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Multi-objective optimization for fast charging design of lithium-ion batteries using constrained Bayesian optimization

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HIGHLIGHTS

- A method is proposed to minimize charging time while maximizing battery lifetime.
- A constrained Bayesian optimization is utilized to explore the parameter space.
- The method is sample-efficient and does not require first-principles models.
- The convergence rate of method in fast-charging optimization is quantified.

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ABSTRACT

Fast charging of lithium-ion battery accounting for both charging time and battery degradation is key to modern electric vehicles. The challenges of fast charging optimization are (i) the high dimensionality of the space of possible charging protocols while the experiment budget is often limited; and (ii) the limited quantitative description of battery capacity fade mechanisms. This article proposes a data-driven multi-objective charging approach to minimize charging time while maximizing battery cycle life, in which a Chebyshev scalarization technique is used to transform the multi-objective optimization problem into a group of single objective problems, and a constrained Bayesian optimization (BO) is then utilized to effectively explore the parameter space of charging current as well as handle the constraint of charging voltage. Moreover, continuous-varied-current charging protocols are introduced into the proposed charging optimization approach by the utilization of polynomial expansion technique. The effectiveness of the proposed charging approach is demonstrated on a porous electrode theory-based battery simulator. The results show that the proposed constrained BO-based approach possesses superior charging performance and higher sample efficiency, compared with the state-of-the-art baselines including constrained optimization by linear approximations (COBYLA) and covariance matrix adaptation evolutionary strategy (CMA-ES). In addition, the increase in the charging performance and its uncertainty with an increasing number of degrees of freedom used in charging protocols is discussed.

1. Introduction

Fast charging technology has become an essential component of modern electric vehicles (EVs) as it enables drivers to recharge their vehicles in a shorter time, making EVs more convenient [1,2]. However, fast charging can cause a significant amount of stress on batteries, which results in capacity loss and reduced overall lifespan. Therefore, it is crucial to design fast charging approaches that minimize charging time while maximizing battery lifetime (i.e., minimizing battery degradation) [3]. Fast charging optimization methods can be divided into two kinds: model-based and data-driven methods. The model-based optimization method involves utilizing electrochemical models to optimize charging strategy, whereas the data-driven method relies solely on electrochemical data, without the need for first-principles models. For the model-based fast charging design method [3,4], Ouyang et al. [5] formulated a multi-objective optimization problem taking into account the battery energy loss, safety-related constraints, economic cost, and user demand, by using a coupled electrothermal model, and a barrier method is then proposed to optimize charging protocols to adjust the charging current with the peak-valley time-of-use electricity price and

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user demand. Liu et al. [6] proposed a multi-objective evolutionary algorithm to design charging protocols that balance the objectives of minimizing charging time, battery energy loss and temperature rise, by the utilization of an electrochemical model comprising both the electrical and thermal characteristics. Liu et al. [7] also put forward a high-fidelity battery model that is synthesized from individual electrical, thermal, and aging models, and used multi-objective optimization method to deal with the conflict between battery health, charging time and energy conversion efficiency.

However, the electrochemical model-based charging method faces the following challenges: (i) Current battery models have limitations in describing all degradation mechanisms [8,9], which deteriorates the performance of model-based charging methods; and (ii) the degradation modes of Li-ion batteries are typically described by using hundreds or even thousands of partial differential equations in electrochemical models [9], which results in a costly large-scale optimization problem when utilizing these models to design fast charging protocols.

The issues mentioned above can be addressed by applying a model-free data-driven optimization for fast charging design. One approach to optimizing battery charging strategies involves using electrochemical data directly, without explicitly constructing battery models. This type of approach is known as black-box optimization, where charging phases are divided into segments and the optimal charging current is determined for each segment by comparing different currents that yields the best charging performance. Grid search is a commonly used black-box optimization method which is to create a grid of possible parameter values for charging currents and exhaustively search all the combinations of these values to determine the combination that yields the best performance in terms of charging speed and battery degradation. However, it can be computationally and experimentally burdensome, especially when dealing with a large number of parameters and a large search space. To address this issue, Bayesian optimization (BO) is proposed that is a sequential decision-making approach that can solve black-box optimization problems with much fewer experiments than grid search.

BO is a well-known data-driven approach used to globally optimize black-box objective functions. It is particularly useful in cases where the objective function evaluation cost is expensive and possibly noisy [10]. The BO algorithm comprises two main steps: (i) building a cheap probabilistic surrogate model for the expensive objective function from available data; and (ii) constructing an acquisition function based on the built surrogate model to determine where the objective function should be evaluated next. By constructing an appropriate acquisition function, we can obtain an excellent balance between the exploration (i.e., testing the area where the model predictions are uncertain) and the exploitation (i.e., testing the area where the model performance is promising) of the parameter space of charging protocols.

For single-objective optimization problems, commonly used acquisition function strategies in BO include promotion-based strategies such as expected improvement (EI) and probability of improvement (PI), confidence boundary strategies such as upper confidence bound (UCB), and information-based strategies such as Thompson sampling (TS). For multi-objective optimization, it can be decomposed into a set of single-objective optimization problems using techniques such as linear scalarization or Chebyshev scalarization [11]. Alternatively, using multi-objective acquisition functions such as expected hypervolume improvement [12] can directly estimate the Pareto front. However, such methods tend to be computationally expensive.

BO is widely applied in many fields including chemical design, crystal structure prediction, and amino acid conformer search [13–15]. Application of BO to fast charging design is however limited. In our previous works [16,17], we use the standard acquisition function of EI, PI and UCB based Bayesian optimization to handle the single objective problem of minimizing battery charging time while ensuring that the voltage and temperature in the charging process meets the constraints.

In this work, we investigate a multi-objective optimization problem to balance charging time and battery degradation, and impose the constraint on the charging process. Since batteries degrade faster at higher voltages (e.g., >4.15V) [18], the constraint on voltage is imposed. To resolve such multi-objective charging problem, a Chebyshev scalarization technique, which can deal with non-convex Pareto front cases, is first utilized to decompose the multi-objective problem into a group of single-objective optimization problems with different weights applied. Subsequently, a constrained BO approach is proposed to explore the parameter space of charging current in a sample-efficient manner. In addition, by adopting the polynomial function expansions technique, a continuous-varied-current charging protocols are introduced into the proposed constrained BO-based charging optimization approach. The proposed approach is evaluated on the PETLION, a porous electrode theory-based battery simulator [19].

The main contribution of this work is that the proposed multi-objective Bayesian optimization-based charging approach is sample-efficient and does not need information of battery electrochemical dynamics, which shows an advantage over the electrochemical model-based optimization techniques which are constrained by the accuracy of the models that detail battery degradation mechanisms. Additionally, the proposed approach is more efficient than data-driven methods such as grid search, which often involve testing protocols across parameter spaces to account for variability—thus being costly in terms of testing cells (i.e., sample inefficient).

The rest of this article is organized as follows. The Chebyshev decomposition method and the BO method are stated in Section 2. The proposed BO approach for the multi-objective fast charging design is developed in Section 3. The effectiveness of the proposed approach is demonstrated on a porous electrode theory-based battery simulator in Section 4, followed by conclusions in Section 5.

2. Method

2.1. Multi-objective optimization

A multi-objective optimization problem is for optimizing multiple real-valued functions $f_i(\boldsymbol{x})$, $i = 1, \ldots, k$, over some bounded domain $\mathscr{X} \subset R^d$, where $f_i(\boldsymbol{x})$ is the ith objective function, k is the number of objective function, and d is the dimensionality of the input. For a minimization objective, a solution $\boldsymbol{x}$ is said to *Pareto dominate* $\boldsymbol{x}'$ if $f_i(\boldsymbol{x}) \le f_i(\boldsymbol{x}')$, $\forall i$, with at least one of the inequalities being strict. The Pareto set $\mathscr{X}^*$ is then the subset of non-dominated points in $\mathscr{X}$, i.e., the set such that $\forall \boldsymbol{x}^* \in \mathscr{X}^*$, $\forall \boldsymbol{x} \in \mathscr{X}$, $\exists j \in 1, \ldots, k$ for which $f_j(\boldsymbol{x}^*) \le f_j(\boldsymbol{x})$. The Pareto set is usually infinite, and most methods aim at finding a finite set to approximate it.

When preferences regarding tradeoff among different objective functions can be obtained prior to optimization, multi-objective optimization can be changed to a single objective problem by explicitly maximizing the desired criterion. This is called scalarization technique. A commonly used way is linear scalarization. The minimum of a linear scalarization is guaranteed to lie on the Pareto frontier; however, not every Pareto optimal point can be recovered in this manner unless the frontier is strictly concave. An alternate way is to use Chebyshev scalarization L_∞ technique that is defined as [20]

$$\min_{x \in R^d} L_\infty(x) = \max_{i=1,\ldots,k} \left(w_i \cdot \left| f_i(x) - z_i^* \right| \right) \tag{1}$$

where z_i^* is a utopian point. In this article, z_i^* is selected as the optimal value of single objective optimization for the ith objective function. w_i is the scalarization weight. It is worth mentioning that the Chebyshev scalarization (i) is advantageous in finding Pareto optimal solutions regardless of whether the shape of the frontier is concave or non-concave, and (ii) is robust to the actual weights used [21,22].

2.2. Bayesian optimization

Bayesian optimization (BO) is a type of machine learning technique that aims to optimize objective functions that are costly to evaluate and possibly noisy [10,23]. These characteristics are particularly relevant in the objective function of fast-charging optimization problem for lithium-ion batteries. A BO method comprises a surrogate model and an acquisition function. The surrogate model is a cost-effective probabilistic model that approximates the expensive objective function [10]. Gaussian process (GP) is a commonly used surrogate model owing to its versatility as a non-parametric model capable of representing various functions, and its accurate and analytical posterior uncertainty estimates [24].

For an objective function $f(\boldsymbol{x})$, it can be modelled by GP as

$$f(\boldsymbol{x}) \sim GP\left(m_f(\boldsymbol{x}), \kappa_f(\boldsymbol{x}, \boldsymbol{x}')\right) \tag{2}$$

where the variable $\boldsymbol{x}$ is the parameters of charging protocol, and $f(\boldsymbol{x})$ means the battery performance from the charging protocol $\boldsymbol{x}$; and $m_f(\cdot)$ and $\kappa_f(\cdot,\cdot)$ are a mean function and a covariance function, respectively.

The selections of $m_f(\cdot)$ and $\kappa_f(\cdot,\cdot)$ mainly depend on *a priori* knowledge and data. A commonly used zero mean and Gaussian kernel is used in this work [24]. We often use maximum likelihood estimation algorithms to estimate the parameters of GP model from data. After the parameters learned, the posterior distribution inferred based on the GP model, given the dataset $\mathscr{D}$, can be obtained as [24]

$$f(\boldsymbol{x})\big|\ \mathscr{D} \sim \mathscr{N}\left(\mu(\boldsymbol{x}; \mathscr{D}), \sigma^2(\boldsymbol{x}; \mathscr{D})\right) \tag{3}$$

where

$$\mu(\boldsymbol{x}; \mathscr{D}) = \boldsymbol{K}_f^T(\boldsymbol{x})\left(\Sigma_f + \sigma_n^2 \boldsymbol{I}\right)^{-1} y \tag{4}$$

$$\sigma^2(\boldsymbol{x}; \mathscr{D}) = \boldsymbol{K}(\boldsymbol{x}, \boldsymbol{x}) - \boldsymbol{K}_f^T(\boldsymbol{x})\left(\Sigma_f + \sigma_n^2 \boldsymbol{I}\right)^{-1} \boldsymbol{K}_f \tag{5}$$

with $\boldsymbol{K}_f(\boldsymbol{x}) = [\kappa_f(\boldsymbol{x}, \boldsymbol{x}^{(1)}), \ldots, \kappa_f(\boldsymbol{x}, \boldsymbol{x}^{(N)})]^T$, and $[\Sigma_f]_{i,j} = \kappa_f(\boldsymbol{x}^{(i)}, \boldsymbol{x}^{(j)})$..

In terms of acquisition function, it is for efficiently sampling the parameter space by balancing exploration and exploitation. In the multi-objective setting, popular acquisition functions include expected hypervolume improvement [12,25,26], and information-theoretic-based methods [27]. Recently Thompson sampling (TS) has been shown to have strong empirical performance with scalarized objectives [28,29]. TS [30] is a randomized strategy for online decision making under uncertainty. At step j, TS samples $\boldsymbol{x}_j$ according to the posterior probability that is the optimum. In this article, an acquisition function of constrained TS (cTS) [31] is used for probing the parameter space of charging protocol. cTS extends the acquisition function of TS to handle black-box constraints (e.g., voltage constraint), in which a separate GP model is applied to learn a constraint function.

Assume $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_r$ be the sampled candidate points, the acquisition function of cTS samples a realization $(\widehat{f}(\boldsymbol{x}_i), \widehat{c}_1(\boldsymbol{x}_i), \ldots, \widehat{c}_s(\boldsymbol{x}_i))$ for all $\boldsymbol{x}_i$ with $1 \le i \le r$ from the respective GP posterior distributions on the functions $f, c_1, \ldots, c_s$, where s is the number of constraints. Let the set of points whose realizations are feasible be defined as $\widehat{F} = \{\boldsymbol{x}_i | \widehat{c}_l(\boldsymbol{x}_i) \le 0\}$, for $1 \le l \le s$. If $\widehat{F} \ne \varnothing$ holds, cTS chooses a point based on $\mathrm{argmin}_{x \in \widehat{F}} \widehat{f}(\boldsymbol{x})$. Otherwise, cTS chooses a point according to the criterion of minimum total violation $\sum_{l=1}^{s} \max\{\widehat{c}_l(\boldsymbol{x}), 0\}$. Feasible points can be effectively determined by using such selection criterion for smooth constraints [31].

3. Battery fast charging problem

This section briefly discusses battery degradation models and the multi-objective charging problem formulated within the Bayesian optimization framework.

3.1. Porous electrode theory-based battery degradation model

The main governing equations are summarized here, with some equations applying to both cathode and anode. The diffusion of lithium ions within each solid particle is described by [16,32,33].

$$\frac{\partial}{\partial t} c_s(z,t) = \frac{1}{z^2} \frac{\partial}{\partial z}\left[z^2 D_{\mathrm{eff}}^s \frac{\partial}{\partial z} c_s(z,t)\right] \tag{6}$$

with boundary conditions

$$\frac{\partial}{\partial z} c_s(z,t)\bigg|_{z=0} = 0, \frac{\partial}{\partial z} c_s(z,t)\bigg|_{z=R_s} = -\frac{j(z,t)}{D_{eff}^s} \tag{7}$$

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

$$\mathrm{SOC}(t) := \frac{1}{L_n c_s^{max,n}} \int_0^{L_n} c_s(z,t) dz \tag{8}$$

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

The voltage of the Li-ion cell can be obtained as

$$V(t) = \Phi_s(0,t) - \Phi_s(L,t) \tag{9}$$

where $\Phi_s(z,t)$ is the solid potential and $z=0$ and $z=L$ correspond to the current collector at the cathode and anode sides. The solid potential $\Phi_s(z,t)$ is described by the conservation of charge in the electrodes as

$$\frac{\partial}{\partial z}\left[\sigma_{\mathrm{eff}} \frac{\partial}{\partial z} \Phi_s(z,t)\right] = aFj(z,t) \tag{10}$$

where F is Faraday's constant, and σ_{eff} is the effective conductivity of the electrodes.

In terms of battery degradation modelling, this work uses the similar degradation modelling as [34], which considers SEI growth and lithium plating as side reactions in the graphite-based anode. A total of three electrochemical reactions can therefore happen in the graphite anode, and the volumetric current density j comprises the transfer current density of lithium intercalation, the local current density of SEI formation reaction, and the transfer current density of the lithium deposition reaction.

This work uses PETLION [19] as a battery simulator that is a Julia implementation of the above electrochemical model based on the finite volume method. More details on the electrochemical model and its software implementation can be found in Refs. [19,35]. It is worth mentioning that the porous electrode theory-based battery model used here is only being used to define "ground truth" for evaluation of the proposed BO-based charging approach.

3.2. Multi-objective fast charging problem

The objective is to maximize battery cycle life while minimizing charging time without violating operational constraints. The fast-charging problem is formulated as

$$\begin{cases} \min\limits_{I(t)} \ t_f - t_0 \\ \max\limits_{I(t)} \ L_f \end{cases} \tag{11a}$$

$$\text{subject to} \begin{cases} \text{battery dynamics in } (6)-(10) \\ \mathrm{SOC}(t_0) = \mathrm{SOC}_0 \\ \mathrm{SOC}(t_f) = \mathrm{SOC}_f \\ V(t) \le V^{max} \end{cases} \tag{11b}$$

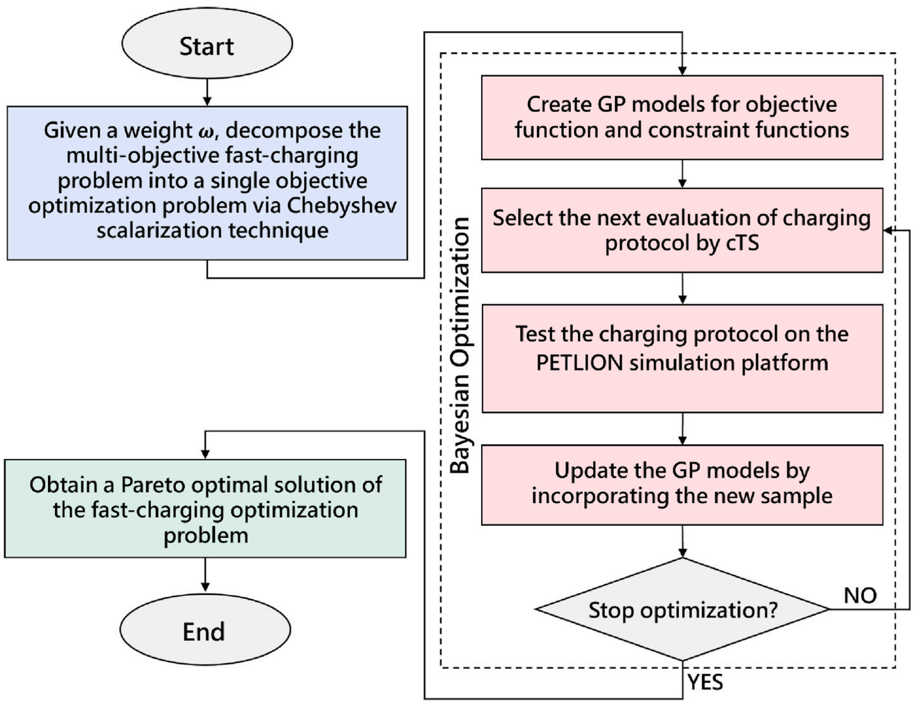


Fig. 1. Schematic of the proposed cTS-BO approach for the multi-objective optimization of fast charging problem.

where t_f is the charging time taken to charge the battery from the state of charge of SOC_0 to SOC_f in each cycle, and L_f is the battery cycle life that is defined as the number of cycles corresponding to a reduction in the battery capacity to 80% of the nominal capacity. V^{max} is the upper bound for cell voltage.

The optimization problem (11a)-(11b) can be decomposed into a set of single objective optimization problems via Chebyshev scalarization technique mentioned in Section 2.1. By using the technique of Chebyshev scalarization L_∞, the sub-optimization problem can be formulated as

$$g = \max_{I(t)} \left\{ \omega \cdot \left| t_f - t_f^* \right|, (1-\omega) \cdot \left| L_f - L_f^* \right| \right\} \tag{12}$$

and the multi-objective Pareto optimal solutions can be solved by minimizing g in eqn. (12), in which t_f^* and L_f^* are chosen as the optimal values of single objective optimization for minimizing the objective function of charging time and for maximizing the objective function of battery cycle life, respectively [21].

In addition, continuous-varied-current charging protocols are used in this work that is defined as

$$I(t) = \sum_{j=0}^{p} \beta_j \varphi_j(t) \tag{13}$$

where φ_j are basis functions, β_j are the corresponding parameters that need to optimize, and p is the order of the basis. The choice of basis function often reflects desired properties required for charging. For simplicity, the basis functions are in the form of polynomials (i.e., $\varphi_j(t) = t^j$). In this work, the order $p = 0$, 1 and 2 are considered, which correspond to constant, linear and quadratic basis functions respectively. A higher order typically corresponds to a more complex function, which could potentially fit more intricate charging patterns. Specifically, (1) for the case of $p = 0$ (i.e., $I(t) = \beta_0$), the current is to remain constant throughout the charging process, which represents a straightforward constant current charging; (2) for the case of $p = 1$ (i.e., $I(t) = \beta_1 t + \beta_0$)), the current might vary linearly, allowing for a protocol where the charging current changes at a constant rate; (3) for the case of $p = 2$ (i.e., $I(t) = \beta_2 t^2 + \beta_1 t + \beta_0$), the current variation is quadratic, potentially accommodating more nuanced charging patterns.

The workflow of the proposed multi-objective constrained BO-based charging approach is shown in Fig. 1. Firstly, given a scalarization weight ω, the optimization problem (11a)-(11b) can be decomposed into a single objective optimization problem by using the Chebyshev scalarization technique. Secondly, surrogate GP models are built for the objective function and constraint functions of the single objective charging problem, and the acquisition function of constrained Thompson sampling (cTS) is then constructed from the learned GP models to sample-efficiently probe the parameter space of charging current to obtain the next evaluation sample. The new sample is then incorporated to update the GP models. The above processes are repeated until a Pareto optimal solution of the fast-charging problem is obtained or the maximum number of iterations is reached. Note that the proposed Bayesian optimization-based charging approach is a model-free method, which does not require electrochemical models.

4. Results and discussion

This section is (i) to verify the efficacy of the proposed cTS-BO approach for multi-objective fast charging optimization, and (ii) to evaluate the performance of various continuous-varied-current charging protocols for the fast-charging design. Our goal is to optimize the charging protocol that charges the battery from 30% state of charge (SOC) to 80% SOC in minimal time while maximizing battery cycle life. Meanwhile, the cell terminal voltage is required to meet the operational constraint (i.e., $V(t) \leq V^{max}$and $V^{max} = 4.15V$ is used in this work). The bound interval for charging protocol coefficients in eqn.(14)are $\beta_0 \in [0.5, 2.5], \beta_1 \in [-5 \times 10^{-5}, 5 \times 10^{-5}], \beta_2 \in [-3 \times 10^{-9}, 3 \times 10^{9}]$. It is worth noting that our optimized charging protocol differs from the battery formation cycling protocol. The former is applied during battery usage, while the latter serves as a crucial step in battery manufacturing.

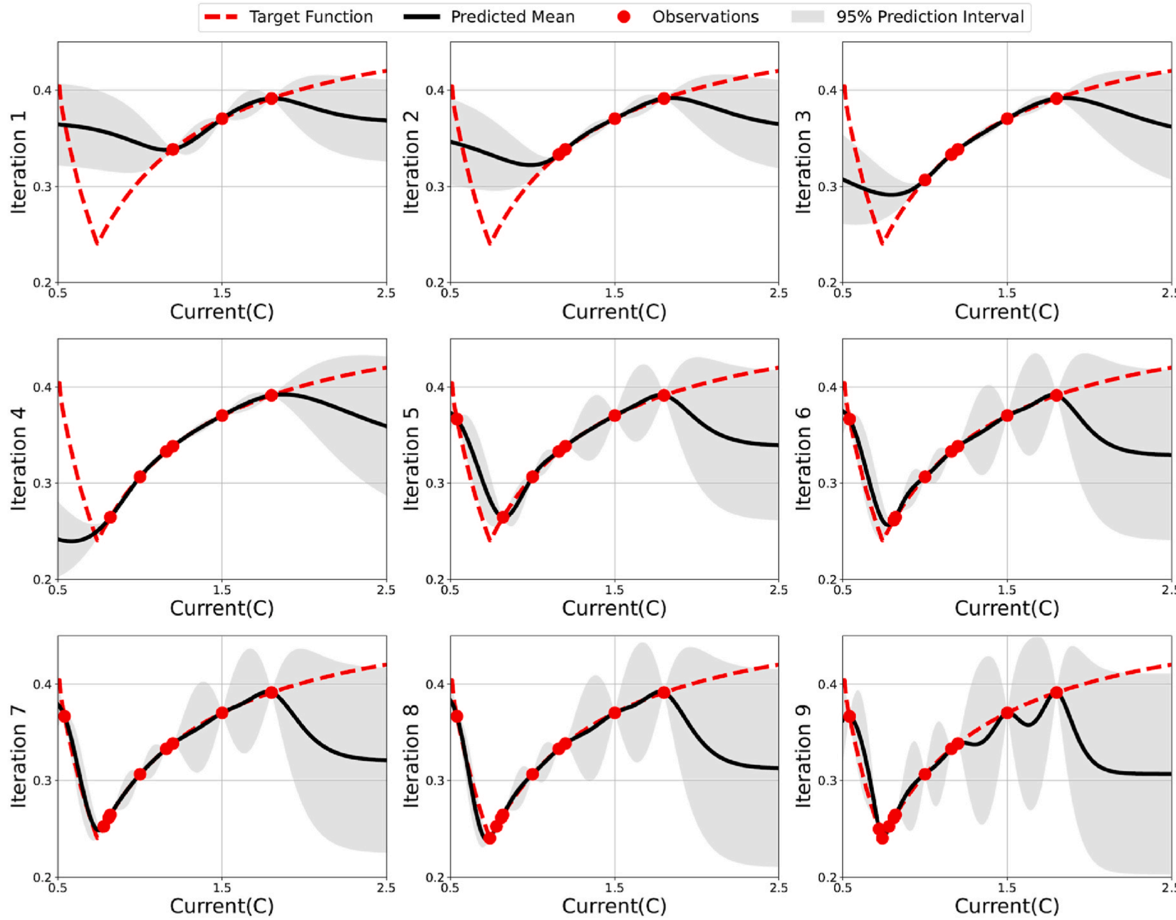


Fig. 2. The iteration process of the proposed cTS-BO charging approach for the optimization of charging protocol $p = 0$. $\omega = 0.7$ is used in this case.

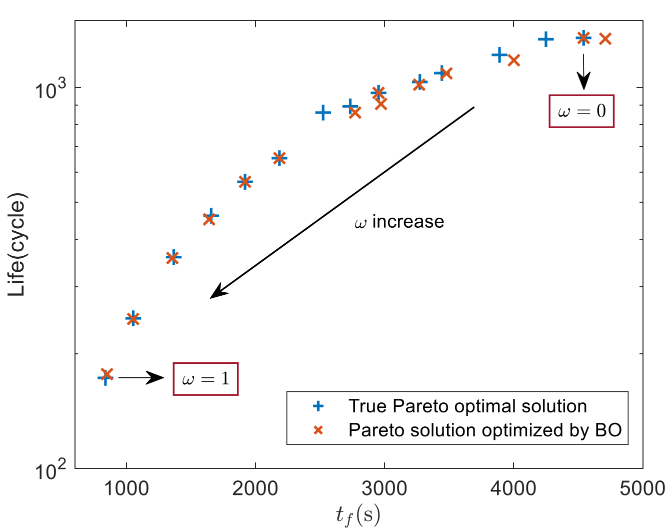


Fig. 3. The Pareto optimal solutions obtained by the proposed cTS-BO method with charging protocol $p = 1$ after 75 iterations. The true Pareto optimality is from the grid search method.

4.1. Performance of the constrained BO approach for fast charging optimization

Let's first consider the case of fast charging optimization using the proposed constrained BO approach with charging protocol $p = 0$. The iteration process of the proposed BO approach for exploring the parameter space of charging current is depicted in Fig. 2. Initially, three data samples are randomly selected for building surrogate GP models, and the cTS acquisition function is constructed based on the GP models to sample the next evaluation point. The GP models are then updated by including the new sample, and the process are repeated. As shown in Fig. 2, the sampling behavior of cTS-BO automatically provides a trade-off between the exploration (i.e., testing the region of charging current parameter space with high uncertainty) and exploitation (i.e., testing the region of charging current space with promising performance). The confidence of cTS-BO in the high-performing region is gradually improved from the first to sixth iterations. After only six iterations, the optimal charging current (i.e., 0.75C) is determined by the proposed approach. Through exploiting the structure information of the parameter space, cTS-BO avoids evaluating the parameter space of charging current with low performing regions and spends most of resources on the high performing regions. The results show the proposed cTS-BO approach for the optimization of fast charging in a sample-efficient manner.

For the case of charging profile $p = 1$, by selecting different value of ω, the Pareto front solutions for the multi-objective fast-charging optimization problem using the proposed cTS-BO method can be obtained and are displayed in Fig. 3, in which $\omega = 0$ corresponds to maximizing only battery cycle life, and $\omega = 1$ corresponds to minimizing only charging time. The result associated with an intermediate value of ω between the two extreme cases of $\omega = 0$ and $\omega = 1$ indicates a different trade-off between charging time and battery degradation. A larger value of ω means that more weight is put on charging time and less on battery degradation and vice versa. For example, for $\omega = 0.3$, the optimized charging time is 4121 s and the corresponding battery cycle life is 1236 cycles, while for $\omega = 0.7$, the optimized charging time is 2425 s, and the

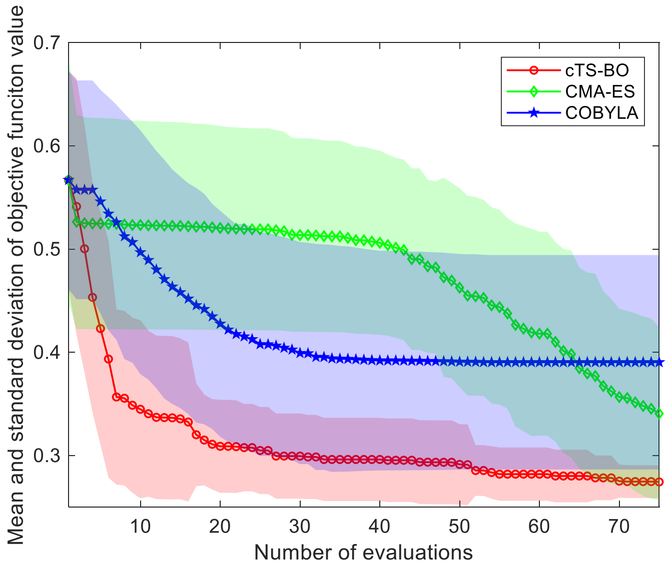


Fig. 4. The performance of the fast-charging optimization by the cTS-BO, CMA-ES, and COBYLA methods using the charging protocol $p = 1$. The results are averaged over 15 experiments.

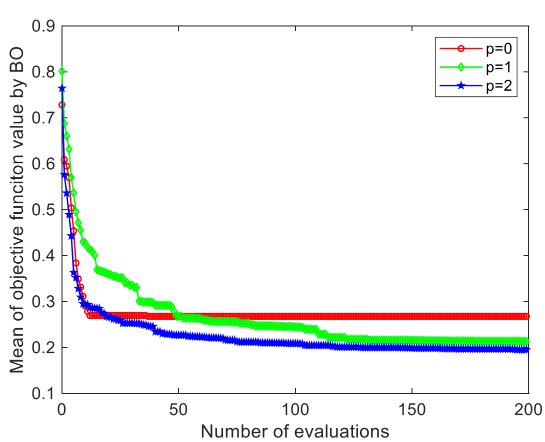
corresponding cycle life is 734 cycles.

In addition, as shown in Fig. 3, the results show that the Pareto solutions optimized by the proposed cTS-BO approach (red markers) is pretty close to the true Pareto optimal solutions (blue markers), which verify the efficacy of the proposed approach for the optimization of the multi-objective charging problem.

To further demonstrate the effectiveness of the proposed cTS-BO method for fast-charging design, two state-of-the-art baselines (i.e., COBYLA [38] and CMA-ES [39]) are selected as comparison to the proposed approach. The Constrained Optimization BY Linear Approximations (COBYLA) optimizes a simplex within a trust region of the parameter space using linear approximations of the target and constrains function [40], and Covariance Matrix Adaptation Evolutionary Strategy (CMA-ES) is a population-based optimization method that draws samples from a multivariate Gaussian distribution whose parameters are adapted online [40]. The three methods were performed on the fast-charging optimization problem for the case of charging protocol $p = 1$ and $\omega = 0.5$. The mean and standard deviation of the charging performance as a function of evaluation number by the three methods are displayed in Fig. 4, in which the cTS-BO method is significantly superior to the other two methods. As shown in Fig. 4, CMA-ES is conservative in the early stage of optimization (its mean decreased only by 6.6% from the 1st iteration to the 40th iteration, compared to 47.8% to cTS-BO), and COBYLA is more easily trapped in the local optimal regions (its mean decreased by 0.4% from the 40th iteration to the 75th iteration, compared to 7.3% to cTS-BO). After 75 evaluations, the mean of the objective function value of cTS-BO is 0.27, which are a factor of 1.26 and 1.44 improved on the charging optimization performance in contrast to CMA-ES and COBYLA, respectively. In addition, compared to CMA-ES and COBYLA, the standard deviation of the objective function value of cTS-BO is lower by 81.1%and 84.8%, respectively. The results show that the proposed cTS-BO charging approach is more efficient and consistent than the CMA-ES and COBYLA methods on the optimization of fast charging protocols.

4.2. Performance of various charging profiles for fast-charging design

The fast-charging optimization performance performed by the proposed cTS-BO approach for the charging protocols $p = 0$, 1, and 2 are provided in Fig. 5. From Fig. 5(a), it can be found that a more complex charging protocol used, a smaller optimal value of the objective function can be obtained by the cTS-BO method, which means that a more complex charging protocol can obtain a longer battery lifetime under the same charging time, or it can obtain a shorter charging time to maintain a similar battery performance on lifetime. Fig. 5(b) displays the variation of standard deviation throughout the optimization of various charging protocols. Clearly, protocols with a higher-dimensional parameter space require a larger number of samples or in other words, more iterations for optimization. Consequently, the associated standard deviation for these optimizations is typically higher. Interestingly, within the initial 120 iterations, the standard deviation for the charging protocol $p = 2$ is less than that of $p = 1$. This can be explained by the increased potential combinations in the protocol $p = 2$, which brings forth more local optimal solutions. As a result, the BO method is more prone to converge to these local optima during initial iterations, leading to a reduced standard deviation. By varying the value of weight ω, the Pareto front optimized by the proposed approach for the charging protocols $p = 0$, 1, and 2 is depicted in Fig. 6. Each marker corresponds to one optimization run by cTS-BO. As shown in Fig. 6, the Pareto front optimized for the charging protocol $p = 2$ performed best, followed by the charging protocols $p = 1$ and $p = 0$, which shows that a more complex charging protocol has a better charging performance as more degrees of freedom of parameters become available for optimization.



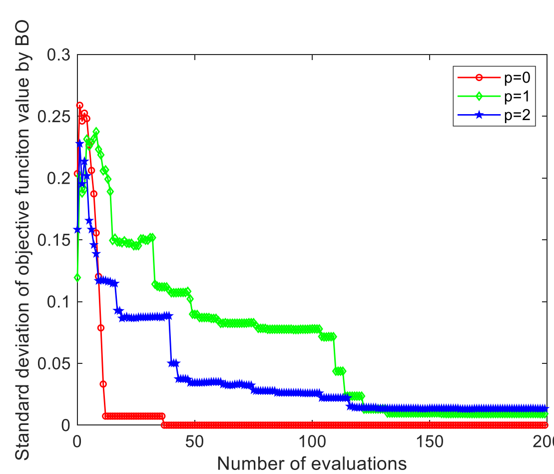


Fig. 5. The mean and standard deviation of the charging performance provided by the cTS-BO method as a function of evaluation number for the optimization of charging protocols $p = 0$, 1, and 2 for the case of $\omega = 0.5$. The results were averaged over 15 experiments: (a) mean, and (b) standard deviation.

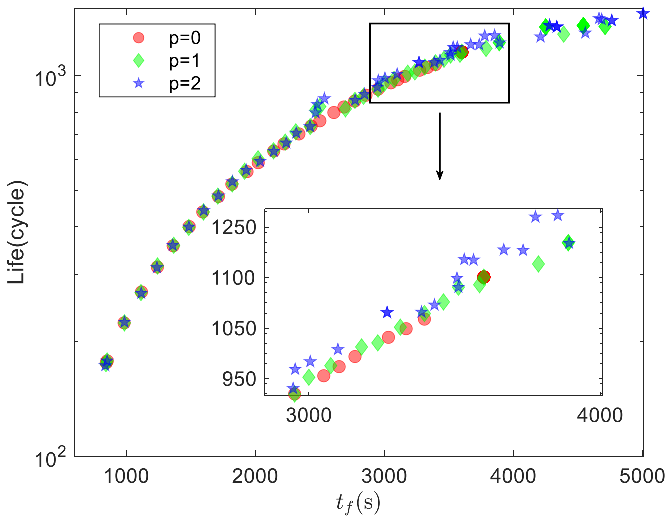


Fig. 6. The Pareto optimal solutions obtained by the proposed multi-objective BO charging method for the charging protocols p = 0,1, and 2 after 200 evaluations; The values of the corresponding parameters β_0, β_1, and β_2 optimized by the BO method for the protocols p = 0,1, and 2 are displayed in Table A1.

For example, for the case of ω = 0.5, the charging time and battery lifetime optimized by the cTS-BO approach for the charging protocol p = 1 is 3273 s and 1035 cycles respectively, while that for the charging protocol $p = 2$ is 3190 s and 1039 cycles respectively. The optimized charging time for the protocol $p = 2$ is 83 s less than that of the protocol $p = 1$ for obtaining similar battery lifetime.

For the case of ω = 0.3, the Pareto optimal solution obtained by the proposed multi-objective BO-based charging approach for the charging protocols p = 0, 1, and 2 are displayed in Fig. 7 with the charging current, cell voltage, state of charge (SOC) and cell capacity. As shown in Fig. 7(a), the charging current optimized by cTS-BO for the charging protocols p = 1 and p = 2 gradually decreases throughout the whole charging process, which is consistent with the most fast-charging protocols reported in the literature that charging current decreasing monotonically as a function of SOC are advantageous to limit lithium plating on graphite, a typical capacity fading mechanism during fast charging [36,37]. From Fig. 7cd, it can be found that the optimal charging time and battery lifetime obtained for the charging protocols p = 0, 1, and 2 are (3600 s, 1151 cycles), (4121 s, 1236 cycles), and (3944 s, 1310 cycles), respectively. Although the charging time optimized for the charging protocol $p = 0$ is shortest, its battery lifetime is also largely lower than the other two protocols. Compared with the optimal charging profiles obtained for the charging protocols $p = 1$ and $p = 2$, the protocol p = 2 not only charged 177 s faster but also obtained 74 cycles longer

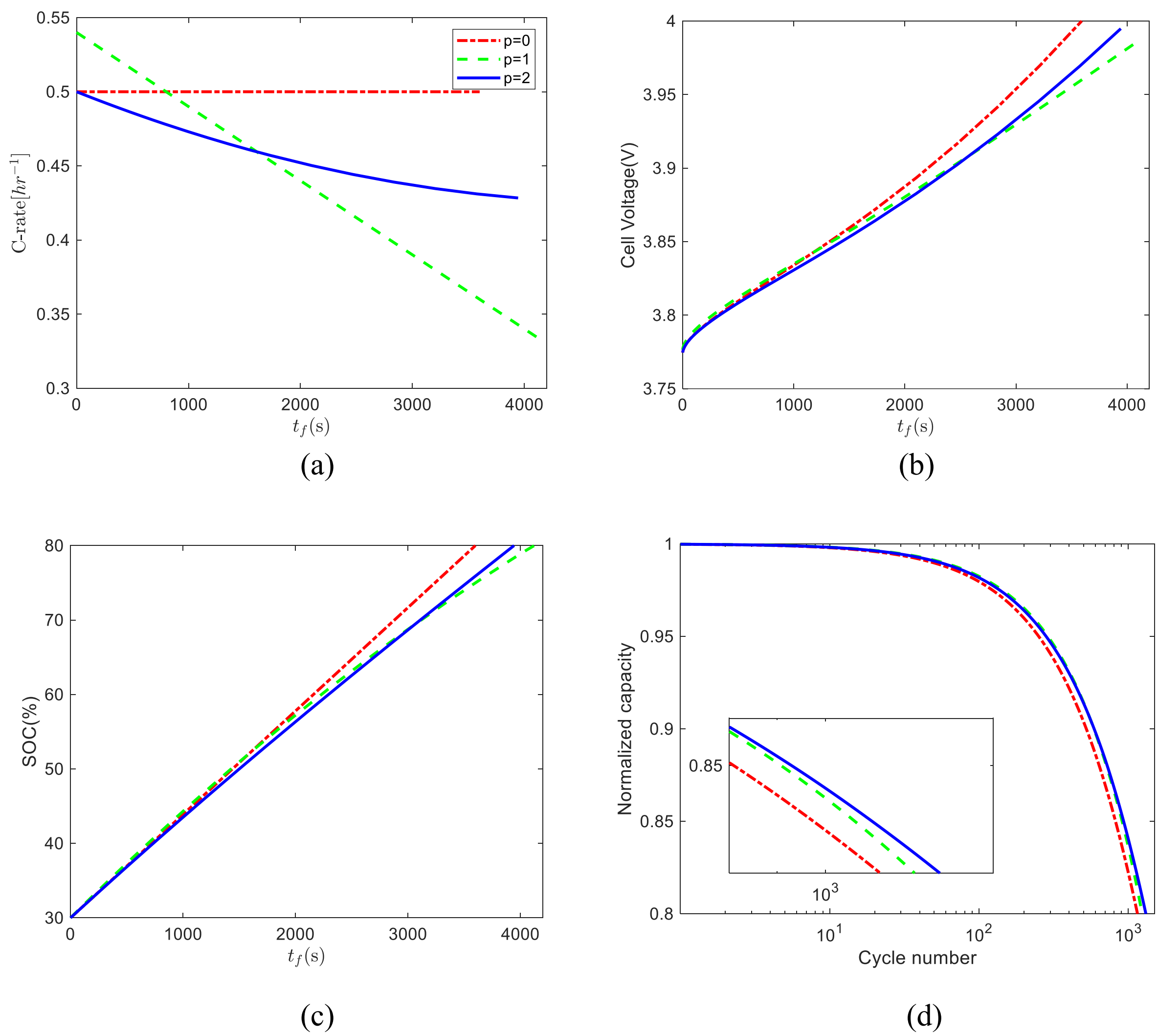


Fig. 7. The optimal charging profiles obtained by the proposed multi-objective BO-based charging approach for the charging protocols p = 0, 1, and 2 after 200 evaluations: (a) C-rate, (b) cell voltage, (c) SOC, and (d) normalized capacity.

lifetime than the charging protocol $p = 1$, which shows that the continuous-varied-current charging protocol $p = 2$ is superior than the protocol $p = 1$ on the performance of both charging time and battery degradation in this case. The reason is that a more complex charging protocol has more degrees of freedom of parameters available for optimization leading to better charging performance.

5. Conclusions

In this article, a constrained Bayesian optimization approach in combination with continuous-varied-current charging profile is proposed for the optimization of multi-objective fast charging problem. The multi-objective optimization problem is changed into a group of single-objective optimization problems by the utilization of Chebyshev decomposition technique, and subsequently the constrained BO method is employed to efficiently explore the parameter space of charging protocols. The multi-objective BO-based charging approach is sample-efficient and does not require first-principles models. The proposed charging approach was evaluated and compared with the state-of-the-art baselines including COBYLA and CMA-ES on the porous electrode theory-based battery simulator. The results verify the efficacy of the proposed approach for the optimization of multi-objective fast charging problems. We also quantify the convergence rate of the constrained BO-based charging approach with an increasing number of degrees of freedom in the optimization of charging protocols. Note that the chosen constraints in equation (11) are heuristics, that is, deviations from the operating range are treated as a surrogate for degradative behavior in the place of difficult-to-measure physical mechanisms such as Li deposition and SEI thickness. If we have more physical knowledge on how to more precisely formulate the constraints regarding the issues of controlling Li deposition and physical mechanisms for different battery materials [41,42], the proposed model free BO-based charging approach is also workable. In addition to fast-charging design, the proposed multi-objective constrained BO approach can also be extended to the optimization of the next-generation battery chemistries such as Lithium metal electrolyte.

CRediT authorship contribution statement

Xizhe Wang: Conceptualization, Methodology, Software, Writing – original draft. **Benben Jiang:** Methodology, Resources, Writing – review & editing, Supervision.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jpowsour.2023.233602.

Appendix

The results of parameters β_0, β_1, and β_2 optimized by the proposed BO-based charging approach for the charging protocols $p = 0$, 1, and 2 under various weights ω are displayed in Table A1.

Table A1
The values of parameters β_0, β_1, and β_2 obtained by the proposed BO-based method for the charging protocols $p = 0$, 1, and 2 after 200 evaluations.

weight ω	$p = 0$	$p = 1$		$p = 2$		
	β_0	β_1	β_0	β_2	β_1	β_0
0	0.50	-5×10^{-5}	0.51	-3×10^{-9}	-5×10^{-5}	0.50
0.1	0.50	-5×10^{-5}	0.51	-3×10^{-9}	-5×10^{-5}	0.51
0.2	0.50	-5×10^{-5}	0.51	-2×10^{-9}	-5×10^{-5}	0.54
0.3	0.50	-5×10^{-5}	0.54	3×10^{-9}	-2×10^{-5}	0.50
0.4	0.50	0	0.50	3×10^{-9}	-3×10^{-5}	0.55
0.5	0.55	0	0.55	3×10^{-9}	-1×10^{-5}	0.57
0.6	0.63	5×10^{-5}	0.59	3×10^{-9}	5×10^{-5}	0.58
0.7	0.74	1×10^{-5}	0.73	-2×10^{-9}	3×10^{-5}	0.71
0.8	0.93	5×10^{-5}	0.89	3×10^{-9}	5×10^{-5}	0.89
0.9	1.32	4×10^{-5}	1.29	3×10^{-9}	4×10^{-5}	1.29
1	2.13	-5×10^{-5}	2.17	1×10^{-9}	-5×10^{-5}	2.17

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