On the Use of Transient Information for Static Real-Time Optimization

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Optimal operation of chemical processes is key for meeting productivity, quality, safety and environmental objectives. Both model-based and data-driven schemes are used to compute optimal operating conditions [1]:

- The model-based techniques are intuitive and widespread, but they suffer from the effect of plant-model mismatch. For instance, an inaccurate plant model leads to operating conditions that typically are not optimal for the plant and may violate constraints. Furthermore, even with an accurate model, the presence of disturbances generally leads to a drift of the optimal operating conditions, and adaptation based on measurements is needed to maintain plant optimality.
- The data-driven optimization techniques rely on measurements to adjust the optimal inputs in real time. Consequently, real-time measurements are typically used to help achieve plant optimality. This field, which is labeled real-time optimization (RTO), has received growing attention in recent years. RTO schemes can be of two types: explicit schemes solve a numerical optimization problem repeatedly, while implicit schemes adjust the inputs on-line in a control-inspired manner.

Explicit RTO schemes solve a numerical optimization problem repeatedly. For example, the two-step approach uses (i) measurements to update the model parameters, and (ii) the updated model to perform the numerical optimization [2]. It has also been proposed to update the model differently. Instead of adjusting the model parameters, input-affine correction terms can be added to the cost and constraint functions of the optimization problem so that it shares the first-order optimality condition with the plant. The main advantage of the technique, labeled modifier adaptation (MA), lies in its proven ability to converge to the plant optimum, even in the presence of structural plant-model mismatch [3]. Furthermore, MA is capable of detecting the correct set of active plant constraints without additional assumptions. As a static optimization method applicable to continuous plants, MA requires waiting for steady state before taking measurements, updating the correction terms and repeating the numerical optimization. Hence, several iterations are generally required to achieve convergence. The main difficulty lies in the estimation of the steady-state plant gradient at each iteration.

In contrast, *implicit RTO schemes*, such as extremum-seeking control [4], self-optimizing control [5] and NCO tracking [6], propose to adjust the inputs on-line in a control-inspired manner. In the absence of constraints, or when assumptions can be made regarding the set of plant constraints that are active at the optimum, implicit RTO methods reduce to gradient control, as the degrees of freedom are adjusted in real time to drive the plant cost gradient to zero. Here again, the difficulty lies in the estimation of the steady-state plant gradient, which, in addition, must be performed during transient operation. This is achieved via either low-frequency plant excitation and corresponding cost measurements (as in extremum-seeking control) or the use of transient measurements together with a model of the steady-state gradient (as in self-optimizing control and NCO tracking via neighboring extremals, where the required steady-state measurements are simply replaced by the corresponding transient measurements) [7]. Implicit RTO is much more challenging when the set of active constraints is unknown, as not only the cost gradient has to be inferred from the measurements but also the set of active constraints and the constraint gradients.

This contribution proposes a framework for using MA during the transient phase toward steady state, thereby attempting to reach optimality in a single iteration to steady state. With this approach, a modified optimization problem is solved repeatedly at each optimization instant during transient, with the input-affine correction terms, which theoretically depend on steady-state plant quantities, being estimated on the basis of transient measurements. Note that such an attempt has already been documented in the literature but, as for the aforementioned implicit methods, the "steady-state" gradients were estimated using transient information in the framework of both multiple units and neighboring extremals [8]. In contrast, this work estimates the steady-state outputs from transient outputs and then uses these estimates "correctly" in the expressions for computing the steady-state gradients. For this, we propose to use the best available dynamic model and perform state estimation using an Extended Kalman Filter (EKF) framework [9]. Since the model is typically not perfect, one key parameter related to the static gain is made adjustable for each input-output pair. This way, the EKF feeds on the transient plant outputs and estimates, at the current time t, the corresponding *steady-state* outputs, which leads to the computation of the *static* gradient. The dynamic model at hand can be seen as a surrogate model that, although not sufficiently accurate globally for process optimization, can process measurements to generate an estimate of the local gradients. The approach will be illustrated on various numerical examples and then applied to the optimization of a continuous stirred-tank reactor.

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