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Quadratic interpolation based teaching-learning-based optimization for chemical dynamic system optimization

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A B S T R A C T

Optimal design and control of industrially important chemical processes rely on dynamic optimization. However, because of the highly constrained, nonlinear, and sometimes discontinuous nature that is inherent in chemical processes, solving dynamic optimization problems (DOPs) is still a challenging task. Teaching-learning-based optimization (TLBO) is a relative new metaheuristic algorithm based on the philosophy of teaching and learning. In this paper, we propose an improved TLBO called quadratic interpolation based TLBO (QITLBO) for handling DOPs efficiently. In the QITLBO, two modifications, namely diversity enhanced teaching strategy and quadratic interpolation operator, are introduced into the basic TLBO. The diversity enhanced teaching strategy is employed to improve the exploration ability, and the quadratic interpolation operator is used to enhance the exploitation ability; therefore, the ensemble of these two components can establish a better balance between exploration and exploitation. To test the performance of the proposed method, QITLBO is applied to solve six chemical DOPs include three parameter estimation problems and three optimal control problems, and compared with eleven well-established metaheuristic algorithms. Computational results reveal that QITLBO has the best precision and reliability among the compared algorithms for most of the test problems.

1. Introduction

Optimization problems encountered in chemical engineering processes often involve dynamic variables whose values change in time [1], and these problems are called dynamic optimization problems (DOPs)[1] which can be modeled by differential and algebraic equations. The DOPs exist in the areas of optimal control, parameter estimation for dynamic models, reactor network synthesis where the dynamic models arise from the differential modeling of the chemical reactors [2]. Their highly constrained, non-linear and sometimes non-smooth nature often causes non-convexity, and therefore global optimization methods are needed to find suitable solutions [3].

Due to the importance of dynamic optimization in industrial and engineering practices, a number of methods have been proposed for solving the DOPs efficiently in the last two decades, including the iterative dynamic programming, deterministic methods and stochastic methods.

Iterative dynamic programming proposed by Luus [4] can get the global optimum for multimodal optimization problems, but the computational expense of this method is very large, since it needs to discretize both states variables and control variables [5]. Deterministic methods includes the gradient-based algorithms [6,7] and branch and bound algorithms [8,9]. The gradient-based algorithms such as Newton's algorithms and sequence quadratic program can converge rapidly, but they also have the possibility of getting trapped at local optimum depending upon the degree of nonlinearity and initial guess [10]. The branch and bound algorithms require rigorous values for the parameters needed or rigorous bounds on these parameters, thus lead to difficulty in implementation [10]. More details about deterministic methods and their applications can be found in the literature [11].

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[1] Dynamic optimization problems in this paper refer to the problems with differential and algebraic constraints.

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Stochastic methods are gaining more attentions for solving chemical DOPs in recent years, and they are found to have better global perspective than the deterministic methods. Stochastic methods primarily include metaheuristic algorithms, and they are primarily nature inspired and apply either population or single solution to explore the search space [12]. These algorithms make few assumptions about the optimization problem being solved, and so they may be usable for DOPs with characteristics such as non-differentiable, multimodal, or mathematical implicit. The genetic algorithm (GA) [13–15], differential evolution (DE) [16–19], simulated annealing (SA) [20, 21], ant colony optimization (ACO) [22,23], particle swarm optimization (PSO) [24–27], scatter search(SS) [28–30], artificial bee colony (ABC) [31], biogeography-based optimization (BBO) [32], line-up competition algorithm(LCA) [33], and cuckoo search (CS) [34] have been applied to dynamic optimization of chemical processes by different researchers.

Teaching-learning-based optimization (TLBO) is a relative new metaheuristic optimization algorithm proposed by Rao et al. [35], which is based on the philosophy of teaching and learning. TLBO has emerged as one of the simplest and most efficient techniques, and it has been empirically shown to perform well on many optimization problems [36]. TLBO and its modified versions have been extended to function optimization [37,38], engineering optimization [39,40], multi-objective optimization [41,42], parameters identification [43], clustering [44], and other fields.

However, as a useful optimization tool, the report of the application of TLBO in chemical engineering is relatively few, especially in chemical dynamic optimization. To the best of our knowledge, TLBO has not been evaluated for solving chemical DOPs. Therefore, this study aims to extend the TLBO for the chemical dynamic optimization. To provide a more efficient balance between exploration and exploration for TLBO, we introduce two modifications to the basic TLBO, namely diversity enhanced teaching strategy and quadratic interpolation (QI) operator. Therefore, a variant of TLBO called quadratic interpolation based teaching-learning-based optimization (QITLBO) is proposed for handling DOPs efficiently. In QITLBO, the diversity enhanced teaching strategy is used to enhance the exploration, and the QI operator is employed to improve the exploitation.

The main contributions of this paper are as follows:

(1) A modified version of TLBO called QITLBO is proposed by integrating the diversity enhanced teaching strategy and QI operator. The integration of these two components can provide a better balance between exploration and exploration for the algorithm.
(2) To the best of our knowledge, it is the first attempt to apply the TLBO-based algorithms for dynamic optimization problems in chemical engineering. The proposed QITLBO is used to solve three dynamic parameter estimation problems and three optimal control problems.
(3) The performance of QITLBO is compared with those of eleven well-established metaheuristic algorithms, including three TLBO algorithms and eight non-TLBO algorithms.

The rest of this paper is organized as follows. Section 2 briefly introduces the formulation of dynamic optimization problems. Section 3 gives a literature review of TLBO. Section 4 presents the proposed QITLBO in detail. Section 5 displays the simulation results and analysis on case studies. Section 6 provides further discussions for the QITLBO. Finally, Section 7 concludes this paper.

2. Problem statement

This paper addresses the DOPs with both differential and algebraic constraints, as given in the following formulation [28]:

$$\min \phi(\boldsymbol{x}(t), \boldsymbol{u}(t), \boldsymbol{p}) \tag{1}$$

subject to

$$\begin{cases} \boldsymbol{f}(\dot{\boldsymbol{x}}(t), \boldsymbol{x}(t), \boldsymbol{u}(t), \boldsymbol{p}) = \boldsymbol{0} \\ \boldsymbol{x}(t_0) = \boldsymbol{x}_0 \\ \boldsymbol{h}(\boldsymbol{x}(t), \boldsymbol{u}(t), \boldsymbol{p}) = 0 \\ \boldsymbol{g}(\boldsymbol{x}(t), \boldsymbol{u}(t), \boldsymbol{p}) \le 0 \\ \boldsymbol{u}^L \le \boldsymbol{u}(t) \le \boldsymbol{u}^U \\ \boldsymbol{p}^L \le \boldsymbol{p} \le \boldsymbol{p}^U \\ t \in [t_0, t_f] \end{cases} \tag{2}$$

where $\phi(\boldsymbol{x}(t), \boldsymbol{u}(t), \boldsymbol{p})$ is the objective function; $\boldsymbol{x}(t)$ are the time-dependent state variables; $\boldsymbol{u}(t)$ are the time-dependent control variables; $\boldsymbol{p}$ are the undetermined parameters; $\boldsymbol{f}$ are the set of differential equations describing the system dynamics; $\boldsymbol{h}$ and $\boldsymbol{g}$ are, respectively, the equality and inequality constraints.

The optimization variables in a generalized DOP include both the time-dependent control variables $\boldsymbol{u}(t)$ and time-independent undetermined parameters $\boldsymbol{p}$. In this study, the DOPs are divided into two types: dynamic parameter estimation problems and optimal control problems. In dynamic parameter estimation problems, only the undetermined parameters $\boldsymbol{p}$ exist, while the control variables $\boldsymbol{u}(t)$ do not exist [30]. By contrast, in optimal control problems, the control variables $\boldsymbol{u}(t)$ must exist, while the undetermined parameters $\boldsymbol{p}$ usually do not exist [6].

The dynamic parameter estimation problems can be easily translated into nonlinear programming problems. However, for the optimal control problems, the time-dependent control variables $\boldsymbol{u}(t)$ cannot be optimized directly, and the control vector parameterization(CVP) approach [6,45] is needed to discretize the control variables $\boldsymbol{u}(t)$. In CVP, the time interval is divided into several stages, and the control variables $\boldsymbol{u}(t)$ in each subinterval are expressed control piece-wise basis functions in, such as constant function, linear functions, wavelet-based functions, and so on. Then, the optimal control problems can be translated into nonlinear programming problems.

After the original DOPs are translated into nonlinear programming problems, there only exist undetermined parameters to be optimized. Then, the optimization algorithms such as metaheuristics can be applied. During the solution process, the optimization parameters need to be taken into Eq. (2), and use differential equation integrator to obtain the objective function value. Finally, the solution of the DOPs is output. The solution process of DOPs is illustrated in Fig. 1.

3. Related work on TLBO

3.1. Basic TLBO

TLBO is a population-based optimization method which mimics the teaching and learning process of a typical class [46]. There are two important phases in the algorithm: a teacher phase and a learner phase. In the teacher phase, the best solution in the entire population is considered as the teacher of the class, and the teacher shares his or her knowledge to improve the performance of the whole class. In the learner phase, learners learn through the interaction and communication among themselves to further improve their performance. The TLBO process is carried out through the two basic operations of the teacher phase and learner phase, which are briefly described in the subsequent paragraphs.

3.1.1. Teacher phase

In the teacher phase, the teacher provides knowledge to the learners to increase the mean result of the class. For an objective function $f(\boldsymbol{x})$ with D-dimensional variables, $\boldsymbol{x}_i = (x_i^1, \cdots, x_i^d, \cdots, x_i^D)$ represents the position of the ith learner. Thus, the mean position of a class with NP learners can be represented as $\boldsymbol{x}_{mean} = \frac{1}{NP}\sum_{i=1}^{NP} \boldsymbol{x}_i$.