Computers and Chemical Engineering 51 (2013) 172–180

Contents lists available at SciVerse ScienceDirect

Computers and Chemical Engineering

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

On the role of the necessary conditions of optimality in structuring dynamic real-time optimization schemes

Dominique Bonvin[a,*], Bala Srinivasan[b]

[a] Laboratoire d'Automatique, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland
[b] Department of Chemical Engineering, Ecole Polytechnique Montreal, Montreal, Canada

ARTICLE INFO

Article history:
Received 28 March 2012
Received in revised form 9 July 2012
Accepted 12 July 2012
Available online 2 August 2012

Keywords:
Dynamic real-time optimization
Plant-model mismatch
Modeling for optimization
Input parameterization
Plant model
Solution model

ABSTRACT

In dynamic optimization problems, the optimal input profiles are typically obtained using models that predict the system behavior. In practice, however, process models are often inaccurate, and on-line model adaptation is required for appropriate prediction and re-optimization. In most dynamic real-time optimization schemes, the available measurements are used to update the plant model, with uncertainty being lumped into selected uncertain plant parameters; furthermore, a piecewise-constant parameterization is used for the input profiles. This paper argues that the knowledge of the necessary conditions of optimality (NCO) can help devise more efficient and more robust real-time optimization schemes. Ideally, the structuring decisions involve the NCO as follows: (i) one measures or estimates the plant NCO, (ii) a NCO-based input parameterization is used, and (iii) model adaptation is performed to meet the plant NCO. The benefit of using the NCO in dynamic real-time optimization is illustrated in simulation through the comparison of various schemes for solving a final-time optimal control problem in the presence of uncertainty.

1. Introduction

Optimization is important in science and engineering as a way of finding the best solutions, designs or operating conditions. Optimization is typically performed on the basis of a mathematical model of the object of attention. For example, engineers might be interested in the optimal operation of processes that either operate at steady state or undergo transient changes. The object of attention, or reality, is called the "plant", whereas the "model" is a set of algebraic, differential or differential-algebraic equations.

In practice, optimization is complicated by the presence of uncertainty in the form of plant-model mismatch and unknown disturbances. Without uncertainty, one could use the model at hand, optimize it numerically off-line and implement the optimal inputs in an open-loop fashion. However, because of uncertainty, additional information such as uncertainty description or plant measurements must be included. In the former case, robust optimization computes a set of inputs that guarantees feasibility either for all possible realizations or with a desired probability level, however at the expense of a conservative solution (Srinivasan, Bonvin, Visser, & Palanki, 2003; Terwiesch, Agarwal, & Rippin, 1994). In the latter case, the inputs are updated in real-time based on measurements. This is the field of *real-time optimization*, which is labeled RTO for static optimization problems (Marlin & Hrymak, 1997) and DRTO for dynamic optimization problems (Biegler, 2009). This paper deals with two major implementation issues in DRTO, namely, model quality and computational aspects.

The issue of *model quality* raises an important question: Does good performance require a good model? This is not necessarily the case for control, since errors resulting from a poor model can be offset by the action of feedback. In optimization, without feedback to make up for modeling errors, the model needs to represent the reality accurately, in particular the optimality conditions of the plant. The situation is slightly different in real-time optimization since the measurements available on-line represent some form of feedback. However, this feedback is only partial as it is typically limited to output information. Furthermore, it is important to adapt the model appropriately, that is, there where it matters most for the purpose of optimization. These issues of measurement location and input update in the context of imperfect model are crucial for reaching optimality. It is argued in this paper that the necessary conditions of optimality (NCO) predicted by the model need to match those of the plant for plant optimality. We will discussed how the NCO measurements can be incorporated in a model so as to be most useful for optimization.

The *computational aspects* are also crucial for implementation. A very reliable optimization scheme is model predictive control (MPC), which incorporates state feedback, uses a receding horizon and carries out the optimization repeatedly at each sampling

* Corresponding author. Tel.: +41 21 693 3843; fax: +41 21 693 2574.
E-mail address: dominique.bonvin@epfl.ch (D. Bonvin).

0098-1354/$ – see front matter © 2012 Elsevier Ltd. All rights reserved.
http://dx.doi.org/10.1016/j.compchemeng.2012.07.012

time (Rawlings & Mayne, 2009). MPC was initially developed to track a reference trajectory by minimization of a quadratic error term. It has recently been extended to "economic MPC" that uses a non-quadratic cost function (Heidarinejad, Liu, & Christofides, 2012; Rawlings & Amrit, 2009). Furthermore, there has been considerable efforts in recent years to speed up the computations by formulating convex optimization problems and also using algorithms that exploit the structure of the problem (Diehl, Ferreau, & Haverbeke, 2009; Richter, Morari, & Jones, 2011; Wang & Boyd, 2010). On the other hand, recent trends in DRTO have included attempts to move the heavy computations off-line, where time and computational power are more available, and limit the on-line operations to quick decisions and easy computations. For example, multi-parametric programming generates off-line a lookup table of control laws, which are then used on-line based on the estimated states of the plant (Bemporad, Morari, Dua, & Pistikopoulos, 2002; Pistikopoulos, Georgiadis, & Dua, 2007; Zeilinger, Jones, & Morari, 2011). Also, "advanced step NMPC" strategies have been proposed, which solve the detailed optimization problem in background and apply sensitivity-based update on-line (D'Amato, Kumar, Lopez-Negrete, & Biegler, 2012; Zavala & Biegler, 2009). Another approach is the nonlinear real-time iteration scheme, which uses a continuation Newton-type framework and solves one QP at each iteration (Diehl, Bock, & Schlöder, 2005; Diehl et al., 2002). This allows for multiple active set changes and thus ensures that the nonlinear MPC algorithm cannot perform worse than a linear MPC controller. Yet a different approach is NCO tracking, which uses a NCO-based parameterization of the input profiles to design a multivariable feedback scheme that tracks the first-order optimality conditions, thereby pushing the system toward optimality (Srinivasan & Bonvin, 2007).

This paper deals with the model-quality issue in DRTO. In the presence of significant plant-model mismatch, the use of a fixed nominal model is typically insufficient to drive the *plant* to optimality. With MPC for example, the estimated states are often inaccurate, and one would need to update the model, which is difficult to do in closed-loop operation due to the so-called dual control problem (Aström & Wittenmark, 1995). This work adopts the viewpoint that, in real-time optimization, the model is a vehicle to process plant measurements and compute the optimal inputs. This step involves two major decisions, namely, the choice of the measured quantities and the choice of a finite number of decision variables via input parameterization. Note that these choices can benefit from knowledge of the NCO since the NCO are intimately linked to plant optimality. The structure of the optimal solution and the corresponding NCO can be determined off-line by numerical optimization. These measurement and input-parameterization issues are briefly addressed next.

Measurements and uncertainty description. The measurements are typically the plant outputs y_{plant}. The uncertainty, which is observed as the difference between the plant measurements and the corresponding model predictions, can be represented as parametric variations of the plant model. Alternatively, if the NCO elements can be measured, say y_{NCO}, the model uncertainty can be expressed as the difference between the measured and the predicted y_{NCO} values. It is interesting to notice the close relation between the type of measurements (the plant outputs y_{plant} vs. the NCO elements y_{NCO}) and the uncertainty description (the plant parameters θ_{plant} vs. the NCO deviations Δ_{NCO}).

Parameterization and update of the inputs. The traditional way of parameterizing infinite-dimensional inputs is control vector parameterization (CVP), whereby the inputs are approximated as piecewise-constant profiles. The main advantage is universality, that is, any solution can be closely approximated by introducing a sufficient number of pieces (barring certain numerical issues such as ringing around discontinuities). However, CVP typically contains a large number of piecewise-constant input values, denoted here π_{CVP}. In contrast, a parsimonious input parameterization, π_{NCO}, can be obtained from the knowledge of the NCO, that is, the input elements correspond to switching times between arcs and input values associated with certain arcs. The way the inputs are parameterized impacts on the way there are updated. With π_{CVP}, the only efficient way to compute the inputs is through numerical optimization. With π_{NCO}, the few input parameters can be adjusted via feedback control to regulate the deviation Δ_{NCO} to zero.

		Input Parameterization	
		π_{CVP}	π_{NCO}
Measurements	y_{plant}	$y_{plant} \xrightarrow{\text{Ident}} \theta_{plant} \xrightarrow{\text{Opt}} \pi_{CVP}$ (*two-step approach, CVP*)	$y_{plant} \xrightarrow{\text{Ident}} \theta_{plant} \xrightarrow{\text{Opt}} \pi_{NCO}$ (*two-step approach, NCO*)
	y_{NCO}	$y_{NCO} \xrightarrow{\text{Diff}} \Delta_{NCO} \xrightarrow{\text{Opt}} \pi_{CVP}$ (*modifier adaptation*)	$y_{NCO} \xrightarrow{\text{Diff}} \Delta_{NCO} \xrightarrow{\text{Control}} \pi_{NCO}$ (*NCO tracking*)

Fig. 1. Measurement and input-parameterization features of various DRTO schemes. The measured plant outputs are labeled y_{plant}, the measured NCO elements y_{NCO}; the inputs are parameterized via control vector parameterization, π_{CVP}, or via the elements of the NCO, π_{NCO}. Plant-model mismatch can be absorbed in the plant model parameters θ_{plant} or via an additive disturbance to the NCO values, Δ_{NCO}. "Ident" means the use of parameter identification, "Diff" the computation of a difference, "Opt" the use of numerical optimization, and "Control" the use of feedback control.

Various DRTO schemes are possible based on the choice of the measurement and input-parameterization options, some of which are illustrated in Fig. 1 and discussed next.

- In the "two-step approach" of repeated parameter identification and performance optimization, the measurements are used to adapt the model parameters and estimate the current states. The estimated states serve as initial conditions for the optimization that is repeated on-line with the updated model (Chen & Joseph, 1987; Eaton & Rawlings, 1990). The input parameterization is of the CVP type.
- In the modifier-adaptation approach, modifier terms are added to the cost and constraint functions. Upon measurement of y_{NCO}, the modifiers are updated in order for the model and the plant to have matching first-order optimality conditions (Chachuat, Srinivasan, & Bonvin, 2009; Marchetti, Chachuat, & Bonvin, 2007). These schemes use the measurements y_{NCO} and the inputs π_{CVP} for optimization.
- It is also possible to perform numerical optimization using a NCO-based input parameterization. Such a scheme has been developed by Schlegel and Marquardt (2006a) and applied to an industrial polymerization process in Schlegel and Marquardt (2006b). The corresponding DRTO scheme consists in measuring y_{plant} and updating the model parameters accordingly, followed by numerical optimization using the π_{NCO} parameterization.
- Finally, NCO tracking uses the measurements of y_{NCO} to update π_{NCO} using feedback control to meet the plant NCO (Srinivasan & Bonvin, 2007).

This paper considers the implementation of optimal control in the presence of significant uncertainty in the form of plant-model mismatch, which requires some form of adaptation based on plant measurements. Three possible adaptation strategies are considered, namely adaptation of the process model, adaptation of the