	1.2	0.9	0.9	1.1	1.1
log_slope_2pt9V_corr	0.0	1.0		1.9	2.2	2.0	2.2	2.6	3.0
log_int_2pt9V_corr	0.4	0.1		1.6	2.0	2.0	2.2	3.1	3.3
log_DeltaQ_mean	0.7	2.8		2.1	2.1	1.4	1.9	1.7	2.5
log_DeltaQ_var	2.1	1.2	4.6	3.0	2.4	1.8	2.4	1.9	3.3
log_IR_min	4.7	4.7		3.1	1.9	1.6	2.3	3.0	2.4
log_IR_diff	1.9	1.4	0.6	1.2	1.2	1.5	1.3	1.0	0.7

Cycle number; Feature weight * 100

- **We can reduce # cycles required!**
- As expected, error generally increases with decreasing cycle number; some overfitting
- **Random forest** performs best
- Elastic net feature selection
  - *Low cycle numbers* (20-40): Charge time, surface fits, capacity, internal resistance (primarily time-independent features)
  - *High cycle numbers* (60-100): Line cuts, change in capacity (primarily degradation features)

Future work, contributions, references

Future work:

- Incorporate features from other components of dataset (rest periods, charging)
- Apply CNNs to X-ray images taken before cycling (manufacturing defects?)
- Classify cells into high/low lifetimes (preliminary screening applications)
- Using reinforcement learning to find optimal fast charging policies

Contributions: All authors contributed to data exploration, feature generation, model development, and poster/report creation.

References: S. J. Harris, D. J. Harris, C. Li. *J. Power Sources* 342, 589-597 (2017).
K. Severson*, P. Attia*, W. Chueh, R. Braatz *et al*. In review.