CNN-based Online Diagnosis of Knee-point in Li-ion Battery Capacity Fade Curve

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Abstract: Accurate monitoring of capacity degradation of a lithium-ion battery is important as it enables the user to manage its usage for optimal performance/lifetime and also to take preemptive actions against any potential explosion or fire. Battery capacity fades gradually through repetitive charging and discharging until it reaches the so called 'knee-point' after which it goes through rapid and irreversible deterioration to reach its end-of-life. It is crucial to forecast the knee-point early and accurately for safe and economic use of the battery. Machine learning based methods have been used to predict the knee-point with early cycle data. Despite some notable progress made, the existing methods make the unrealistic assumption of constant cycle-to-cycle charge/discharge operation. In this study, a deep learning method is developed for online knee-point prediction under the more realistic scenario of variable battery usage. A CNN-based model extracts temporal features of data across past and current cycles to sort out those cells in an urgent state that calls for close monitoring, and then predict the number of cycles left to reach the knee-point. The proposed method extracts features from dynamic data and thus the extracted features reflect dynamic changes in battery properties, thereby improving the prediction performance under realistic scenarios.

Keywords: Lithium-ion batteries, Knee-point, Convolutional neural networks, Feature extraction

1. INTRODUCTION

As the global markets for electric vehicles and energy storage systems grow, the demand for lithium-ion batteries is exponentially increasing. Consequently, ensuring stability of the battery cells has become a major issue, not only to lengthen their lifetime but also to prevent catastrophic explosions. Battery capacity degrades with repeated charging and discharging until the cell reaches 80% of its initial capacity, marking the end of its lifetime. For safety and economic reasons, it is important to monitor a battery's state of health (SOH) and predict its remaining lifetime. Particularly, an occurrence of sudden capacity degradation can lead to serious problems. General Motors issued a recall resulting in a significant economic loss due to such a problem in 2017 (Zhang et al., 2019). In general, battery capacity tends to fade gradually before it reaches a critical transition point, called 'knee-point', after which the degradation greatly accelerates. Since irreversible deterioration occurs after that, predicting the knee point in advance is therefore critical in ensuring safe use and prolonging its lifetime.

There have been few research studies on methods for predicting the knee-point; instead most studies have focused on predicting remaining useful life (RUL). Accurate RUL estimation can certainly be helpful in achieving more predictable battery performance. However, more active measures would be possible if the nature of battery degradation mechanism is better known. Prediction of the knee-point rather than the number of cycles left to the end-of-life would make enable an earlier detection of accelerated health degradation and more timely predictive maintenance. This motivates us to address the problem of predicting the knee point. Battery SOH prognostics can be broadly grouped into two categories: model-based methods and data-driven methods. The former category tries to develop an aging model based on fundamental electrochemical principles and then fits the model parameters to available data. On the other hand, the latter tries to extract certain fingerprints from available data that can be useful for monitoring and predicting the nature of battery degradation. Many stress factors exist that affect a battery's aging process, and it is very difficult to describe all the involved mechanisms mathematically. This limitation makes the data-driven approach easier and perhaps more practical as it can extract patterns which are results of phenomena yet to be discovered. Recently, various early prediction models of the knee-point based on machine learning have been put forward. The quantile regression method was employed for knee-point recognition but it cannot be used for advance prediction in cases of nonlinear fade (Zhang et al., 2019). A novel method to identify the knee-point and knee-onset was proposed using a prediction model of these points based on early-cycle data (Fermín-Cueto et al., 2020). Knee-onset, a term newly defined in this work, represents the point marking the beginning of nonlinear capacity degradation. A convolutional neural networks (CNN) model was proposed to predict a full capacity fade curve interpolating some key points including the kneepoint and the knee-onset from one cycle data (Strange and Dos Reis, 2021). However, the existing models are valid only under the restrictive assumption of a constant charge/discharge pattern from one cycle to next, which is highly unrealistic. Insitu alert of an impending reaching of the knee-point to the end user is needed, with operating conditions changing from one cycle to another.



Fig. 1. Proposed two-step CNN-based online knee-point diagnosis method, which first identifies the cells with less than 100 cycles left to the knee-point and then predicts the number of cycles left to the knee-point.

In this study, a deep learning method is developed for online knee-point prediction under a more realistic scenario of variable charge/discharge operation. A CNN-based model extracts temporal features across past and current charge/discharge cycle data to sort out those cells that are likely to reach the knee point early on (i.e., earlier than normal), and then predict the number of cycles left to the knee-point in real time. The proposed approach is the first of its kind enabling online knee-point prediction.

The paper is structured as follows: Section 2 describes the data preparation process and model development based on deep layers of CNN. In Section 3, performance of the prediction model is analyzed and compared with the method that uses manually extracted features. Section 4 concludes the paper.

2. MODEL DEVELOPMENT

2.1 Data preprocessing

To develop an online knee-point prediction model, raw measurement data of voltage, current, and temperature during charging and discharging cycles are used as input. Given the different lengths of cycle data available to us, interpolation was used to fill in missing time points such that each cycle is represented by 200 data points. Outlier removal and noise filtering were performed. Data from 3 consecutive cycles is collected as a vector and used as the input as patterns seen in consecutive cycling data contain time-wise trends of the battery degradation. The input data matrix is given as

$$\mathbf{x}_{N}^{(i)} = \begin{bmatrix} V_{N-2,1}^{(i)} & \cdots & V_{N-2,200}^{(i)} & \cdots & V_{N,1}^{(i)} & \cdots & V_{N,200}^{(i)} \\ I_{N-2,1}^{(i)} & \cdots & I_{N-2,200}^{(i)} & \cdots & I_{N,1}^{(i)} & \cdots & I_{N,200}^{(i)} \\ T_{N-2,1}^{(i)} & \cdots & T_{N-2,200}^{(i)} & \cdots & T_{N,1}^{(i)} & \cdots & T_{N,200}^{(i)} \end{bmatrix}_{3\times 600}$$

where $V_{N,j}^{(t)}$, $I_{N,j}^{(t)}$, and $T_{N,j}^{(t)}$ indicate voltage, current, and temperature at the *j*-th point from the current *N*-th cycle of the *i*-th battery cell. Since input data includes data collected from previous two cycles before the current cycle, *N* can take on a value between 3 and the number right before the knee-point.

The knee-point of each cell was calculated by the Bacon-Watts model (Fermín-Cueto et al., 2020), which is shown to be effective on data containing a large amount of noise. Capacity degradation is represented in a two-piecewise linear function with unknown parameters of the slopes and the transition point (which represents the knee-point) fitted to the data. Each input data is labeled with the number of cycles left to the knee-point, *Y*, defined as

$$Y = C_{knee-point} - N$$

where $C_{knee-point}$ is the cycle number at the knee-point and N is the current cycle index. For the first stage classification task, the labels are given to the cells, depending on how early the knee-points are reached, as described in a later section.



Fig. 2. Identifying the knee-point on a capacity degradation curve of a sample cell

2.2 Model architecture

CNN automatically extract features from data through mathematical convolution operations. While CNNs have been extensively applied in the field of computer vision, it also has huge potential for use in handling time-series data (Jiang and Zavala, 2021). Once data are represented in a grid form, they can highlight hidden features among them. Therefore, CNN is used as a base model architecture to extract temporal features across the raw data. A proposed CNN-based deep learning method works in two steps: classification of knee-onset state and prediction of cycles left to the knee-point. Although accurate prediction of the knee-point is critical, it is not efficient to build a predictor that performs the prediction at every single cycle from the start of cycle life. If we interpret the knee-point as the transition point from a gradual deterioration to a rapid one, it would be better to notify the end user immediately when signs of an accelerated degradation appear. Therefore, the classification model first sorts out the cell according to the knee-onset state. The knee-onset of each cell was calculated by the double Bacon-Watts model (FermínCueto et al., 2020) and they were about 100 cycles before the knee-point on average. When input data are given, the classification model determines whether more than 100 cycles are left before reaching the knee-point (*class 0*) or not (*class 1*) starting from the current state. Then, only for those cells belonging to *class 1*, the predictor estimates how many cycles are left to the knee-point so as to enable any remedial action to prolong its life and prevent catastrophic failures.



Fig. 3. CNN model architecture

Each input variable has a close correlation within its own measurements through repetitive cycles of charging and discharging. Therefore, it is important to capture features, i.e., fingerprints, embedded in them that can represent current state of the cell using all the available data up to that point. In this work, dilated CNNs are used to boost up learning, which are proven to be efficient when processing long sequences of timeseries data (Oord et al., 2016). A dilated convolution is a convolution skipping input values at certain steps and defined as

$$y[i] = \sum_{l=1}^{L} x[i+d \cdot l]h[l],$$

where x[i] and y[i] is the input and output value at timestep *i*, h[l] is the filter of length *L*, and *d* is the dilation rate. Dilation increases the receptive field so that less information is lost along long-term data. Deep layers of a dilated CNN enable the learning of the patterns hidden in the augmented input data.

The prediction model is composed of six consecutive CNN blocks followed by fully connected (FC) layers (see Fig. 3). Batch normalization was used to stabilize the training process and max pooling was operated in the first two CNN blocks. Detailed configuration of the model is described in Table 1. To train the classification model, the binary cross entropy (BCE) term is used as the loss function.

$$BCE = -\omega_n [y_n \log x_n + (1 - y_n) \log(1 - x_n)],$$

where ω_n is the class weight, y_n and x_n are the ground-truth and the score for *class* 0 and $(1 - y_n)$ and $(1 - x_n)$ are for *class 1*. Due to the imbalance in data amount between the two classes, class weight ω_n is manually calculated from the number of samples in each class and added on the loss term to improve the model performance. To train the regression model to predict the knee-point, the mean square error (MSE) loss function is used:

$$MSE = \frac{1}{n} \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2$$

where *n* is the number of training samples, Y_i is prediction output of the model, and \hat{Y}_i is the ground-truth of the sample.

Table 1. Configuration of the model

Layer name	Filter size	Number of kernels	Dilation
Input	3×600	-	-
Conv.1	15	16	2
Maxpooling1	2	16	-
Conv.2	15	32	2
Maxpooling2	2	32	-
Conv.3	15	32	2
Conv.4	15	32	2
Conv.5	15	32	2
Conv.6	1	1	-
FC1	16	-	-
FC2	output size	-	-

3. MODEL EVALUATION

3.1 Data description

The dataset provided by Severson et al. (2019) was used in this study. The dataset is generated from 124 commercial Li-ion phosphate (LFP)/graphite cells cycled until end-of-life, at which capacity degrades to 80% of the nominal capacity. The cells have a nominal capacity of 1.1 Ah and a nominal voltage of 3.3 V. Each cell was cycled under different one-step or two-step fast-charging policies ranging from 3C to 8C but was discharged with an identical 4C discharging condition. Measurement data of the voltage, current, temperature, and internal resistance are recorded over every cycle.

3.2 Knee-point prediction result

The dataset was randomly split into three sets: 104 cells for training, 10 cells for validation, and another 10 cells for testing. Adam optimizer was used for training 200 epochs with a batch size of 1024. Training stopped when the validation loss showed no improvement after 6 epochs.

The prediction result of the model is given in Table 2. It achieved 91% of accuracy for classifying *class* 0 and *class* 1. According to the confusion matrix in Fig. 3 (a), recall for *class* 1 was 99% implying that the model is accurate in terms of classifying cells in an urgent state. The case that should be avoided most in terms of safety is to misclassify the dangerous *class* 1 cells as *class* 0. Fortunately, such case represented only 1%. For those cells with 100 cycles left to the knee-point, the



Fig. 3. (a) Confusion matrix for the classification model. (b) Error in predicting how many cycles are left to the knee point vs different input lengths used. The results are averages over 100 random seeds. (c) Training time per epoch overdifferent input lengths. Also averaged over 100 random seeds. Total training time was divided by the number of epochs for an easy comparison because each random seed resulted in a different epoch number where the training stopped.

model predicted the number of cycles left with an average error of 14.60 cycles.

	Precision	Recall	F1-Score	Support
Class 0	1.00	0.89	0.94	4115
Class 1	0.69	0.99	0.81	1000
Accuracy		0.91		5115
Prediction r	esult			
MAE (cycle)		1	4.60	

Table 2. Result of online knee-point diagnosis framework

In addition, model performance with different input cycle lengths was compared (Fig. 3 (b)) to evaluate the sensitivity of the model to the amount of input data used. 1 to 10 cycle long data were tested as the input vector. As the cycle length increased, the error decreased since the model can potentially extract more information from the longer historical data. However, the computational load also increases with the data length, so a proper cycle length should be selected (Fig. 3 (c)).

3.3 Comparison with model using manually selected features

To demonstrate the effectiveness of the proposed method, the knee-point prediction model with manually selected features based on Severson et al. (2019) is compared. Several features are extracted to predict cycle life based on expert knowledge. We take these features to build a prediction model based on multilayer perceptron (denoted as MLP model) which can validate automatic feature extraction of CNN model. The MLP model is establish by removing the CNN blocks in charge of feature extraction (Fig. 1) and feeding the manually selected features as input to the latter FC layers.

Table 3. 7 manually selected features for knee-point prediction. All features are extracted from the same raw input data used in the CNN model for fair comparisons. N is the current cycle

number and k represents the input cycle length, ranging from 3 to 10.

Corresponding raw data	Features
V, I (Discharging)	Variance of discharge voltage curve difference between cycle $N - k + 1$ and cycle N Minimum of discharge voltage curve difference between cycle $N - k + 1$ and cycle N Slope of linear fit to the capacity fade curve, cycles $N - k + 1$ to cycle N Intercept of linear fit to the capacity fade curve, cycles $N - k + 1$ to cycle N Discharge capacity at current cycle
V, I (Charging)	Average charge-time during k cycles
T	Integral of temperature over time, cycles $N - k + 1$ to cycle N

7 features that can be constructed from the charge/discharge V, I, T data are chosen and modified to fit to the online prediction model (see Table 3). These features are then fed into the shallow MLP model replacing the automatically extracted features by CNN.



Fig. 4. Comparison between the proposed CNN model and the MLP model with manually selected features (Severson et al., 2019)

According to Fig. 4, our CNN model outperforms the MLP model when input information of less than 5 cycle length is used. This implies that it is able to extract key fingerprints for the capacity degradation from unrefined measurement data. As more information is given, the MLP model shows slightly better performance. However, it has a critical limitation that features can be extracted only after a full cycle is finished. The statistical features of the discharge voltage curve and capacity fade curve become available after discharging is completed to the end. On the contrary, the CNN model using raw data is free from those constraints, making itself more suitable for online prediction. Moreover, regarding the essence of battery management system, longer input data length might be burdening and sometimes infeasible due to memory management issues.

4. CONCLUSIONS

As monitoring the status of battery degradation is becoming crucial, efficient early on-line prediction of the knee-point has become important. The unrealistic assumption of constant cycle-to-cycle charge/discharge operation has been relaxed in the proposed CNN-based deep learning method, which diagnoses a battery cell's health and predicts the number of cycles left to the knee-point in real-time. The method extracts the relevant patterns in the dynamic charging/discharging profiles to enable more accurate and flexible prediction of the knee point. The framework has well-classified the cells about to be on the knee-point, which then needs to be watched closely. For those cells, accurate prediction of knee-point was possible thanks to the CNN model's capability to extract key degradation fingerprints hidden in measurement data. Its effectiveness was demonstrated by comparison with the MLP model which replaced the automatically extracted features with manually selected features in the published literature.

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