Optimally Invariant Variable Combinations for Nonlinear Systems

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Abstract: In this article we present an "explicit RTO" approach for achieving optimal steady state operation without requiring expensive online calculations. After identifying regions of constant active constraints, it is shown that there exist some optimally invariant variable combination for each region. If the unknown variables can be eliminated by measurements and system equations, the invariant combinations can be used for control. Moreover, we show that the measurement invariants can be used for detecting changes in the active set and for finding the right region to switch to. This explicit RTO approach is applied to a CSTR described by a set of rational equations. We show how the invariant variable combinations are derived, and use polynomial reduction to eliminate the unknown variables to obtain the measurement invariants which are used for control.

Keywords: Optimizing control, Polynomial systems, Real-time optimization, Explicit RTO, Self-optimizing control, Optimally invariant measurement combinations, Changing active sets

1. INTRODUCTION

Optimal operation of chemical processes becomes increasingly important in order to be able to compete in the international markets and to minimize environmental impact. A well established tool to achieve this goal is real-time optimization (RTO), where the optimal set-points are computed on-line, based on measurements taken at given sample times. This involves setting up and maintaining a real-time computation system, which can be very expensive and time consuming.

An alternative approach is to use off-line calculations and analysis to minimize or avoid complex on-line computations for example by finding optimally invariant measurement combinations ('self-optimizing' variable combinations, (Narasimhan and Skogestad (2007)). Controlling these combinations to their setpoints guarantees to operate the process optimal or close to optimal, with a certain acceptable loss (Skogestad (2000)). The combinations can be controlled by a simple control structure based on PI controllers. The conventional real-time optimization problem can either be replaced completely or partially by controlling invariant variable combinations. In practice, many processes are operated by something similar to this alternative approach, although not always consciously. That is, the optimization problem is not formulated explicitly and the control variables are chosen from experience and engineering intuition.

This publication presents two main results. The first one is extending the idea of self-optimizing control from unconstrained linear problems to constrained nonlinear problems. To the authors knowledge, optimally invariant variable combinations have been considered systematically only for linear plants with quadratic performance index (see e.g. Alstad et al. (2009)). A second contribution is the proof that using controlled variable to identify new sets of active constraints will always identify the correct active set. Although measurement invariants have been used before for active set identification (Manum et al. (2007)), it has not been proved that this holds for nonlinear problems, too.

2. GENERAL PROCEDURE

We consider a plant at steady state and assume the plant performance can be modelled as an optimization problem with a performance index J together with equality and inequality constraints, $g(\mathbf{u},\mathbf{x},\mathbf{d})$ and $h(\mathbf{u},\mathbf{x},\mathbf{d})$:

$$\min_{\mathbf{u},\mathbf{x}} J \quad \text{s.t} \quad \begin{cases} g(\mathbf{u},\mathbf{x},\mathbf{d}) = 0 \\ h(\mathbf{u},\mathbf{x},\mathbf{d}) \leq 0 \end{cases} \tag{1}$$

The variables $\mathbf{u}$, $\mathbf{x}$, $\mathbf{d}$ denote the manipulated input variables, the internal states, and the disturbance variables, respectively. In addition, we assume that there are measurements $\mathbf{y}(\mathbf{x},\mathbf{u},\mathbf{d})$, which provide information about the internal states and the disturbances of the process.

In order to obtain optimal operation we do not optimize the model on-line at given sample times. Instead, we use the structure of the problem to find optimally invariant variable combinations for the system. Since the available number of degrees of freedom changes when an inequality constraint becomes active, we have to find a new set of invariant measurement combinations for each set of constraints that becomes active during operation of the plant. This makes it necessary to define separate control structures for each region. Therefore, the first step is to partition the operating space into regions defined by the set of active constraints, i.e. the system is optimized for all possible disturbances $\mathbf{d}$ and the active constraints in each region are identified.

In the second step, we determine (nonlinear) variable combinations which yield optimal operation when kept at their constant setpoint. The variables resulting from this step cannot be used for control directly, because they contain unknown disturbance variables and internal states which are not known. To be able to control the system, we attempt to "model" the variable invariants by expressions which only contain known variables. These can then be used for control in feedback loops.

The last step in this procedure is to define rules for detecting and switching regions when the active constraints change. In many cases this can be done by monitoring the controlled variables of the neighbouring region and switching when the controlled variable of the neighbouring region reaches its optimal value.

3. DETERMINING INVARIANT VARIABLE COMBINATIONS

3.1 Invariants for systems with quadratic objective and linear inequality constraints and linear measurements

To illustrate the idea of finding invariant variable combinations we first consider a problem with a quadratic objective and linear constraints. After having identified n_r regions of active constraints, we can define an equality constrained optimization problem for each region.

Given $\mathbf{z} \in \mathbb{R}^{n_z \times 1}$ and $\mathbf{d} \in \mathbb{R}^{n_d \times 1}$, consider the constrained optimization problem:

$$\min_{\mathbf{z}} J = \min_{\mathbf{z}} [\mathbf{z}^{\mathbf{T}}\, \mathbf{d}^{\mathbf{T}}] \begin{bmatrix} \mathbf{J_{zz}} & \mathbf{J_{zd}} \\ \mathbf{J_{zd}}^{\mathbf{T}} & \mathbf{J_{dd}} \end{bmatrix} \begin{bmatrix} \mathbf{z} \\ \mathbf{d} \end{bmatrix} \tag{2}$$

subject to

$$\mathbf{A}_z \mathbf{z} + \mathbf{A}_d \mathbf{d} = \tilde{\mathbf{A}} \begin{bmatrix} \mathbf{z} \\ \mathbf{d} \end{bmatrix} = 0 \tag{3}$$

where we have $\mathbf{A}_z \in \mathbb{R}^{n_c \times n_z}$ has rank n_c, $\mathbf{A}_d \in \mathbb{R}^{n_c \times n_d}$, $\tilde{\mathbf{A}} = [\mathbf{A}_z\, \mathbf{A}_d]$, and $\mathbf{J_{zz}} > 0$.

Eq. (3) may include the model equations as well as active (equality) constraints. Instead of using (3) to eliminate n_c internal states to obtain an unconstrained problem, we keep the constraints explicit in the formulation as this more general formulation will be used later when presenting the nonlinear case (where the internal states are not easily substituted). The Karush-Kuhn-Tucker first order optimality conditions give

$$\nabla_z L = \nabla_z J + \mathbf{A}_z^{\mathbf{T}} \lambda = \tilde{J} \begin{bmatrix} \mathbf{z} \\ \mathbf{d} \end{bmatrix} + \mathbf{A}_z^{\mathbf{T}} \lambda = 0, \tag{4}$$

where $\tilde{J} = [\mathbf{J_{uu}}\, \mathbf{J_{ud}}]$, and λ is the vector of Lagrangian multipliers. Therefore, from (4) we have that

$$\mathbf{A}_z^{\mathbf{T}} \lambda = -\tilde{J} \begin{bmatrix} \mathbf{z} \\ \mathbf{d} \end{bmatrix}. \tag{5}$$

$\mathbf{A}_z$ is not full column rank, so let $\mathbf{N}_z$ be a basis for the null space of $\mathbf{A}_z$ with dimension $n_{DOF} = n_z - n_c$. Then $\mathbf{N}_z^{\mathbf{T}} \mathbf{A}_z^{\mathbf{T}} = 0$, and at the optimum we must have

$$\mathbf{c}^v(\mathbf{z}, \mathbf{d}) \triangleq \mathbf{N}_z^{\mathbf{T}} \tilde{J} \begin{bmatrix} \mathbf{z} \\ \mathbf{d} \end{bmatrix} = 0 \tag{6}$$

for the system (5) to be uniquely solvable for λ. Keeping $\mathbf{c}^v(\mathbf{z}, \mathbf{d})$ at zero (in addition to the active constraints), is always optimal. However, it cannot be used for control directly, as it contains unknown (unmeasured) variables. For control, we need a function of measurements $\mathbf{c}(\mathbf{y})$, such that the difference between the invariant and the measurement combination is minimal. Here, we want to "model" $\mathbf{c}^v(\mathbf{z}, \mathbf{d})$ perfectly, such that

$$\mathbf{c}(\mathbf{y}) = \mathbf{c}^v(\mathbf{z}, \mathbf{d}). \tag{7}$$

Then controlling $\mathbf{c}(\mathbf{y}) = 0$ yields optimal operation. If we have $n_z + n_d$ independent linear measurements

$$y = \mathbf{G}^y \begin{bmatrix} \mathbf{z} \\ \mathbf{d} \end{bmatrix}, \tag{8}$$

where $\mathbf{G}^y$ is invertible, we can use them with (6) to give

$$\mathbf{c}(\mathbf{y}) = \mathbf{N}^{\mathbf{T}} \tilde{J} [\mathbf{G}^y]^{-1} \mathbf{y}. \tag{9}$$

However, note that we actually only need $n_z - n_c + n_d = n_{DOF} + n_d$ measurements, since the model equations (3) can be used to eliminate the constrained degrees of freedom (internal states). This is shown in Appendix A.

Remark 1. In the unconstrained case, the optimal invariant variable combination is simply the gradient, such that we have $\mathbf{c}(\mathbf{y}) = \mathbf{H}\mathbf{y} = \nabla_u J$, and $\mathbf{H} = \tilde{J}[\tilde{\mathbf{G}}^y]^{-1}$.

3.2 Invariants for polynomial and rational systems

An analog approach may be taken for obtaining invariant variable combinations for more general systems described by polynomials. Since rational equations can be transformed into polynomials by multiplying with the common denominator, the method is applicable to rational systems, too.

Initially, all regions defined by constant active constraints are determined. For each region we then have:

Theorem 1. (Nonlinear invariants). Given $\mathbf{z}, \mathbf{d}$ as in section 3.1, consider the nonlinear optimization problem

$$\min_{\mathbf{z}} J(\mathbf{z}, \mathbf{d}) \quad \text{s.t} \quad g_i(\mathbf{z}, \mathbf{d}) = 0, \quad i = 1 \ldots n_g, \tag{10}$$

and implicit measurement relations

$$m_j(\mathbf{y}, \mathbf{z}, \mathbf{d}) = 0 \quad j = 1 \ldots n_y, \tag{11}$$

where $\mathbf{y}$ is the measured variable. If the Jacobian $\mathbf{A}_z(\mathbf{z}, \mathbf{d}) = [\nabla_z g]$ has full rank n_g at the optimum throughout the region, following holds:

(1) There exist $n_{DOF} = n_z - n_g$ independent invariant variable combinations $\mathbf{c}^v$ with

$$\mathbf{c}^v = [\mathbf{N}_z(\mathbf{z}, \mathbf{d})]^{\mathbf{T}} \nabla_z J(\mathbf{z}, \mathbf{d}), \tag{12}$$

where $\mathbf{N}_z(\mathbf{z}, \mathbf{d})$ denotes the null space of the Jacobian of the active constraints $g(\mathbf{z}, \mathbf{d})$.

(2) If there exist polynomials $\alpha_i(\mathbf{z}, \mathbf{d})$ and $\beta_j(\mathbf{z}, \mathbf{d})$, such that element of $\mathbf{c}^v$ can be expressed by

$$c^v = \sum_{i,j} (\alpha_i(\mathbf{z}, \mathbf{d}) g_i(\mathbf{z}, \mathbf{d}) + \beta_j(\mathbf{z}, \mathbf{d}) m_j(\mathbf{y}, \mathbf{z}, \mathbf{d})) + c(\mathbf{y}), \tag{13}$$

then the term $c(\mathbf{y})$ is the desired self-optimizing variable which when controlled to zero yields optimal operation.

Proof. Calculate the Jacobian of the constraints:

$$\mathbf{A}_z(\mathbf{z}, \mathbf{d}) = \left[\, [\nabla_z g_1(\mathbf{z}, \mathbf{d})]^{\mathbf{T}}, \,\cdots\,, \,[\nabla_z g_{n_g}(\mathbf{z}, \mathbf{d})]^{\mathbf{T}} \,\right]^{\mathbf{T}} \tag{14}$$