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Tracking the necessary conditions of optimality with changing set of active constraints using a barrier-penalty function

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Abstract

In the framework of process optimization, the use of measurements to compensate the effect of uncertainty has become an active area of research. One of the ideas therein is to enforce optimality by tracking the necessary conditions of optimality (NCO tracking). Most techniques assume that the set of active constraints remains the same even in the presence of uncertainty and disturbances. Consequently, changes in the active set are difficult to handle. In this paper, this assumption on active set tracking is relaxed by using a logarithmic-linear barrier-penalty function. This way, none of the constraints is active and no assumption regarding the active set is required. Optimization with this barrier-penalty function is shown to have the same convergence properties as optimization with the standard barrier function while, at the same time, avoiding a separate logic to guarantee feasibility. Thus, the adaptation can be more aggressive and lead to better performance. The gradient of the augmented objective function is computed using finite perturbations and forced to zero with PI-type controllers. The approach is illustrated in simulation via the static optimization of an isothermal continuous stirred-tank reactor.

Keywords: Static optimization; Measurement-based optimization; NCO tracking; Barrier function; Penalty function; Interior point methods

1. Introduction

Measurement-based optimization has gained popularity in recent years as it uses measurements to compensate the effect of uncertainty – in the form of both model mismatch and process disturbances – occurring at the time of implementation (Abel & Marquardt, 1998; Eaton & Rawlings, 1990; Ruppen, Benthack, & Bonvin, 1995). Among the many techniques that are available for this purpose, the method that tracks the necessary conditions of optimality (NCO) shows promise since it adapts the inputs directly, i.e. without having to update a process model and re-optimize the process (Clarke-Pringle & MacGregor, 1998; Srinivasan, Bonvin, Visser, & Palanki, 2003; Srinivasan, Palanki, & Bonvin, 2003).

The NCO contain two parts: (i) the active constraints and (ii) the sensitivities, i.e. the reduced gradients of the objective function with respect to the manipulated variables. The NCO-tracking method enforces the active constraints and pushes the sensitivities to zero. This can be done for static optimization (François, Srinivasan, & Bonvin, 2002, 2005) as well as for dynamic optimization (Srinivasan et al., 2003a, 2003b). Alternate methods have been proposed that push the sensitivities in static optimization problems to zero, e.g. the self-optimizing control approach (Skogestad, 2000), where outputs that are nearly invariant to uncertainty are chosen for tracking. However, these methods do not work if the set of postulated active constraints is incorrect due to model mismatch or process disturbances. For example, if the set of active constraints changes, the NCO-tracking scheme will keep the "old" set of active constraints active, which obviously is no longer optimal. This problem can be especially serious if the active set is nonunique.

There has been a recent surge of interest in extremum-seeking (Kristic & Wang, 2000) and adaptive extremum-seeking (DeHaan & Guay, 2004a, 2004b; Zang, Guay, & Dochain, 2001) techniques that force the sensitivities to zero. The concept of barrier function is typically used to eliminate the presence of active constraints. As a result, the NCO include only sensitivities, i.e. the gradient of the augmented objective function with respect to the decision variables. Though an important

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issue – the need to define the active constraint set – can be sorted out with this barrier-function approach, the problem has in fact been made more difficult to solve, since forcing sensitivities to zero is typically more difficult to implement than keeping given constraints active. Also, the key point is that the process outputs are required to remain in the strict interior of the feasible region, since the barrier function is undefined otherwise. This features requires special care, which restricts the extremum-seeking control scheme to convex constraints.

The idea used in this paper is to eliminate the concept of active constraints by using a barrier-penalty function. The reason for this new formulation is that a barrier function must be evaluated in the strict interior of the feasible region since it is undefined at active constraints and infeasible points. Hence, separate logic for adjusting the step size is necessary to maintain feasibility. In contrast, the proposed barrier-penalty function allows us to address a more general class of problems since it does not need to remain in the strict interior of the feasibility region. This is an important advantage for soft constrained formulations where violations are inevitable due to noisy outputs. Moreover, the form of the barrier-penalty function allows considering nonconvex inequality constraints as well.

It is well known that exact penalty function approaches have difficulties with convergence due to discontinuity of the derivatives. In this paper, we deal with this difficulty through a smoothing approach and develop a *logarithmic-linear barrier–penalty function* that guarantees continuous derivatives and automatically pushes the solution back to the feasible region.

The paper is organized as follows. Section 2 formulates the optimization problem and introduces the concepts of NCO tracking, barrier and exact penalty functions. The features of a combined barrier-penalty function are discussed in Section 3, and its suitability for NCO tracking is investigated in Section 4. The proposed methodology is illustrated in simulation on a CSTR example in Section 5, and Section 6 concludes the paper.

2. Optimization problem formulation

The *static* optimization problem considered in this paper can be formulated in reduced form as follows:

$$\min_{u} \quad \phi(u) \tag{1}$$

such that

$$S(u) \leq 0 \tag{2}$$

where ϕ is the smooth scalar cost function to be minimized, u the n_u-dimensional vector of inputs, and S is the n_s-dimensional vector of inequality constraints. We assume that the inputs are mapped smoothly into the outputs, the objective and the constraint functions. A sufficient condition for this is that the (eliminated) state and output equations, $f(x, u) = 0$, $y = g(x, u)$, which map the manipulated variables to the state and output variables form a smooth injective mapping. As a result, we assume that the matrix $\partial f(x, u)/\partial x$ is nonsingular for all x and u.

The NCOs for problems (1) and (2) read:

$$\frac{\partial \phi}{\partial u} + \mu^{\mathrm{T}} \frac{\partial S}{\partial u} = 0 \tag{3}$$

$$\mu^{\mathrm{T}} S = 0, \quad S \leq 0, \quad \mu \geq 0 \tag{4}$$

where μ are the n_s-dimensional Lagrange multipliers for the constraints. Let us introduce the following standard assumptions:

Assumption 1. Optimization problem (1) and (2) has a solution that satisfies the NCO (3) and (4). Let $\mathcal{A}$ be the set of active constraints, i.e. $\mathcal{A} = \{j | S_j(u^*) = 0\}$. In addition, at the solution (u^*, μ^*), we assume:

- The gradients of the active constraints are linearly independent, which implies that μ^* are bounded and unique.
- μ^* are strictly complementary, i.e. $\mu_j^* S_j(u^*) = 0$ implies $\mu_j^* - S_j(u^*) > 0 \ \forall j$. This property is needed for regularity of the Karush-Kuhn-Tucker system.
- The second-order sufficient conditions are satisfied, i.e. $(\partial^2\phi(u^*)/\partial u^2) + \sum_j \mu_j^* (\partial^2 S_j(u^*)/\partial u^2)$ is positive definite in all allowable directions p such that $(\partial S_j/\partial u)p = 0, \forall j \in \mathcal{A}$.

2.1. Optimization via NCO tracking

Measurement-based optimization via NCO tracking enforces the necessary conditions of optimality (3) and (4) using measurements. As shown in François et al. (2002, 2005), one first determines the set of active constraints $\bar{S}$. The inputs are then partitioned into (i) the constraint-seeking inputs $\bar{u}$ and (ii) the sensitivity-seeking inputs $\tilde{u}$. The $\tilde{u}$ correspond to input directions that have no influence on the active constraints, i.e. $\partial\bar{S}/\partial\tilde{u} = 0$, and $\bar{u}$ are orthogonal to $\tilde{u}$. Hence, the NCO can be written as:

$$\bar{S} = 0 \tag{5}$$

$$\frac{\partial \phi}{\partial \tilde{u}} = 0 \tag{6}$$

$$\frac{\partial \phi}{\partial \bar{u}} + \mu^{\mathrm{T}} \frac{\partial \bar{S}}{\partial \bar{u}} = 0 \tag{7}$$

Condition (5) indicates that the active constraints should be kept active in the presence of perturbation using the constraint-seeking inputs $\bar{u}$. Condition (6) deals with the adaptation of $\tilde{u}$ to push the sensitivities to zero. Note that $\partial\phi/\partial\tilde{u}$ corresponds to the reduced gradient of ϕ. Condition (7) is less important since it is only there to determine the Lagrange multipliers μ, which are not needed in the NCO-tracking scheme. The main assumption for this NCO-tracking scheme to work is that the set of active constraints is known a priori for the real process and does not change with perturbations.

We note that partitioning the inputs into these two sets is not always straightforward, especially as the active set of constraints changes. In the next section, we see that the barrier-penalty approach eliminates the need for this partitioning.