Journal of Process Control 68 (2018) 195–204

Contents lists available at ScienceDirect

Journal of Process Control

journal homepage: www.elsevier.com/locate/jprocont

Real-time Optimization with persistent parameter adaptation using online parameter estimation☆

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ARTICLE INFO

Article history:
Received 7 November 2017
Received in revised form 24 April 2018
Accepted 31 May 2018

Keywords:
Real-time optimization
Steady-state detection
Nonlinear state estimation

ABSTRACT

One of the major drawbacks of traditional Real-time Optimization (RTO) is the steady-state wait before estimating the parameters. This paper proposes an alternative solution called Real-time Optimization with Persistent Adaptation (ROPA), which integrates on-line parameter estimation in the optimization cycle, avoiding the SS detection step. Essentially, the idea is to use transient information to update the steady-state economic optimization problem and, then, by continuously solving it, the calculated optimal solution would reach the actual plant steady-state optimum in a given time horizon. ROPA provides an intermediary solution between static and dynamic optimization schemes. While it approximates the optimal trajectory, ROPA design enables the application of techniques to plant-wide optimization and the use of well-established static RTO commercial solutions. The new methodology benefits are illustrated with a case study, in which the traditional RTO and ROPA schemes are applied to the Williams–Otto reactor. Their performance is compared based on profit loss and deviation from the actual optimal decisions. The results show that the refinement of the prediction capacity by decreasing the time between two sequential optimization leads to a better economic performance and enhances the disturbance detection of the optimization cycle.

1. Introduction

Optimization of chemical processes has drawn attention of the academic and industrial communities due to the difficulties in achieving profitable operating conditions, while meeting constraints imposed by the equipment, product specifications, and safety/environmental regulations [1,2].

Usually in the standard Real-time Optimization (RTO) implementation, Model Parameter Adaptation (MPA), nonlinear rigorous steady state models are optimized online in order to determine best operating condition for the plant (e.g. maximizing profit, minimizing cost) [3]. In order to operate at the current optimal condition, not in a nominal one, these models are updated with plant measurement information every time the plant reaches steady-state condition [4].

In practice, detecting the stationary condition is a difficult task to be carried out [5]. Generally, steady-state (SS) detection methods rely on statistical or heuristic tests and, even after meeting the methods' criteria, it is hard to determine if the process has actually reached steady-state [4]. The SS detection problem gets even more complex if the size of the process increases. In these cases, choosing a set of measurements that represents the plant state is not trivial. Moreover, the measurement set can contain signals with slower responses, which may not be in phase with other measurements, misleading the steady-state detection [4,5]. Additionally, if the disturbance frequency is higher than the process time constants and/or disturbances are constantly affecting a small section of the process, the global set of measurements is unlikely to pass a steady-state acceptance test.

As the steady-state periods are very difficult to detect, there is a risk that the model is updated with erroneous information (i.e. the stationary model parameters are directly updated with transient data). Under these conditions, the calculated optimal does not correspond to the actual plant optimum, even in cases with a perfect plant model. By optimizing an unsuited model, the RTO obtains aggressive and profitless updates of the setpoints, decreasing the potential benefits of the economic optimization [6].

Hence, avoiding the steady-state detection step in the optimization scheme is a significant advantage. This paper proposes an alternative RTO methodology called Real-time Optimization with Persistent Adaptation (ROPA) that avoids the steady-state wait problem. ROPA continually adjusts the optimal set-point values by

☆ The authors thank CNPq [grant number 140314/2013-0] and Petrobras S.A. [grant number 15014] for the financial support.
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https://doi.org/10.1016/j.jprocont.2018.05.009
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updating the stationary model of the static optimization layer in real time with on-line parameter estimation methods.

Basically, the parameters are estimated with transient measurements, but they are treated as if they represent a steady-state condition. Thus, the methodology does not seek continuous optimization, in a strict sense, rather it seeks to continuously improve the set-points in a manner that in a broader time horizon, the set-points reach the steady-state optimum. Fig. 1 compares ROPA with the classical RTO approach, MPA.

Clearly, ROPA appears as an intermediary solution between static RTO and optimization schemes that calculate optimal trajectories, like Dynamic Real Time Optimization (DRTO) [7] and Economic Model Predictive Control (EMPC) [8–10]. Despite appealing, there are few examples of DRTO and EMPC implementations using large-scale rigorous first-principles models [11–13]. The lack of large-scale models is a problem in cases involving complex processes composed by several units, like a refinery. In these cases, optimizing a single unit or subsystem does not guarantee that the plant global optimum is reached [4]. In addition, estimating states/parameter for dynamic models that encompass the whole unit is a challenging task.

ROPA is the key for decoupling the estimation problem in order to achieve plant-wide optimization. On one hand, ROPA takes advantage of the well-established literature and software of stationary economic optimization (like ROMeo 5.1 (Schneider Electric, Houston, TX), and Aspenplus 7.1 (Aspentech,Burlington, MA) [3]). On the other hand, ROPA asynchronously updates the plant-wide model by applying online estimation to subsections of the plant model that have low parameter update frequency (e.g. highly perturbed sections). Consequently, the steady-state plant-wide optimization problem can be solved at any desired rate.

This paper is the first step towards developing this decoupled optimization scheme. Specifically, the aim of this paper is to understand the benefits and shortcomings of applying online estimation in a static economic optimization context. As shown in the case study, the analysis of the closed-loop behavior of ROPA is very encouraging. It indicates that ROPA has potential to improve the overall economic result when compared to the classical RTO scheme by reducing the RTO frequency and avoiding the SS wait. Thus, ROPA offers an interesting alternative for optimizing chemical processes in real-time.

The paper is organized as follows. First some preliminary information about notation and the models is given. In Section 3, the formulation of the optimization problem along with the RTO (MPA) layer is presented. Then, in Section 4, the online estimation methods are reviewed, the implemented estimator (extended Kalman filter (EKF)) is briefly described, and the ROPA methodology convergence properties assessed. Section 6 presents details of the case-study simulation. Next, the comparison of ROPA with MPA is shown in Section 7. Finally, Section 8 concludes the paper.

2. Preliminaries

The plant is represented by the following steady-state input–output mapping:

$$\mathbf{y}_{p,k}(\mathbf{u}_k, \mathbf{d}_{p,k}, \boldsymbol{\epsilon}_{p.k}) \in \mathbb{R}^{n_y} \tag{1}$$

in which $\mathbf{u}_k \in \mathbb{R}^{n_u}$ are the system inputs, $\mathbf{d}_{p,k} \in \mathbb{R}^{n_d}$ are the deterministic disturbances, and $\boldsymbol{\epsilon}_{p,k} \in \mathbb{R}^{n_n}$ the random disturbances. The subscript k indicates the variable at time t_k assuming a zero-order holder over the interval $[t_k, t_{k+1})$.

Steady-state and dynamic models are developed for the RTO and online estimation layers. They are associated with the subscripts *ss* and *dyn*, respectively. The steady state model is:

$$\begin{aligned} \mathbf{0} &= \mathbf{f}_{ss}(\mathbf{x}, \mathbf{u}, \mathbf{p}) \\ \mathbf{y} &= \mathbf{h}(\mathbf{x}, \mathbf{p}) \end{aligned} \tag{2}$$

where, in addition to the previous notation, $\mathbf{x} \in \mathbb{R}^{n_x}$ are the model state variables and $\mathbf{p} \in \mathbb{R}^{n_p}$ is the set of model parameters. $\mathbf{f}_{ss} : \mathbb{R}^{n_x} \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_p} \to \mathbb{R}^{n_x}$ is a nonlinear function. The lack of time subscripts indicates steady-state values. The dynamic model is represented by:

$$\begin{aligned} \mathbf{x}_{k+1} &= \mathbf{f}_{dyn}(\mathbf{x}_k, \mathbf{u}_k, \mathbf{p}_k) + \boldsymbol{\omega}_k \\ \mathbf{y}_k &= \mathbf{h}(\mathbf{x}_k, \mathbf{p}_k) + \boldsymbol{\nu}_k \end{aligned} \tag{3}$$

In the dynamic case, process and measurement noise, $\boldsymbol{\omega}_k$ and $\boldsymbol{\nu}_k$, are added to the process model. Both are modeled as white Gaussian random noises with zero mean and constant covariance matrices $\mathbf{Q} \in \mathbb{R}^{n_x, n_x}$ and $\mathbf{R} \in \mathbb{R}^{n_y, n_y}$, respectively. Also, the state transition function $\mathbf{f}_{dyn}(\mathbf{x}_k, \mathbf{u}_k, \mathbf{p}_k)$ is a mapping over the interval $[t_k, t_{k+1})$, which represents the solution of the differential model during the period. $\mathbf{f}_{dyn}$ is assumed to be at least once differentiable in all points of the valid operation range. Moreover, $\mathbf{f}_{dyn}$ has the same dimensions as $\mathbf{f}_{ss}$ and both share the same states.

3. Model parameter adaptation (MPA)

MPA, which is the standard RTO approach [3], is implemented in order to be used as a comparison basis to ROPA. Although the MPA cycle can have more elements [3], like gross error detection, only the three steps shown in Fig. 1 were implemented in the case study, namely: steady-state detection; model adaptation (parameter estimation); and steady-state optimization.

3.1. Steady-state detection

The steady state detection method is based on [14], which estimates the variance of the data by two methods. The first method calculates an estimate of the variance between the current measurement and a filtered trend of the same measurement. In turn, the second method calculates the variance between sequential data measurements. Whenever the process reaches a steady state, the variances calculated by both methods will ideally be equal to each other. Therefore, if the process is not at steady state, the variance ratio is significantly larger than unity. The equations of the SS detection method are:

$$\begin{aligned} z_{f,k} &= \lambda_1 z_k + (1-\lambda_1) z_{k-1} \\ \delta^2_{1,f,k} &= \lambda_2 (z_k - z_{f,k-1})^2 + (1-\lambda_2)\delta^2_{1,f,k-1} \\ \delta^2_{2,f,k} &= \lambda_3 (z_k - z_{k-1})^2 + (1-\lambda_3)\delta^2_{2,f,k-1} \\ R &= (2-\delta_1)\delta^2_{1,f,k}/\delta^2_{2,f,k} \end{aligned} \tag{4}$$

in which, z is the given measured variable ($z \in \mathbf{y}_{p,k}$); z_f is its filtered value; $\delta^2_{1,f,k}$ is the variance calculated by the first method, and $\delta^2_{2,f,k}$ by the second; λ_i are the filter factors; and R is the ratio of variances.

If R is larger than a given threshold (R_{crit}), the measurement fails the SS detection test. In the case where two or more measurements are used to indicate the SS, all of them need to pass the test in order to consider the process at steady-state.

3.2. Model adaptation

Once the plant has reached steady state, the model adaptation algorithm starts to run. The parameters are estimated by minimiz-