Supplementary Information for
Identification and machine learning prediction of knee-point and knee-onset in capacity degradation curves of lithium-ion cells

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Supplementary Figures

Supplementary Fig. 1: Knee-point identified in a random sample of 32 cells from the A123 dataset, using three methods: the Bacon-Watts method from the main article and the methods proposed by Satopaa et al. and Diao et al.
Supplementary Fig. 2: Knee-onset identified in a random sample of 32 cells from the A123 dataset, using two methods: the intersection between the first segment of the Bacon-Watts model and the capacity fade data and the double Bacon-Watts model.
Supplementary Fig. 3: Comparison of single transition point in Bacon-Watts model ($x_1$, blue cross) in relation to the two transition points of the double Bacon-Watts ($x_0$ and $x_2$, yellow circle and red plus respectively), for all cells in the A123 dataset. It can be seen that $x_1$ always lies between $x_0$ and $x_2$, i.e. blue cross always above yellow circle and below red plus signs.

Supplementary Fig. 4: Cycle-to-cycle evolution of in-cycle variables used for feature extraction: a current as a function of time, b discharge curve as a function of voltage, c first derivative of b, d first derivative of voltage as a function of discharge capacity, e change in discharge voltage curves between a given cycle and a reference cycle, f similar to e for the voltage as a function of the discharge capacity and g temperature as a function of voltage. Sample data for cell b1c20.
Supplementary Fig. 5: Illustration of feature extraction process for one of the predictors of the regression model. Starting from $dV/dQ$ curves (left), given for each cell and cycle, the area under the curve is computed to extract the cycle-to-cycle evolution of an intermediate variable at a cycle level, for each cell (centre). Lastly, the minimum is calculated to obtain a predictor with one value per cell (right).

Supplementary Fig. 6: Machine learning pipeline and feature extraction for classification problem using first 3 cycles: 2 steps of feature extraction using metrics from time series analysis, selection of relevant features using recursive feature elimination, feature normalisation and support vector machine.
Supplementary Fig. 7: Machine learning pipeline and feature extraction for quantitative prediction problem using first 50 cycles: 2 steps of feature extraction using metrics from time series analysis, selection of relevant features using Bonferroni correction, feature normalisation, Box-Cox transformation, Principal Component Analysis and relevance vector machine enriched with conformal prediction on the last step.
Supplementary References


