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A Bayesian approach for Li-Ion battery capacity fade modeling and cycles to failure prognostics

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HIGHLIGHTS

- Model Li-Ion battery capacity/power fade using Bayesian models to capture various variations.
- Systematic method for battery performance prediction including predictor and model selection.
- Compare two data input methods for accurate battery capacity fade prognostics.
- Simulate and evaluate the end-of-life battery cycles to failure distributions.

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ABSTRACT

Battery capacity fade occurs when battery capacity, measured in Ampere-hours, degrades over the number of charge/discharge cycles. This is a comprehensive result of various factors, including irreversible electrochemical reactions that form a solid electrolyte interphase (SEI) in the negative electrode and oxidative reactions of the positive electrode. The degradation mechanism is further complicated by operational and environmental factors such as discharge rate, usage and storage temperature, as well as cell-level and battery pack-level variations carried over from the manufacturing processes. This research investigates a novel Bayesian method to model battery capacity fade over repetitive cycles by considering both within-battery and between-battery variations. Physics-based covariates are integrated with functional forms for modeling the capacity fade. A systematic approach based on covariate identification, model selection, and a strategy for prognostics data selection is presented. The proposed Bayesian method is capable of quantifying the uncertainties in predicting battery capacity/power fade and end-of-life cycles to failure distribution under various operating conditions.

1. Introduction

Li-ion batteries are used in a variety of applications, such as satellites, automobiles, laptops, and other electrical equipment. In order to extend the lifetime of batteries, extensive research has been conducted to explore new battery materials for electrodes and electrolytes, designing new electrode structures, and investigating various battery aging mechanisms [1–3]. Capacity fade prediction over repetitive charge/discharge cycling based on quantitative mathematical models is another important research topic. Accurate estimation and prediction of battery failure time provides the decision information for timely replacement of degraded batteries before the batteries reach the end of their useful life.

Battery capacity fade is mainly attributable to electrochemical reactions, and the associated factors causing such reactions can be leveraged for accurate performance degradation prediction [4]. These factors include charge–discharge protocol, temperature, state of charge (SOC), and materials of electrode and electrolyte. For different types of batteries, capacity fade mechanisms are usually dominated by unique aging mechanisms [5–7]. For example, it has been demonstrated that active lithium loss due to electrolyte decomposition forming the solid electrolyte interphase (SEI) in the carbon negative is the dominant aging mechanism for $LiFePO_4$ batteries [5]. It has also been shown that a substantial decrease in the surface conductivity in lithium nickel cobalt aluminum oxide ($LiNi_{0.8}Co_{0.15}Al_{0.05}O_2$) cells dominate the cells aging processes [6]. In addition, Broussely et al. [7] observed that the anode's structural

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Notation and acronyms

i	index for the observed capacity data
j	index for each individual battery cell
n_J	the number of observed capacity fade data
α	intercept of the fixed effect model
α_j	intercept of the random effect model
β_{kj}	slope parameters of the square root of cycle, logarithm cycle and interaction,$k = 1,2,3$
ε_i	random errors in the mixed effect capacity fade model
Σ	covariance matrix in the random effect model for intercept and slope parameters
SEI	Solid Electrolyte Interphase
BIC	Bayesian Information Criterion
MAD	Mean Absolute Deviation

instability due to volumetric change induced stress during repeated charge/discharge cycling can also lead to accelerated capacity fade. Smith et al. [8] interpreted the degradation mechanism of Li-ion cells using a lithium inventory model to account for the unwanted parasitic reactions during the battery charge and discharge cycling process. Parasitic processes and reactions, including the solid electrolyte interphase (SEI) growth and repair at the negative electrode, the electrolyte oxidation at the positive electrode, the dissolution of transition metal ions, and the rate of positive electrode damage, are incorporated in the proposed lithium inventory model.

Extensive research has been conducted to understand capacity fade and predict battery life. Generally, these works can be classified into three types: physics-based methods, data-driven methods, and hybrid methods of combining both methods [9]. Under physics-based performance degradation modeling, Santhanagophlan et al. [10] applied an unscented filter algorithm to model the electrochemical reactions that cause the battery's capacity fade based on a rigorous electrochemical model proposed by Doyle et al. [11]. Safari et al. [12] proposed a multimodal physics-based model that considers solvent-decomposition reaction as the source of capacity fade. Ning et al. [13] developed a physics-based model based on the loss of active lithium ions and the rise of anode film resistance.

Physics-based capacity fade and prediction models can accurately predict capacity fade through knowledge of the electrochemical changes in batteries. However, these models are usually limited to specific type of batteries. On the other hand, data-driven models, which are less dependent on the physics-of-failure mechanisms, have been extensively investigated [14–19]. For example, Jin et al. [14] employed a Bayesian framework for on-line degradation assessment and residual life prediction of secondary batteries in spacecraft. Liu et al. [15] used Gaussian process functional regression in capacity fade modeling. He et al. [16] estimated parameters in a capacity fade model using the Bayesian Monte Carlo method. The deficiency of data-driven models is their difficulty in interpreting the model parameters and predicting variables.

A more suitable method for battery performance modeling is the hybrid method, which integrates physics-of-failure mechanisms and data-driven models. Hybrid methods usually have better interpretability for capacity fade mechanisms. Broussely et al. [7] studied the losses at the negative electrode and fitted a rate-determining step model with experimental data. Jungst et al. [20] developed an inductive model that modeled the capacity loss as a function of state of charge (SOC), storage temperature, and time, based on experimental data from 18650 cells. Thomas et al. [21] suggested a methodology for estimating the mean cell life with uncertainty bounds that uses both a degradation model and an error model based on accelerated degradation test data. However, the existing physics-based and data-driven hybrid models only model the longitudinal uncertainty of capacity fade and ignore the between-battery variations. The proposed Bayesian method incorporates physics-of-failure-based covariates and is able to quantify the uncertainty of both within-battery and between-battery variations.

Compared with independently observed data, the dependency of within-battery observations over cycles contains important longitudinal structure information that independently observed data do not possess. In the proposed Bayesian capacity fade prognostic method, such dependency and variations within a micro-level unit, such as the observed capacity data for a single battery over a certain period of time, is modeled using appropriate functional forms with the identified physics-of-failure-based covariates. On the other hand, when multiple battery units are tested, the between-battery variation and uncertainty structure need to be well modeled. Between-battery variations usually come from the manufacturing process due to material and process variations. In the proposed Bayesian model, the random effects for the coefficients of the functional capacity fade model are capable of modeling such between-battery variations. Thus, both within-battery and between-battery variations can be statistically modeled using the proposed Bayesian models with random effects. In addition, this paper investigates the optimal data selection strategy for accurate capacity fade prediction, which has been less studied in the literature. Two data usage schemes for capacity fade prediction—cumulative data input and moving window data input-are compared, and an optimal moving window length for using historical capacity data is determined for accurate capacity fade prediction. Fig. 1 shows the overall research scheme. The proposed methodology for battery capacity fade modeling and health prognostics follows three major steps, i.e., covariates selection, model selection and health prognostics. During the covariate selection, predicting variables are identified based on the reviewed literature and physics-of-failure failure mechanisms. The model selection part evaluates and compares both fixed and random effect models for capacity fade modeling. Finally, two data input methods for battery health prognostic are investigated using the selected random effect capacity fade model from step 2.

The performance of Li-ion battery can also be expressed in term of Watt-hours which is the unit of energy measurement indicating how much energy can be drawn from the battery for a certain number of hours. Thus, power fade becomes a more meaningful indicator of battery performance in applications such as hybrid electric vehicles. In certain external environments, power fade is directly related to the increase of impedance as well as the active material loss during microchemical reactions over cycles [22]. Both impedance rise and active material loss are related to the number of cycles. Theoretically, Watt-hour and Ampere-hour can be converted to each other via the formula: $Wh = Ah \times V$. As a result, power fade modeling and prediction can utilize the same functional forms as used for the capacity fade models.

The remainder of the paper is constructed as follows. Section 2 describes the battery testing data and investigates the covariates for building predictive models using designed experiments. Section 3 compares a set of various capacity fade models by incorporating various combinations of identified prediction variables. The model's performance with random effects and without random effects is compared in terms of the Bayesian information criterion. Section 4 investigates two types of a data input scheme for battery