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Experimental gradient estimation of multivariable systems with correlation by various regression methods and its application to modifier adaptation

Dong Hwi Jeong[a], Chang Jun Lee[b], Jong Min Lee[a,*]

[a] School of Chemical and Biological Engineering, Institute of Chemical Processes, Seoul National University, 1 Gwanak-ro, Gwanak-gu, Seoul 08826, Republic of Korea
[b] Department of Safety Engineering, Pukyong National University, 45, Yongso-ro, Nam-gu, Busan 48513, Republic of Korea

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ABSTRACT

In process optimization, model-plant mismatch is an important issue because it is closely related to the economic competitiveness of the product. To handle this issue, experimental gradient-based methods, such as modifier adaptation scheme, that ensure the necessary conditions of optimality for the plant equations have been utilized. However, gradient estimation methods may not work properly for the conventional modifier adaptation scheme in the case of multivariable systems with correlation. In this paper, we compare the optimization performance of gradient estimation for conventional modifier adaptation approaches and regression methods, such as multivariable linear regression, partial least squares regression, and principal component analysis. The moving average input update strategy and latent variable space model based algorithm are proposed to suppress excessive updates and improve the convergence rate and stability near the Karush-Kuhn-Tucker (KKT) point. Several simulation results of fed-batch operation of a bioreactor show that regression-based methods, especially latent variable space modelling, outperform conventional methods in the optimization of the multivariable system with correlation. In addition, the simulations show that both fast convergence and stability near the KKT point can be achieved by using the proposed latent variable space model-based algorithm.

1. Introduction

Intensifying global competition has necessitated operations optimization in the process industry. Process optimization typically utilizes a mathematical model to numerically compute optimal solutions [5]. Therefore, building a reliable mathematical model is important for obtaining accurate results. However, construction of an accurate process model is almost impossible in practice. This inherent issue is referred to as model-plant mismatch, which is caused by unknown disturbances occurring during actual process operations or by the variables that were not reflected in the model. If model-plant mismatch exists, the optimal solutions based on this erroneous model will differ from those of the actual plant, and such solutions may even become infeasible.

In order to optimize the process under a model-plant mismatch, two approaches have been applied. Implicit methods do not use a process model but directly adjust inputs in a control-inspired manner to seek a plant optimum or use the process model in off-line manner [2]. For example, Box and Draper [1] propose an algorithm that mimics an iterative numerical optimization algorithm and successively determines optimal operating points. Other implicit methods using the process model off-line are the self optimizing control (SOC) and necessary conditions of optimality (NCO) tracking approach, which adjust inputs by tracking the NCO of the modified model [8]. If no constraints exist, the implicit methods can be seen as gradient control [9]. However, these model-free methods cannot consider constraints when the active constraint set is changed during iterative optimization [6]. For chemical process applications, this is disadvantageous because respecting constraints is more important than finding the optimum.

In contrast, explicit (or fixed-model) methods use actual plant measurements given a model. The measured outputs are compared to model predictions and incorporated into the model. The most conventional method, known as the two-step approach, involves

* Corresponding author.
E-mail addresses: cacaca26@snu.ac.kr (D.H. Jeong), changjunlee@pknu.ac.kr (C.J. Lee), jongmin@snu.ac.kr (J.M. Lee).

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parameter update followed by optimization of the updated model in a repeated manner [12]. In this way, the updated model is expected to yield a better description of the actual plant at a given operating point. However, the two-step approach works well only provided that (1) there are few structural problems other than parametric mismatch and (2) the operating condition can be sufficiently changed to provide enough perturbations for parameter estimation. Unfortunately, such conditions are rarely met in practice [13]. On the other hand, there are other explicit methods that update the model structure by adding error terms between the measurement and model prediction [12]. The integrated system optimization and parameter estimation (ISOPE) was first proposed to converge the solution to a Karush-Kuhn-Tucker (KKT) point by modifying the gradient of the model objective [2]. Recently, a new scheme called modifier adaptation, which adds zeroth- and first-order modification terms both to the objective and constraints, was proposed [13]. Modifier adaptation has been proven to converge to the plant KKT point for the more various types of model-plant mismatches than the conventional two-step approaches. For the large structural model-plant mismatch case, the two-step approaches generally fail to converge to the plant KKT point, while the modifier adaptation can converge to the plant KKT point provided the model adequacy is guaranteed [6].

A key element of the implicit and explicit approaches is estimating the gradients of the plant given input variables, referred to as experimental gradients [6]. Various methods have been proposed for appropriate gradient estimation. In the case of parametric mismatch, a model-based gradient estimation approach, called the neighboring extremal method, can be utilized [26]. For more general cases, a straightforward approach exists for individually perturbing each input around the current operating point and estimating the corresponding gradient [2,28]. Roberts' algorithm using the finite difference is the most representative case [2]. However, these approaches are not practical because they require that a perturbation be performed for each input variable at each iteration [27]. Meanwhile, there are other gradient estimation methods that do not require input perturbations but use one or several past operating points instead. Brdyś and Tatjewski firstly proposed a different way of implementing a finite difference approximation of the gradient based on past operating points [10,11]. Compared to the original ISOPE proposed by Roberts [2], this algorithm is called dual ISOPE because it has two conflicting objectives, the primal objective of improving the plant operation and the dual objective of estimating the experimental gradient [27]. In order to avoid the ill-conditioned or non-singularity problem, the dual ISOPE includes a constraint related to the condition number of updated input matrix. However, introducing additional constraints to compensate for the matrix inversion problem can also lead to nonconvex optimization [25]. In addition, the conventional gradient estimation techniques may not work well, especially in the case of multivariable systems with highly correlated data. To solve this multivariable system's optimization problem, directional modifier adaptation is recently proposed [36]. In this algorithm, a few privileged directions are selected and the modifier adaptation scheme is applied only to these directions for finding a suboptimal solution which satisfies the KKT conditions in these directions. In this way, the required update number can be reduced and fast improvement of optimization performance can be achieved in the multivariable system. However, the directional modifier adaptation has a limitation that the choice of the privileged direction cannot be ensured when the model-plant mismatch is not the small parametric uncertainty. In addition, measurement noise is not considered in this algorithm.

On the other hand, combining the advantages of model-based and model-free methods, regression models can be effectively used to optimize unconstrained processes [4,14]. Camacho et al. [4] employ partial least squares regression to estimate experimental gradients with several input and output data points. The estimates are further used to update the operational strategy, e.g., feed rate, in a run-to-run fashion. Compared with model-free approaches, regression models achieve faster convergence to the plant optimum. However, their algorithm does not deal with the constraints in the framework of the conventional constrained optimization problem as the modifier adaptation, but only suppresses the updated inputs in an ad hoc manner. Thus, it has a limitation of not considering the convergence to the KKT points of plant equations.

In this work, we extend the regression-based method proposed by Camacho et al. for unconstrained optimization to the constrained case by combining it with the modifier adaptation scheme. We evaluate the resulting method by simulating a multivariable system with correlation comprising run-to-run optimization of a fed-batch bioreactor having 50 manipulated variables, constraints, and model-plant mismatches. Compared to conventional methods of gradient estimation, the regression-based gradient estimation shows improved performance of optimization. Especially, several latent variable space model-based approaches, such as the partial least squares and principal component analysis, outperform the other ones in the case of optimizing the multivariable systems having correlated data. The effects of the number of principal components and data points for gradient estimation on the optimization performance are studied under several simulations when using the latent variable space-based approaches. Based on these results, a moving average input update strategy and an algorithm that satisfies both fast convergence and stability near the KKT point are proposed.

The remainder of the paper is organized as follows. Section 2 introduces an example of fed-batch bioreactor optimization and motivates the problem of optimization with a large number of manipulated variables and model-plant mismatches. Section 3 explains the loss of optimality caused by model-plant mismatch and introduces one of its solutions, i.e., the modifier adaptation scheme. Section 4 details conventional gradient estimation methods and their application to the optimization of the multivariable system having correlated data. In Section 5, various regression methods are utilized to estimate the experimental gradient of the multivariable system with correlation, and optimization performance is compared. Section 6 discusses the key factors affecting the optimization performance based on regression gradient estimation and an algorithm based on latent variable space modeling for fast convergence and stability near the KKT point is proposed. Finally, Section 7 provides concluding remarks.