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A Three-section Algorithm of Dynamic Programming Based on Three-stage Decomposition System Model for Grade Transition Trajectory Optimization Problems ☆

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ABSTRACT

This paper introduces a practical solving scheme of gradetransition trajectory optimization (GTTO) problems under typical certificate-checking–updating framework. Due to complicated kinetics of polymerization, differential/algebraic equations (DAEs) always cause great computational burden and system non-linearity usually makes GTTO non-convex bearing multiple optima. Therefore, coupled with the three-stage decomposition model, a three-section algorithm of dynamic programming (TSDP) is proposed based on the general iteration mechanism of iterative programming (IDP) and incorporated with adaptivegrid allocation scheme and heuristic modifications. The algorithm iteratively performs dynamic programming with heuristic modifications under constant calculation loads and adaptively allocates the valued computational resources to the regions that can further improve the optimality under the guidance of local error estimates. TSDP is finally compared with IDP and interior point method (IP) to verify its efficiency of computation.

1. Introduction

Nowadays, diverse polymer products have been widely used in many standard applications including automobile industries, electronics and packaging materials [1,2]. These polymers are in demand with different physical and chemical specifications, *i.e.*, different grades. Therefore, to meet the various requirements and high quality standards from industrial consumers, many different products must be produced and transitions are inevitable. However, during transitions, two different kinds of products are mixed with long reactor residence time (*e.g.*, 2–4 h), thus resulting in a long transition time (*e.g.*, 5–30 h) and a large amount of off-spec polymers, which have to be sold at a much lower price[2,3]. Over the last three decades, the need to increase profitability in polymer industrial productions has given rise to many attracting research problems such as dynamic modeling of polymerization reactors (or quality index) [4,5], reference trajectory optimization offline [6–8], monitoring quality index online and hierarchical integration optimization [9]. Among these topics, the dynamic models of processes and trajectory optimization are the basal but challenging problems, which will be the concern in this paper.

For these basic dynamic optimization problems, one common used method is sequential method with non-linear differential/algebraic equations (DAEs), in which only the control variables are discretized. McAuley employed a gradient based nonlinear programming problem (NLP) optimizer updating feasible solutions which are integrated to determine the resulting trajectories of the state variables based on first-principle models [7]. Takeda and Ray proposed the methodology that utilized a dynamic process simulator embedded in the algorithm iterations, and coupled to a sequential quadratic programming (SQP) [8]. Wang and Yang presented a grade transition model with state constraints and chosen SQP to solve it [6]. Related studies can be referred to He *et al.* (2012) [10], Wang and Yang (2003) [6] and Fei *et al.*[11]. However, Lee *et al.* pointed out that non-linear and multimodal chemical systems had difficulties in the convergence to the global optimum and therefore, they proposed a modified differential evolution algorithm [12,13].

Biegler *et al.* believed that sequential methods with repeated integration of the DAE may become time-consuming [14,15]. Therefore, they adopted simultaneous approaches which discretized state and control variables and transformed the original problem into a much larger non-linear programming problem (NLP) which was solved by the interior point strategy [15]. Fei *et al.* indicated that the development of mechanism models based on rigorous theoretical knowledge of physicochemistry was usually quite difficult and may be impractical [11]. Considering the difficulties and practicality of modeling, they proposed a new data-based model using ARX (AutoRegressive with eXogenous inputs) combined with neural network under partial least squares framework (ARX-NNPLS), in which less specific knowledge of the process was required but the input and output data [11]. The summary of the up-to-now research work is illustrated in Table 1.

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Table 1
The summary of the up-to-now research work

Methods	Dynamic system models	Optimization solver
Sequential method with DAEs	DAEs	Gradient based NLP optimizer[7,8]
Stochastic methods with DAEs	DAEs	GA, DE, *et al.*[12,13,16,17]
Simultaneous methods with DAEs	DAEs	Interior point method [14,15,18,19]
Sequential method with data-driven models	Data-driven models	NLP algorithm [11]

As quality demands have gradually increased in recent years, they cause great pressure and motivations to make polymer productions more efficient and cost-effective. Thus, the accuracy of quality measurements and the flexibility and profitability of grade transitions have to be promoted further[1].

For the expressions of dynamic system models, DAEs are often difficult to establish and will cause time-consuming evaluation processes for feasible solutions, whereas, data-driven models as local models fit training sets well but may mismatch the true systems over a wide range. Thereby, if structural knowledge and data-driven methods can be incorporated, it will share advantages of these two kinds of approaches. Due to the physical structural information involved, the model can capture the nature of the wide range of process fluctuations, while on the other hand, the unknown non-linearities, dynamics of highly complicated kinetic behavior along with unknown noises can be approximated by the data-driven methods. A three-stage decomposition model based on structural information to describe the dynamic non-linear behavior of dynamic transitional processes has been developed and the estimation accuracy is validated to be effective in comparison with black-box modeling methods [20].

For optimization algorithms, dynamic programming (DP) is a typical solution method for dynamic optimization problems. The advantages are independence on problem structures and gradient information, and can obtain optimal solutions based on the principle of optimality. However, in most cases, the lack of closed form solutions of Bellman equations always leads to the use of computational methods—such as value iteration and policy iteration—to solve those equations, typically requiring computation time and memory that grow exponentially in the number of state variables, decision variables and random variables that affect the system in each time period, which are "curses of dimensionality" [21]. Just these difficulties render DP infeasible for high-dimensional problems of extensively practical use [21].

In recent years, in order to overcome the "curses of dimensionality", iterative dynamic programming (IDP) and adaptive grid scheme for DP have been proposed. IDP is first proposed by Luus [22] and has been extensively applied [23,24]. The procedure of IDP is performed for a number of iterations of DP. The optimal control policy from the previous iteration gives the central values of the search regions at each stage of the current iteration. The radii of corresponding regions are contracted by a constant to provide a finer resolution. Grune and Semmler proposed an adaptive grid scheme for the discretization of state space to find the global solutions of discrete time Bellman equations [25,26]. Local posteriori error estimates were established to guide the computation to the refinement on certain critical regions of the whole space.

For IDP, search regions at each time stage are contracted by a constant factor which is assigned in advance. Therefore, the computational resources may not be adaptively adjusted to concentrate on the interesting regions. For an adaptive grid scheme, the task of algorithm is just to solve a fixed-point equation without a practical trajectory used for operations, therefore neglecting some heuristic improvements at certain stages of the time horizon. Contrarily, if the local posteriori error estimate equations proposed by Grune can be incorporated into IDP, it will lead us to select a finer region and concentrate on the computations, and consequently the approximately optimal solutions can be achieved under a certain amount of calculations. Also, if the heuristic modifications can be performed at a particular time stage, a better solution in a short time can also be obtained [27]. Thereby, on one hand, relying on the principle of optimality of dynamic programming, optimal or approximately optimal solutions can be obtained in principle, while on the other hand, iteration mechanisms of IDP coupled with the adaptive grid scheme and heuristic modifications can efficiently allocate computational resources and overcome the curse of dimensionality.

In order to increase the algorithmic efficiency of grade transition problems, a three-section algorithm of dynamic programming (TSDP) coupled with the three-stage system model is proposed in this paper. Similarly with IDP, this novel algorithm starts from a DP algorithm of coarse discretization with fast computation characteristics. The following idea that improves efficiency is to design iteration cycles with heuristic modifications under limited calculation loads and to allocate adaptively the valued computational resources to the regions that can further improve the optimality of feasible solutions with the guidance of local posteriori error estimates.

2. Problem Formulations

The grade transition problem in polymerization industries is a dynamic optimization problem. The goal is to find the input trajectories during transitions to have the best dynamic performance under certain objective functions, considering states and outputs of a system in a dynamical process [8]. Therefore, system models should be included.

The general continuous grade transition optimization problem can be written as the following formulation.

$$
\begin{aligned}
& f(\boldsymbol{s}_0) = \min_{\boldsymbol{u}\in\boldsymbol{U}} \sum_{t=0}^{t_f} \alpha_t v(\boldsymbol{s}(t), \boldsymbol{u}(t)) \\
& \text{s.t.} \\
& \quad \boldsymbol{s}(t+1) = \boldsymbol{T}(s(t), \boldsymbol{u}(t)) \\
& \quad \boldsymbol{s}(0) = \boldsymbol{s}_0 \in \mathbb{R}^n \\
& \quad \boldsymbol{U}^{\min} \le \boldsymbol{u}(t) \le \boldsymbol{U}^{\max} \\
& \quad \boldsymbol{S}^{\min} \le \boldsymbol{s}(t) \le \boldsymbol{S}^{\max}
\end{aligned} \tag{1}
$$

where $\boldsymbol{s}(t)$ is the m-dimensional state vector and $\boldsymbol{u}(t)$ is the n-dimensional input vector. The objective function is the integration form of continuous state and input trajectories from start time 0 to the end time t_f, in which $v(\boldsymbol{s}(t), \boldsymbol{u}(t))$ is the current cost function of state $\boldsymbol{s}(t)$ and input $\boldsymbol{u}(t)$ at time t, and $\alpha(t)$ is the time-weight factor.

The most challenging problem for dynamic optimization problems is the complicated non-linear dynamic system behavior due to the polymerization kinetics and energy effects [16]. On one hand, it is difficult to accurately describe the unknown non-linearity over a wide range. On the other hand, the non-linearity usually makes grade transition a non-convex optimization problem bearing multiple optima [16]. The complexity of algorithm applied up to now that intends to find optimal solutions will always grow exponentially with respect to the size of the input. Therefore, approximation algorithm is an alternative approach that is less ambitious to aim in finding exact optimal solutions.

The offline optimization strategy research is typically performed using a dynamic model in conjunction with optimization. In the search for feasible solutions, two algorithms are usually designed to finish the optimization, which are the certificate-checking algorithm around solutions at hand and the updating algorithm to find new solutions as illustrated in Fig. 1[28]. Many progresses have been made under this generally accepted framework [7,8,13–15].

The certificate-checking algorithm around solutions at hand is mainly the scheme dealing with the complex system constraints. The objectives of the algorithm are checking whether the solutions are