

Constrained Bayesian Optimization for Minimum-Time Charging of Lithium-Ion Batteries

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Abstract—The fast charging of lithium-ion batteries while minimizing battery degradation is a key challenge to battery community. Difficulties in this optimization are the high dimensionality of parameter space of charging strategies, significant variability between batteries (even from the same production line), and limited quantitative information on battery degradation mechanisms. Current approaches to addressing these challenges are model-based optimization and grid search. Model-based methods are limited by the insufficient complexity and accuracy of electrochemical models – especially in the early stage of development when a new battery chemistry is being introduced to the market – and grid search methods are expensive in terms of testing time and cells. This article proposes a data-driven Bayesian optimization (BO) approach for minimum charging time problem, in which an acquisition function of constrained expected improvement is employed to explicitly handle constraints that limit degradation. In addition, continuous-varied-current charging protocols are introduced into the proposed BO approach by utilizing the technique of polynomial function expansions. The effectiveness of the proposed approach is demonstrated on the LIONSIMBA, a porous electrode theory-based battery simulator. The simulation results show that the proposed BO-based charging approach with continuous current profile outperforms the commonly used constant current constant voltage (CC-CV) method for the minimum charging time problem. Moreover, the decrease in the minimum charging time and increase in its variance with increasing number of degrees of freedom used in charging protocols is also quantified.

Index Terms—Data-driven optimization, fast charging, lithium-ion battery, energy systems, machine learning.

I. INTRODUCTION

WITH electric vehicles (EVs) recently gaining popularity, range anxiety and long charging time are becoming common concerns and are considered to be the main barriers

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for wider adoption of EVs [1]–[3]. Fast charging capability has therefore been of growing interest in the community of batteries and EVs [4], [5]. However, charging at high currents was observed to accelerate the degradation of battery capacity [1], [2], [5]. Charging strategies or protocols, which determine how the current densities used during the charging process that best balance the desire for fast charging while minimizing battery degradation, is of importance to solve the issues of long charging time and range anxiety.

Common challenges in optimization of charging strategies are high dimensionality of parameter space, and high manufacturing variability. Two approaches for probing a large battery operating parameter space are grid search [6], [7] and model-based optimization [8], [9]. Grid search, which largely samples protocols from across the parameter space and experimentally tests them multiple times, is accurate but expensive in terms of testing time and cells. Using physics-based battery models to optimize operating conditions has been proposed as a way to reduce experimentation time. Lam *et al.* [9] utilized a single shooting optimization method to design fast charging of minimizing both charging time and reaction rates of solid electrolyte interphase (SEI) formation, in which a coupled electrochemical-thermal-aging model is used to capture the growth of the SEI layer. Xavier [10] proposed a model predictive control (MPC) method in combination with a reduced-order model to design fast-charging strategies in the presence of no-plating constraints. Torchio *et al.* [11] put forward a quadratic dynamic matrix control approach to optimize charging protocols in real time subjecting to the battery temperature and voltage constraints. Xu *et al.* [12] proposed a multi-stage charging approach for lithium-ion batteries to minimize capacity degradation with constraints on SEI layer growth, in which a dynamic programming algorithm based on electrochemical-thermal-capacity fading model is used to optimize charging current profiles.

However, optimization based on electrochemical models has the following difficulties: (i) Model-based methods are limited by the insufficient complexity and accuracy of electrochemical models, which do not comprise all of the details of the degradation mechanisms and the effects of manufacturing variations [13], [14]. (ii) The electrochemical models that describe the details of degradation mechanisms in lithium-ion batteries often comprise of hundreds or even thousands of states [14], leading to an expensive large-scale optimization problem when used to compute charging protocols. The issues above can be addressed by applying a model-free Bayesian optimization framework for fast charging design.

Bayesian optimization (BO) is a commonly used data-driven approach for performing global optimization of black-box objective functions that are expensive to evaluate and possibly noisy [15], [16], just as the characteristics of objective function in the fast-charging optimization problem for lithium-ion batteries. A BO approach comprises of surrogate models and acquisition functions. A surrogate model, which is often a cheaper probabilistic model such as Gaussian process regression, is used for approximating original objective functions that are of expensive evaluation [16]. An acquisition function is for efficiently probing the space of parameters by balancing exploration and exploitation [15], [16]. In the absence of constraints, acquisition functions such as expected improvement (EI), upper confidence bound (UCB), and predictive entropy search (PES) are widely used [16]. For the case with constraints, the most established acquisition function to circumvent constrained BO is constrained EI (cEI) [17], in which separate regression models are applied to learn the constraint functions, and the standard EI acquisition function is modified to account for additional information of constraint uncertainties. Constrained PES (cPES) is another acquisition function for BO with constraints. However, cPES is difficult to implement and its computation is expensive [17]. Shahriari *et al.* [16] and Gelbart [17] provide good reviews on BO methods.

BO approaches have been widely used in various field such as autonomous driving policy determination [18], crystal structure prediction [19], and robot path planning [20]. However, investigation on the application of BO to fast charging design is limited. In one study [6], a standard BO algorithm is utilized to efficiently optimize fast charging protocols by formulating the charging problem as to maximize battery cycle life in a fixed charging time, in which an unconstrained version of acquisition function (upper confidence bound) is utilized.

In this work, we formulate the fast-charging problem in a different manner, namely, the optimization objective is the minimization of the charging time while imposing constraints on the charging introduced by degradation concerns. It is widely acknowledged that cells degrade faster at elevated temperatures (e.g., $>40^\circ\text{C}$) or higher voltages (e.g., $>4.15\text{ V}$), depending on the battery chemistry (e.g., graphite/lithium iron phosphate) [21], [22], constraints on the maximum temperature and voltage are therefore imposed. Then a data-driven constrained BO methodology is proposed to minimize charging time while guaranteeing the constraints of voltage and temperature, in which an acquisition function of cEI is utilized to account for the uncertainty information of voltage and temperature constraints. In addition, continuous-varied-current charging protocols are introduced into the proposed BO approach by incorporating the polynomial function expansions technique. The proposed constrained BO-based charging approach is tested by using a LIONSIMBA-based battery simulator using the representation of pseudo-two-dimensional model [23].

The contributions of this work are summarized as following.

(i) A constrained BO approach is put forward to optimize fast charging while meeting constraints that limit battery capacity fading. The constrained BO-based charging approach is sample-efficient and does not need first-principles models.

(ii) Continuous-varied-current charging protocols are introduced into the proposed BO approach and their performance is compared and discussed for the minimum time charging problem with application to a simulated graphite/LiCoO₂ battery. The decrease in the minimum charging time and increase in its variance with increasing number of degrees of freedom used in charging protocols is quantified.

The rest of this letter is organized as follows. The constrained BO approach is stated in Section II. The proposed BO approach with cEI acquisition function for the minimum charging time optimization is developed in Section III. The effectiveness of the proposed approach is demonstrated in a porous electrode theory-based battery simulator in Section IV, followed by conclusions in Section V.

II. CONSTRAINED BAYESIAN OPTIMIZATION APPROACH

The objective of the Bayesian optimization in this work is to minimize a target black-box function:

$$y = f(\mathbf{x}) + \varepsilon \quad (1)$$

subject to the constraints

$$c_i(\mathbf{x}) \leq \delta_i, \quad i = 1, 2, \dots, k \quad (2)$$

where $\mathbf{x} \in \mathbb{R}^d$, δ_i is the limit for the i th constraint and ε is measurement noise following $\varepsilon \sim N(0, \sigma^2)$.

A. Gaussian Process Regression

Gaussian processes (GPs) are distributions over functions that are specified by a mean and covariance function [24]. GPs are used to model both the objective function $f(\mathbf{x})$ and the constraint functions $c_i(\mathbf{x})$, $i = 1, 2, \dots, k$. $f(\mathbf{x})$ and $c_i(\mathbf{x})$ are assumed to be provided by independent Gaussian processes priors.

For the objective function $f(\mathbf{x})$, its GP model can be provided as

$$f(\mathbf{x}) \sim GP(m_f(\mathbf{x}), \kappa_f(\mathbf{x}, \mathbf{x}')) \quad (3)$$

where $m_f(\mathbf{x})$ is the mean which is often specified to be zero [24], and $\kappa_f(\mathbf{x}, \mathbf{x}')$ is the covariance function. The choice of the covariance function $\kappa_f(\mathbf{x}, \mathbf{x}')$ depends on *a priori* knowledge and data. A commonly used Gaussian kernel is used in this work [24]. The Gaussian kernel is characterized by its hyperparameters that are often learned from data via maximum likelihood estimation. With the hyperparameters learned, the GP model is then used to infer the posterior distribution $f(\mathbf{x})|\mathcal{D}$ given the data \mathcal{D} as [24]

$$f(\mathbf{x})|\mathcal{D} \sim N(\mu_f(\mathbf{x}; \mathcal{D}), \sigma_f^2(\mathbf{x}; \mathcal{D})) \quad (4)$$

where

$$\mu_f(\mathbf{x}; \mathcal{D}) = K_f^T(\mathbf{x})\Sigma_f^{-1}\mathbf{y} \quad (5)$$

$$\sigma_f^2(\mathbf{x}; \mathcal{D}) = K(\mathbf{x}, \mathbf{x}) - K_f^T(\mathbf{x})\Sigma_f^{-1}K_f(\mathbf{x}) \quad (6)$$

with $K_f(\mathbf{x}) = [\kappa_f(\mathbf{x}, \mathbf{x}^{(1)}), \dots, \kappa_f(\mathbf{x}, \mathbf{x}^{(N)})]^T$, and $[\Sigma_f]_{ij} = \kappa_f(\mathbf{x}^{(i)}, \mathbf{x}^{(j)}) + \sigma^2\delta_{ij}$, where δ_{ij} is the Kronecker delta function.

Similarly, the constraint functions $c_i(\mathbf{x})$ can also be modelled with GPs, whose predicted mean and variance can be obtained by replacing the kernel function of $\kappa_f(\mathbf{x}, \mathbf{x}')$ in (3)-(6) with $\kappa_{c_i}(\mathbf{x}, \mathbf{x}')$. The detailed expression can be found in [17], which is omitted here for brevity.

B. Acquisition Function of Constrained Expected Improvement

Expected improvement (EI) criterion is utilized here to construct an acquisition function for constrained Bayesian optimization [15], [16]. The EI function with respect to the predictive distribution of Gaussian process enables a balance to the tradeoff of exploitation and exploration. The EI acquisition function is to maximize the improvement which is given by [25]

$$\alpha_{\text{EI}}(\mathbf{x}) = \sigma_f(\mathbf{x}) \left((Z_f(\mathbf{x}) \Phi(Z_f(\mathbf{x}))) + \phi(Z_f(\mathbf{x})) \right) \quad (7)$$

where

$$Z_f(\mathbf{x}) = \frac{f(\mathbf{x}^+) - u_f(\mathbf{x})}{\sigma_f(\mathbf{x})} \quad (8)$$

$\Phi(\cdot)$ and $\phi(\cdot)$ are the normal cumulative distribution function and the normal probability distribution function respectively; the incumbent $f(\mathbf{x}^+)$ means the best observation so far, and $u_f(\mathbf{x})$ and $\sigma_f(\mathbf{x})$ are the posterior predictive GP mean and standard deviation for objective function, respectively.

Because the improvement is not feasible when constraints are violated, an acquisition function for constrained Bayesian optimization can be defined by extending the EI in (7) to take into account the additional constraint uncertainties. This results in a constrained EI (cEI) acquisition function, which is expressed as

$$\alpha_{\text{cEI}}(\mathbf{x}) = \alpha_{\text{EI}}(\mathbf{x}) \prod_{i=1}^k \Pr(c_i(\mathbf{x}) \leq \delta_i) \quad (9)$$

where the constrained satisfaction probabilities can be separated owing to assumed independence among $c_i(\mathbf{x})$.

Since each probability $\Pr(c_i(\mathbf{x}) \leq \delta_i)$ is a normal cumulative distribution function, the cEI acquisition function in (9) can be further expressed as [17]

$$\alpha_{\text{cEI}}(\mathbf{x}) = \sigma_f(\mathbf{x}) \left((Z_f(\mathbf{x}) \Phi(Z_f(\mathbf{x}))) + \phi(Z_f(\mathbf{x})) \right) \prod_{i=1}^k \Phi\left(\frac{\delta_i - \mu_i(\mathbf{x})}{\sigma_i(\mathbf{x})}\right) \quad (10)$$

where $\mu_i(\mathbf{x})$ and $\sigma_i(\mathbf{x})$ are the posterior predictive GP mean and standard deviation for constraint $c_i(\mathbf{x})$.

III. BATTERY FAST CHARGING PROBLEM

This section first briefly states a commonly used battery model that describes many of the physicochemical details of battery dynamics, and then describes a fast-charging problem in the formulation of minimum-time charging optimization.

A. Electrochemical Model by Porous Electrode Theory

The porous electrode theory (PET) model is widely used for describing lithium-ion batteries [26]. This article uses LIONSIMBA [23] – a MATLAB implementation of the PET model based on the finite volume method – as a battery simulator.

In the PET model, the diffusion of lithium ions within each solid particle is described by [25], [27]

$$\frac{\partial}{\partial t} c_s(z, t) = \frac{1}{z^2} \frac{\partial}{\partial z} \left[z^2 D_{\text{eff}}^s \frac{\partial}{\partial z} c_s(z, t) \right] \quad (11)$$

with boundary conditions

$$\frac{\partial}{\partial z} c_s(z, t) \Big|_{z=0} = 0, \quad \frac{\partial}{\partial z} c_s(z, t) \Big|_{z=R_s} = -\frac{j(z, t)}{D_{\text{eff}}^s} \quad (12)$$

where t is time, z is the one-dimensional spatial variable; $c_s(z, t)$ is the concentration of the solid particles; R_s is the radius of the solid particles; D_{eff}^s is the effective diffusion coefficients within the particles; and $j(z, t)$ is the ionic flux.

The state of charge (SOC) of the anode is defined as

$$\text{SOC}(t) := \frac{1}{L_n c_s^{\text{max},n}} \int_0^{L_n} c_s(z, t) dz \quad (13)$$

where $c_s^{\text{max},n}$ is the maximum concentration of lithium ions in the negative electrode.

The conservation of charge in the electrodes based on Ohm's law is modeled as

$$\frac{\partial}{\partial z} \left[\sigma_{\text{eff}} \frac{\partial}{\partial z} \Phi_s(z, t) \right] = a F j(z, t) \quad (14)$$

where $\Phi_s(z, t)$ is the solid potential, F is Faraday's constant, and σ_{eff} is the effective conductivity of the electrodes. The voltage of the lithium-ion cell can be computed by

$$V(t) := \Phi_s(0, t) - \Phi_s(L, t) \quad (15)$$

The temperature dynamics are described by

$$\rho C_p \frac{\partial}{\partial t} T(z, t) = \frac{\partial}{\partial z} \left[\lambda \frac{\partial}{\partial z} T(z, t) \right] + Q_{\text{ohm}}(z, t) + Q_{\text{rxn}}(z, t) + Q_{\text{rev}}(z, t) \quad (16)$$

where λ is the thermal conductivity, C_p is the specific heat, ρ is the material density, and the terms $Q_{\text{ohm}}(z, t)$, $Q_{\text{rev}}(z, t)$, and $Q_{\text{rxn}}(z, t)$ are ohmic, reversible, and reaction heat sources [27].

The aforementioned equations are coupled through ionic flux, which is described by the Butler-Volmer equation. More details on the PET-based electrochemical model and its software implementation can be found in [23], [25], [26].

B. Minimum Charging Time Optimization Problem

The objective is to solve the battery charging problem in minimum time without violating operating constraints. The fast charging problem is formulated as

$$\min_{I(t)} \{t_f\} \quad (17)$$

$$\text{subject to} \begin{cases} \text{battery dynamics in (11)–(16)} \\ T_{\text{cell}}(t_0) = T_0 \\ \text{SOC}(t_f) = \text{SOC}_{\text{ref}} \\ V(t) = V^{\text{max}}, T_{\text{cell}}(t) \leq T_{\text{cell}}^{\text{max}} \end{cases} \quad (18)$$

where $t_0 = 0$ and t_f are the initial and final times of the charging process, T_0 is the initial value for the temperature, SOC_{ref} is the reference of SOC at which the charging is considered completed, and V^{max} and $T_{\text{cell}}^{\text{max}}$ are upper bounds for the voltage and temperature.

Continuous-varied-current charging protocols are considered here, which is defined as

$$I(t) = \sum_{j=0}^p \beta_j \phi_j(t) \quad (19)$$

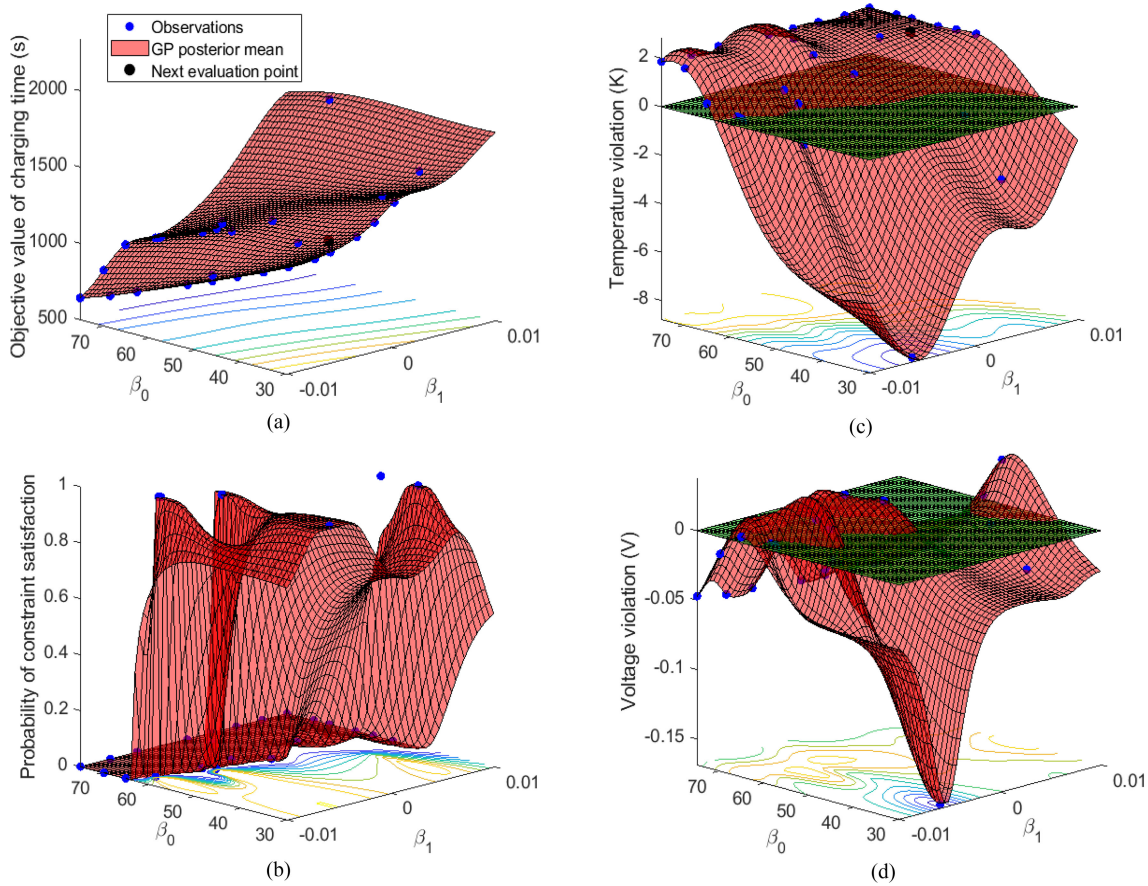


Fig. 1. Sampling behavior produced by the constrained BO method to reach the optimal charging profile for optimization of charging protocol with $p = 1$, along with the corresponding GP modeling for the objective function and voltage and temperature constraints: (a) GP modeling for the objective function, (b) probability of constraint satisfaction $\prod_{i=1}^K \Pr(c_i(x) \leq \delta_i)$, and (c, d) voltage and temperature constraint violations where positive values indicate the constraints are violated.

where ϕ_j are basis functions, β_j are the corresponding coefficients, and p is the order of the basis. The basis functions are often chosen *a priori* to reflect desired properties. For simplicity, the polynomials are used as basis functions (i.e., $\phi_j(t) = t^j$), and the order $p = 0, 1, 2$, corresponding to the constant, linear, and quadratic basis function would be considered in this letter.

The implementation procedure of the proposed BO-based approach is as following: Surrogate models of Gaussian process (GP) are trained on initial datasets; and the learned GP information is used to generate an acquisition function for probing next data samples. The data samples are then contained into the dataset to update the GP models. These procedures are repeated until achieving optimal charging protocols or reaching the maximum iteration step.

If we have *a priori* knowledge on the starting point initialization for the implementation of BO, the proposed approach would converge to the solution of optimal charging protocol faster; if we do not have such *a priori* knowledge, the implementation of proposed BO-based approach may need more evaluations to converge to the same degree of optimality.

IV. RESULTS AND DISCUSSION

In this section, the objective is (i) to validate proposed constrained Bayesian optimization approach for the minimum time charging optimization, and (ii) to evaluate the

TABLE I
MEAN AND STANDARD DEVIATION OF THE MINIMUM CHARGING TIME OPTIMIZED BY CONSTRAINED BO FOR THE CHARGING PROTOCOLS $p = 0, 1$, AND 2 AFTER 30 EVALUATIONS. EACH OPTIMIZATION PROCEDURE WAS REPEATED 20 TIMES FOR EACH CASE

Minimum charging time (s)	$p = 0$	$p = 1$	$p = 2$
Mean (Std)	1162.8 (5.5)	1102.5 (22.9)	1054.2 (40.7)

performance of various continuous-varied-current charging protocols (i.e., $p = 0, 1$, and 2) for the fast-charging problem, in comparison with the commonly used CC-CV charging method. The PET-based electrochemical model in Section III, for a graphite anode/LiCoO₂ (LCO) cathode cell [23] is employed for the evaluation and comparison. Our goal is to obtain a minimum time charging protocol that charges the battery from 20% state of charge (SOC) to 80% SOC, while keeping the cell temperature and cell terminal voltage within operational constraints. The values of the constraint parameters are $V^{\max} = 4.15\text{V}$, and $T_{\text{cell}}^{\max} = 313.15\text{K}$; the bound interval for charging protocol coefficients in (20) are $\beta_0 \in [30, 75]$, $\beta_1 \in [-10^{-2}, 10^{-2}]$, and $\beta_2 \in [-10^{-5}, 10^{-5}]$.

Given the budget of 30 evaluations, the mean and standard deviation of minimum charging time (MCT) for the fast charging problem optimized by using the constrained BO approach for the charging protocols with orders $p = 0, 1$, and 2 are provided in Table I. As shown in Table I, the charging

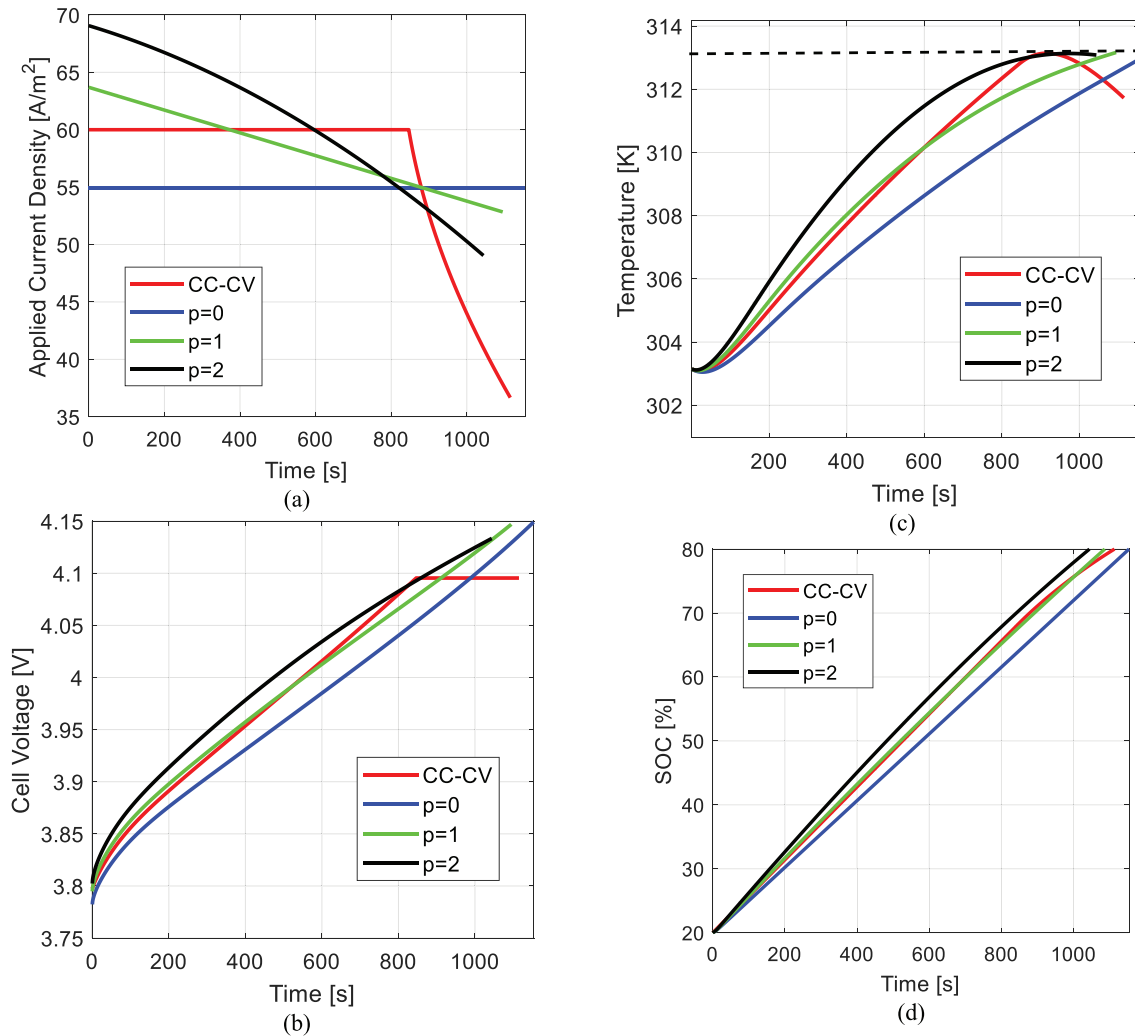


Fig. 2. The optimal charging profiles provided by the constrained BO method for the charging protocols $p = 0, 1$ and 2 after 30 evaluations as well as the optimal charging profile for the CC-CV method: (a) applied current density, (b) cell terminal voltage, (c) cell temperature, and (d) SOC. The dashed lines in the cell temperature are the upper bound of temperature.

protocol $p = 2$ optimized by the constrained BO approach had faster charging time than the charging protocols $p = 0$ and $p = 1$ produced by the same BO method. Specifically, the mean MCT of the charging method $p = 2$ was 1054.2 s, compared to 1162.8 s to the $p = 0$ and 1102.5 s for the $p = 1$. Table I shows that the standard deviation of MCT is larger for the charging method with $p = 2$ than that with $p = 1$, and for the charging method $p = 1$ than $p = 0$. The difference between the standard deviation for the charging method $p = 2$ is 40.7 s, which are 35.2 and 17.8 s larger than that of $p = 0$ and $p = 1$, respectively. The reason is that, for a fixed number of evaluations, the higher dimension of the parameter spaces, the larger the variance of results produced by the constrained BO methods.

Take the case of using the constrained BO method for optimization of charging protocol $p = 1$ as an example, the sampling behavior to reach the optimal charging profile, along with the corresponding GP modeling for the objective function and voltage and temperature constraints, by the utilization of acquisition function of constrained EI is displayed in Fig. 1. Figs. 1bcd visualize how much constraints are violated during

the exploration and exploitation behavior provided by the constrained BO method, in which the probability of constraint satisfaction is calculated by $\prod_{i=1}^k \Pr(c_i(\mathbf{x}) \leq \delta_i)$, and the voltage and temperature constraint violation degrees are computed according to $\max\{V(t) - V^{\max}, \forall t \in [0, t_f]\}$, and $\max\{T(t) - T^{\max}, \forall t \in [0, t_f]\}$, respectively. The results show that infeasible samples (i.e., the sample points whose probability $\cong 0$ in Figure 1b) were produced by the acquisition function of cEI, which occurred because the expected improvement term $\alpha_{\text{EI}}(\mathbf{x})$ in the cEI in eq. (9) is more dominant than the constraint satisfaction probability term $\prod_{i=1}^k \Pr(c_i(\mathbf{x}) \leq \delta_i)$ at those sample points.

The best MCT was achieved by the constrained BO approach for the charging protocols $p = 0, 1$, and 2 , with the applied current density, state of charge, cell voltage, and cell temperature plotted in Fig. 2. As shown in Figs. 2bc, the optimal charging profile of the protocol $p = 0$ first hits the limit of voltage, while the protocols $p = 1$ and 2 first touch the temperature limit. The optimized charging profile for the protocol $p = 2$ exhibits the constant temperature (CT) shape (see Fig. 2c), which can be qualitatively same as the

model-based control results in [28]. The only difference is that the proposed constrained BO-based charging approach do not need the information of model dynamics. As shown in Fig. 2a, for both the charging protocols $p = 1$ and 2, the maximum allowed charging current is applied and then the current gradually decreases until the end of charging, which relaxes high polarization toward the end of charging [5].

The best MCT for the charging protocols $p = 0, 1$, and 2 is 1150.6 s, 1095.2 s, and 1041.5 s, respectively. Compared with the MCTs optimized for the charging protocols $p = 0$ and 1, the optimal charging protocol $p = 2$ charged 109.1 s and 53.7 s faster, respectively. In addition, a commonly used CC-CV charging method [2] is used here as a benchmarking. The CC-CV method would switch the charging from constant current to constant voltage when the cell voltage or temperature during charging reaches their maximum allowed values. It can be obtained that the MCT for the CC-CV method is 1115.4 s (see supplementary information), and the corresponding optimal charging profiles for applied current density, state of charge, cell voltage, and cell temperature are also provided in Fig. 2. Fig. 2 shows that our proposed BO based charging approaches are 73.9 s (protocol $p = 2$) and 20.2 s (protocol $p = 1$) better than the benchmarking CC-CV method. The results further demonstrate the efficacy of the proposed constrained BO approach with continue current protocol for the battery fast-charging design.

V. CONCLUSION

In this article, a constrained Bayesian optimization strategy in combination with continuous-varied-current profile is proposed for the battery minimum charging time problem in the presence of voltage and temperature constraints. The proposed BO-based fast charging approach was demonstrated by a LIONSIMBA-based battery simulator using the representation of pseudo-two-dimensional model. The results show that the proposed charging approach is superior than the benchmarking CC-CV method. For the best-performing charging method, the charging protocol $p = 2$ charged 92.2 s faster than CC-CV. In addition, the decrease in the minimum charging time with increasing number of degrees of freedom used in charging profiles was quantified – the optimal charging protocol $p = 2$ provided by the constrained BO approach charged 109.1 s and 53.7 s faster than that for the charging protocols $p = 0$, and 1, respectively. In addition to the fast-charging design, the proposed constrained BO strategy can also be extended for the optimization of battery design parameters related to next-generation electrolyte chemistries such as solid-state electrolytes.

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