Fast Estimation of Plant Steady State, with Application to Static RTO

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In the operation of continuous processes, many tasks require the knowledge of plant steady state at various operating points. This is for example the case in the context of kinetic modeling, response surface modeling and real-time optimization. If the computational techniques are in principle straightforward, the time needed to reach steady state represents the main limiting factor. This work proposes a novel way of speeding up the *estimation* of plant steady state through the use of feedback control and rate estimation. It must be emphasized here that rate estimation requires only some structural information of the plant and no rate model. Generally speaking, the context of the present investigation corresponds to industrial practice, where there is significant plant-model mismatch, which typically calls for the use of measurements to feed data-driven techniques.

We will illustrate the fast estimation of plant steady state in the context of static optimization of continuous reactors. Real-time optimization (RTO) is typically implemented via some iterative scheme that uses steady-state plant measurements. The cost and constraints of the optimization problem are functions of the input and output steady-state values. At the k^{th} iteration, the constant inputs $\mathbf{u}_k$ are usually applied to the plant in open loop and, once steady state is reached, the outputs $\bar{\mathbf{y}}_k$ are measured and the cost and constraint values are evaluated. However, depending on the dominant time constant of the plant, the time necessary to reach steady state may be rather long. Hence, it would be useful to be able to speed up convergence to steady state, or at least speed up the *estimation* of plant steady state. This will be done in this work through combination of feedback control (to speed up a specific part of the plant) and rate estimation (to estimate the steady-state values of the remaining part of the plant so that the cost and constraint functions can be evaluated).

For this, let us consider a time-invariant dynamic system with the inputs $\mathbf{u}$ and the state variables $\mathbf{x}$ and $\mathbf{z}$ that can be described by the differential equations:

$$\dot{\mathbf{x}}(t) = \mathbf{f}(\mathbf{x}(t),\mathbf{u}(t)) \qquad \mathbf{x}(0) = \mathbf{x}_0$$

$$\dot{\mathbf{z}}(t) = \mathbf{h}(\mathbf{x}(t),\mathbf{u}(t)) - \mathbf{\Omega}(\mathbf{x}(t),\mathbf{u}(t))\, \mathbf{z}(t) \qquad \mathbf{z}(0) = \mathbf{z}_0$$

The particular structure of this dynamic system can be exploited when the *slow* and *fast* states $\mathbf{z}$ and $\mathbf{x}$ are associated with slow and fast dynamics, respectively, and the slow states do not affect the fast states**.** The idea is to use feedback control to speed up the convergence of the fast states $\mathbf{x}$ to $\bar{\mathbf{x}}$ and the inputs $\mathbf{u}$ to $\bar{\mathbf{u}}$, provided that the states $\mathbf{x}$ are accessible, and then compute the steady-state values $\bar{\mathbf{z}}$ of the slow states as:

$$\bar{\mathbf{z}} = \mathbf{\Omega}^{-1}(\bar{\mathbf{x}},\bar{\mathbf{u}})\, \mathbf{h}(\bar{\mathbf{x}},\bar{\mathbf{u}})$$

This computation relies on nonparametric estimation of the rates $\mathbf{h}(\bar{\mathbf{x}},\bar{\mathbf{u}})$ and $\mathbf{\Omega}(\bar{\mathbf{x}},\bar{\mathbf{u}})$ using measurements and structural information of the plant. Note that $\bar{\mathbf{z}}$ can be estimated long before the state variables $\mathbf{z}$ converge to their steady-state values.

RTO is implemented via a two-layer approach. In the inner layer, feedback control is used to rapidly drive $\mathbf{x}$ to the setpoints $\mathbf{x}_{sp}$ by manipulating the inputs $\mathbf{u}$ and rate estimation is used to compute $\bar{\mathbf{z}}$ from $\bar{\mathbf{x}}$ and $\bar{\mathbf{u}}$. In the outer (optimization) layer, the RTO algorithm computes optimal values for the setpoints $\mathbf{x}_{sp}$. The inner layer is described in more detail next for chemical reactors:

- The objective of the control scheme is to drive the fast states $\mathbf{x}$, typically some reactant concentrations, to their constant setpoints in the shortest possible time after a step change in the setpoints $\mathbf{x}_{sp}$. This time is shorter than the time needed by the open-loop plant to reach steady state after a step change in the inputs $\mathbf{u}$, typically inlet flowrates. Multivariable control is implemented via input-output feedback linearization [1], pole placement or optimal control and typically involves the measurement or estimation of $\mathbf{x}$. Note that the gains to control the fast states (reactant concentrations) $\mathbf{x}$ are typically lower than those necessary to control both the fast (reactant) concentrations $\mathbf{x}$ and the slow (product) concentrations $\mathbf{z}$, thereby making the control scheme with $\mathbf{x}$ less sensitive to measurement noise. Also note that the separation into slow and fast states assumes that the rates $\mathbf{f}(\mathbf{x},\mathbf{u})$ are independent of the slow (product) concentrations $\mathbf{z}$.
- The rate estimation relies on the knowledge of the stoichiometry and the inlet concentrations, and on measurements of flowrates, reactor temperature, volume, and some of the concentrations *at steady state*. The rates are computed through numerical differentiation of the reaction variants using a Savitzky-Golay filter [1]. These reaction variants are easily computed from measured concentrations [2]. It will also be shown that the proposed Savitzky-Golay filter is the optimal convolution filter for rate estimation.

A simulated homogeneous CSTR [3] is used to illustrate the implementation of “fast static RTO” and address the following questions: (i) how to best combine feedback control and rate estimation, (ii) which controlled and manipulated variables to choose, (iii) how to eliminate the slow states in the objective and constraint functions, and (iv) how to deal with measurement noise in this measurement-based RTO algorithm.

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