

Supplementary Materials

Comparative Analysis of Commonly Used Machine Learning Approaches for Li-Ion Battery Performance Prediction and Management in Electric Vehicles

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Table S1. Parameters used in regression-based ML models.

Model Number	Model Type	Preset	Model Size (bytes)	Selected Features	Hyperparameters	Optimizer Options
1	Linear Regression	Linear	6414	4	Terms: Linear Robust option: Off	Not applicable
2	Linear Regression	Interactions Linear	9462	4	Terms: Interactions Robust option: Off	Not applicable
3	Linear Regression	Robust Linear	6958	4	Terms: Linear Robust option: On	Not applicable
4	Stepwise Linear Regression	Stepwise Linear	9462	4	Initial terms: Linear Upper bound on terms: Interactions Maximum number of steps: 1000	Not applicable
5	Kernel	SVM Kernel	9212	4	Learner: SVM Number of expansion dimensions: Auto Regularization strength (Lambda): Auto Kernel scale: Auto Epsilon: Auto Standardize data: Yes Iteration limit: 1000	Not applicable
6	Kernel	Least Squares Regression Kernel	9142	4	Learner: Least Squares Kernel Number of expansion dimensions: Auto Regularization strength (Lambda): Auto Kernel scale: Auto Standardize data: Yes Iteration limit: 1000	Not applicable
7	Gaussian Process Regression	Rational Quadratic GPR	1882692	4	Basis function: Constant Kernel function: Rational Quadratic Use isotropic kernel: Yes Kernel scale: Automatic Signal standard deviation: Automatic Sigma: Automatic Standardize data: Yes Optimize numeric parameters: Yes	Not applicable

8	Gaussian Process Regression	Squared Exponential GPR	1882661	4	Basis function: Constant Kernel function: Squared Exponential Use isotropic kernel: Yes Kernel scale: Automatic Signal standard deviation: Automatic Sigma: Automatic Standardize data: Yes Optimize numeric parameters: Yes	Not applicable
9	Gaussian Process Regression	Exponential GPR	1882647	4	Basis function: Constant Kernel function: Exponential Use isotropic kernel: Yes Kernel scale: Automatic Signal standard deviation: Automatic Sigma: Automatic Standardize data: Yes Optimize numeric parameters: Yes	Not applicable
10	Efficient Linear	Custom Efficient Linear	10866	4	Solver: Auto Relative coefficient tolerance (Beta tolerance): 0,0001	Optimizer: Bayesian optimization Training time limit: false Acquisition function: Iterations: 30 Expected improvement per second plus
11	Efficient Linear	Efficient Linear SVM	10934	4	Learner: SVM Solver: Auto Regularization: Auto Regularization strength (Lambda): Auto Relative coefficient tolerance (Beta tolerance): 0,0001 Epsilon: Auto	Not applicable
12	Efficient Linear	Efficient Linear Least Squares	10894	4	Learner: Least squares Solver: Auto Regularization: Auto	Not applicable

					Regularization strength (Lambda): Auto Relative coefficient tolerance (Beta tolerance): 0,0001	
13	Efficient Linear	Efficient Linear SVM	10934	4	Learner: SVM Solver: Auto Regularization: Auto Regularization strength (Lambda): Auto Relative coefficient tolerance (Beta tolerance): 0,0001 Epsilon: Auto	Not applicable
14	Efficient Linear	Custom Efficient Linear	11577	4	Solver: SGD Relative coefficient tolerance (Beta tolerance): 0,0001	Optimizer: Bayesian optimization Acquisition function: Iterations: 30 Training time limit: false Expected improvement per second plus

Table S2. Parameters of DT-based ML models.

Model Number	Model Type	Preset	Model Size (bytes)	Selected Features	Hyperparameters
1	Tree	Fine Tree	1603830	4	Minimum leaf size: 4 Surrogate decision splits: Off
2	Tree	Medium Tree	688034	4	Minimum leaf size: 12 Surrogate decision splits: Off
3	Tree	Coarse Tree	237830	4	Minimum leaf size: 36 Surrogate decision splits: Off
4	Ensemble	Boosted Trees	157041	4	Minimum leaf size: 8 Number of learners: 30 Learning rate: 0,1 Number of predictors to sample: Select All
5	Ensemble	Bagged Trees	26304765	4	Minimum leaf size: 8 Number of learners: 30 Number of predictors to sample: Select All

Table S3. Parameters of SVM-based ML models.

Model Number	Model Type	Preset	Model Size (bytes)	Selected Features	Hyperparameters
1	SVM	Linear SVM	1507475	4	Kernel function: Linear Kernel scale: Automatic Box constraint: Automatic Epsilon: Auto Standardize data: Yes
2	SVM	Fine Gaussian SVM	1618087	4	Kernel function: Gaussian Kernel scale: 0,5 Box constraint: Automatic Epsilon: Auto Standardize data: Yes
3	SVM	Medium Gaussian SVM	1619247	4	Kernel function: Gaussian Kernel scale: 2 Box constraint: Automatic Epsilon: Auto Standardize data: Yes
4	SVM	Coarse Gaussian SVM	1508007	4	Kernel function: Gaussian Kernel scale: 8 Box constraint: Automatic Epsilon: Auto Standardize data: Yes

Table S4. Hyperparameters of ANN-based models.

Model Number	Model Type	Preset	Model Size (bytes)	Selected Features	Hyperparameters	Optimizer Options
1	Neural Network	Narrow Neural Network	5462	4	Number of fully connected layers: 1 First layer size: 10 Activation: ReLU Iteration limit: 1000 Regularization strength (Lambda): 0 Standardize data: Yes	Not applicable
2	Neural Network	Medium Neural Network	6182	4	Number of fully connected layers: 1 First layer size: 25 Activation: ReLU Iteration limit: 1000 Regularization strength (Lambda): 0 Standardize data: Yes	Not applicable
3	Neural Network	Wide Neural Network	9782	4	Number of fully connected layers: 1 First layer size: 100 Activation: ReLU Iteration limit: 1000 Regularization strength (Lambda): 0 Standardize data: Yes	Not applicable
4	Neural Network	Bilayered Neural Network	7262	4	Number of fully connected layers: 2 First layer size: 10 Second layer size: 10 Activation: ReLU Iteration limit: 1000 Regularization strength (Lambda): 0 Standardize data: Yes	Not applicable
5	Neural Network	Trilayered Neural Network	9062	4	Number of fully connected layers: 3 First layer size: 10 Second layer size: 10 Third layer size: 10 Activation: ReLU Iteration limit: 1000 Regularization strength (Lambda): 0 Standardize data: Yes	Not applicable