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A Formulation for Globally Optimal Controlled Variable Selection

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***Abstract*—Self-optimizing control (SOC) is a powerful tool to select controlled variables (CVs) so that when these variables are maintained at constant set-points, the entire process operation is automatically optimal or near optimal (self-optimizing) in spite of the presence of various uncertainties. Over a decade development, many SOC theories and methods have been developed to select optimal CVs. However, all these methods are based on local linearization of the process model at a nominally optimal operating point, hence referred to as local methods.**

Due to the nature of locality, existing SOC methods may cause a large performance loss when the feasible operation region is large and the process is highly nonlinear. In this paper, we propose a global approach to select optimal CVs for nonlinear processes so that the average loss over the entire feasible operation region is minimized. Firstly, the globally average loss minimization problem is formulated and a toy example is solved analytically to explain the difference between the global approach and other local methods. For more complex processes where an analytical solution is not tractable, a numerical approach is proposed to minimize the average loss globally. In the new approach, optimal CV selection is found by solving a regression problem to approximate the necessary conditions of optimality of the objective function. A case study on an exothermic reactor demonstrates the effectiveness of the new approach.

I. Introduction

Traditionally, CVs are selected from a list of available or inferred measurements based on heuristic experiences and understanding of the whole process from an engineering perspective. For example, the variables related to safety regulations and product qualities usually need to be actively controlled and they are naturally chosen as CVs, thus consuming most of the process degrees of freedom (DOF). In many cases, these active constraints will dominate the process operation. However, for processes with extra DOF more than active constraints, self-optimizing control (SOC) [1] showed that the remain DOF can be used for optimization purpose by selecting appropriate CVs. When the selected CVs are maintained at predetermined constant set-points, the entire process operation is automatically optimal or near optimal (self-optimizing) in spite of the presence of various uncertainties, disturbances and measurement errors.

Over a decade development, many SOC theories and methods have been developed to select optimal CVs. Halvorsen et al. [2] derived simple singular value rule and local exact method for CV selection. Recent works have been engaged in finding proper combination matrix H of measurements as CVs to reduce the economic cost. Kariwala [3] minimized the local worst-case loss via singular value and eigenvalue decompositions. Later Kariwala et al. [4] derived optimal H with average loss minimization. Alstad and Skogestad [5] presented a null space method to minimize the loss caused by disturbances. Furthermore, Alstad et al. [6] extended null space method using extra measurements to minimize the loss caused by implementation error. Hori and Skogestad [7] compared maximum gain rule and local exact method and found the former one should be used with care for ill-conditioned plants. All these SOC methods were derived based on linearization of the process model around a normally optimal operating point, hence are referred to as local methods. This means the CVs selected by using these methods may only be optimal in a small neighborhood around the nominal point.

To address the locality issue, this paper aims to select CVs for nonlinear processes to be globally optimal by minimizing the average loss across the entire operation region. The remaining of this paper is organized as follows: Section II briefly reviews the local SOC methods, and Section III presents the formulation of globally average loss minimization problem for CV selection, together with a toy example to explain the difference between the global approach and existing local approaches. In Section IV, a CV selection procedure through regression for more general processes is proposed. The effectiveness of proposed solution is further demonstrated through an exothermic reactor case study in Section V. Finally, Section VI concludes the work together with some suggestions for future works.

II. A Brief Review of Local Methods based Self-Optimizing Control

Consider a generalized static optimization problem for continuous processes, which is given as

$$\begin{aligned} &\min_{u} J(u,d) \\ &\text{s.t. } g(u,d) \leq 0 \end{aligned} \tag{1}$$

with available measurements

$$y = f(u,d) \tag{2}$$

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where J is the scalar objective function; $u \in \mathbb{R}^{n_u}$, $d \in \mathbb{R}^{n_d}$ and $y \in \mathbb{R}^{n_y}$ are manipulated, disturbance and measurement variables, respectively; $g : \mathbb{R}^{n_u \times n_d} \Rightarrow \mathbb{R}^{n_g}$ and $f : \mathbb{R}^{n_u \times n_d} \Rightarrow \mathbb{R}^{n_y}$ are the operational constraints and measurement equations, respectively.

Let c represent the CVs with set-points at c_s. SOC [1] demonstrated that if c are properly selected, then when these variables are perfectly maintained at their optimal values, $c_s = c_{opt}(d)$ in the presence of disturbance, d, manipulated variables, u will approach to their optimal values $u_{opt}(d)$ through feedback control without re-optimizing c_s. To select CV properly, let measurements y at the nominal point be linearized as

$$y = G_y u + G_{yd} W_d d + W_n n \tag{3}$$

where G_y and G_{yd} are the steady state gain matrices of y with respect to u and d, respectively; n is the implementation error due to measurement noise and/or control errors associated with individual measurement; W_d and W_n are diagonal matrices representing magnitudes of d and n respectively.

The selected CVs as linear combinations of full measurements set y can be represented as

$$c = Hy \tag{4}$$

where H is the combination matrix with full row rank of n_u to square the control system. Especially, zero columns in H imply a subset of full y is unused. The worst case loss [2] and the average loss [4] in objective function due to maintaining CVs at constant set-points for uniformly distributed d and n are given in (5) and (6), respectively.

$$L_{\mathrm{wc}} = \frac{1}{2}\sigma^2_{\max}(M) \tag{5}$$

$$L_{\mathrm{av}} = \frac{1}{6(n_d + n_y)}\|M\|^2_F \tag{6}$$

where $\sigma_{\max}(\cdot)$ and $\|\cdot\|_F$ are the maximum singular value and Frobenius norm of a matrix respectively; $M = \left[J_{uu}^{1/2}\left(J_{uu}^{-1}J_{ud} - G^{-1}G_d\right)W_d \quad J_{uu}^{1/2}G^{-1}HW_n\right]$ with $G = HG_y$ and $G_d = HG_{yd}$. Here, $J_{uu} = \partial^2 J/\partial u^2$ and $J_{ud} = \partial^2 J/(\partial u \partial d)$ are the diagonal and off-diagonal Hessian matrices of J evaluated at the nominal point.

CV selection is then characterized as minimizing (5) or (6) with respect to H. Recently, several explicit expressions for H have been reported [5], [3], [4], [6]. For example, if $n_y = n_u + n_d$, the combination matrix H according to null space method proposed by Alstad and coworkers [5], [6] can be selected as

$$H = \left[J_{uu}^{1/2} \quad J_{uu}^{-1/2}J_{ud}\right]\left[G_y \quad G_{yd}\right]^{-1} \tag{7}$$

III. Selection of Globally Optimal Controlled Variables

A. Formulation

In the existing SOC theory, the CV selection problem is solved by assuming measurements in (2) are linearized in (3). This assumption restricts the solution to be local. To avoid this locality, the linear model assumption is discarded in the new global formulation to be presented below. Furthermore, in general, CVs can be either linear (as shown in (4)) or nonlinear combinations of all or a subset of available measurements. Therefore, in this work, the CVs are parameterized by $w \in \mathbb{R}^{n_w}$ as follows.

$$c = \phi(y, w) \tag{8}$$

For simplicity but without loss of generality, it is assumed that $c_s = 0$.

Let the entire operating range defined by the disturbance $d \in \mathcal{D}$ and all possible measurement noise represented by $n \in \mathcal{N}$. It is assumed that d and n are statistically independent. The minimum cost of the optimization problem in (1) is a function of d, $J_{\mathrm{opt}}(d)$, while the actual cost when $c = 0$ is a function of d and n denoted as $J_w(d, n)$. Then, the operation loss in terms of the cost function for $c = 0$ with specific d and n is $L_w(d, n) = J_w(d, n) - J_{\mathrm{opt}}(d)$, whilst the average loss across the entire operation range is a function of design parameters, w as follows.

$$L_{\mathrm{gav}}(w) = E[L_w(d, n)] \tag{9}$$

$$= \int_{n\in\mathcal{N}, d\in\mathcal{D}} \rho(d)\rho(n)L_w(d, n)\mathrm{d}n\mathrm{d}d \tag{10}$$

where $E[\cdot]$ and $\rho(\cdot)$ represent the expected value and the probability density of a random variable, respectively.

Then, the globally optimal CVs can be selected by designing w to solve the following optimization problem

$$\begin{aligned} \min_{w}\ & L_{\mathrm{gav}}(w) \\ \text{s.t. } & y = f(u, d) + n \\ & 0 = \phi(w, y) \\ & d \in \mathcal{D} \\ & n \in \mathcal{N} \end{aligned} \tag{11}$$

The optimization problem in (11) is generally suitable for various $\mathcal{D}$, $\mathcal{N}$ and nonlinear combination, ϕ.

It was shown in [8] that local SOC methods essentially capture necessary conditions of optimality (NCO) locally at the nominal point with a straight line as CV. The aim of this work is to search other curves as CVs, which have better average performance across the whole region. The differences of these methods are illustrated in Figure 1, where c_{loc} is the CV obtained by local SOC method, c_{gav} is the globally optimal CV. As shown in Figure 1(a), the vertical axis is the NCO value when $c = 0$, where the desired value is 0. The curve of NCO for c_{loc} can only be maintained at the nominal point, $d = d^\star$, whereas the deviation goes large as the operation point drifts far away from the nominal point. The curve of NCO for c_{gav} approaches the zero line more closely in an average sense to minimize the overall loss, which can be quantified by the area surrounded by the curve of L and d axis in the disturbance range $[\underline{d}, \bar{d}]$, as shown in Figure 1(b).

From Figure 1, it is clear that the price to gain better average performance across the entire region is the slightly increased loss around the nominal operating point. To help understanding

of the general formulation, a toy example is to be solved as follows.

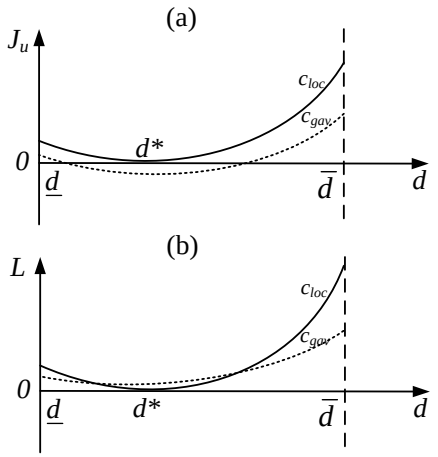

Fig. 1. Comparison of local SOC and globally optimal CV: (a) NCO against d; (b) Loss function L against d

B. A toy example

To illustrate the proposed new framework for globally optimal CVs selection, consider a problem to minimize the objective function

$$J = \frac{1}{2}(u-d)^2 \tag{12}$$

where both u and d are scalars. Two measurements are available as follows.

$$y_1 = u \tag{13}$$

$$y_2 = \frac{1}{4}u^2 + d \tag{14}$$

The nominal disturbance is $d^* = 0$. Correspondingly, the optimal point is then defined by $u^* = 0$, where $J^* = 0$, $y_1^* = 0$ and $y_2^* = 0$. The possible variation of d is uniformly distributed between -1 and 1, *i.e.* $d \in \begin{bmatrix}-1 & 1\end{bmatrix}$.

It is clear that $u_{\text{opt}}(d) = d$ and correspondingly, $J_{\text{opt}}(d) = 0$. Therefore, for a non-optimal input, u, the loss, $L(u,d) = J(u,d) - J_{\text{opt}}(d) = J(u,d)$.

Firstly, the local SOC approach of null space method proposed in [5], [6] is applied to the problem. Since, $J_{uu} = 1$, $J_{ud} = -1$, $G_y = \begin{bmatrix}1 & 0\end{bmatrix}^T$ and $G_{yd} = \begin{bmatrix}0 & 1\end{bmatrix}^T$, the local optimal CV is then obtained using (7), which also minimizes the average loss locally for this problem[4]

$$c_{\text{lav}} = y_1 - y_2 \tag{15}$$

To maintain $c_{\text{lav}} = 0$ through feedback, the corresponding input has two solutions. The one satisfies the nominal operating condition, $u^* = 0$ is

$$u_{\text{lav}} = 2 - 2\sqrt{1-d} \tag{16}$$

Accordingly, the loss is then

$$L_{\text{lav}}(d) = \frac{1}{2}(2 - 2\sqrt{1-d} - d)^2$$

Hence, the expectation of the loss over the entire range is

$$E[L_{\text{lav}}(d)] = \frac{1}{2}\int_{-1}^{1}\frac{1}{2}\left[8(1-d) + d^2 - 4(2-d)\sqrt{1-d}\right]\mathrm{d}d = 0.0183$$

Next, the global CV selection problem in (11) is to be solved for the toy example. For simplicity, consider the CV to be a linear combination of measurements. It can be parameterized as

$$c_{\text{gav}} = \phi(w,y) = y_1 + w_1 y_2 + w_2 \tag{17}$$

When $c_{\text{gav}} = 0$, the corresponding input, which is most close to $u^* = 0$ is

$$u_{\text{gav}} = \frac{2}{w_1}\left(-1 + \sqrt{1 - w_1(w_2 + dw_1)}\right) \tag{18}$$

Inserting (18) into (10) and solve it for optimization problem (11), we obtain the following results using Matlab Symbolic Math and Optimization Toolboxes:

$$w_1 = -0.9231$$
$$w_2 = 0.0705$$

with the minimized average loss

$$\min_w L_{\text{gav}}(w) = 0.00278 \tag{19}$$

The result shows that the minimum global loss is much less than the local counterpart even though CVs of both methods are linear with the same number of parameters. The globally optimal linear CV is

$$c_{\text{gav}} = y_1 - 0.9231 y_2 + 0.0705 \tag{20}$$

which minimizes the average loss over the entire disturbance space.

IV. A Regression Approach for Globally Optimal CV Selection

The toy example is solved analytically through finding the relationships between the loss expectation $E[L]$ and the CV parameters, w. However, finding analytical solution may not be tractable for general self-optimizing control problems. Therefore, it is necessary to develop a numerically effective approach to solve the globally optimal CV selection problem. In the following, we propose a regression approach to approximate the NCO of the optimization problem using CVs so that when these CVs are perfectly controlled at zero, the loss is proportional to the regression error. More specifically, let u_w the control input corresponding to $c_w = \phi(w,y,n) = 0$. Then, the cost function $J(u,d)$ at a specific d can be represented as the Taylor expansion around u_w,

$$J(u,d) = J_w + \eta_w^T \Delta u + 0.5\Delta u^T S_w \Delta u \tag{21}$$

where $\Delta u = u - u_w$, $J_w = J(u_w, d)$,

$$\eta_w = \left.\frac{\partial J(u,d)}{\partial u}\right|_{u=u_w} \tag{22}$$

and

$$S_w = \left.\frac{\partial \eta(u,d)}{\partial u}\right|_{u=u_w} \tag{23}$$

The gradient function can also be expanded similarly.

$$\eta(u,d) = \eta_w + S_w \Delta u \tag{24}$$

At the optimal point, $u_{\text{opt}}(d)$, the above expansion becomes

$$J(u_{\text{opt}},d) = J_w + \eta_w^T \Delta u_{\text{opt}} + 0.5 \Delta u_{\text{opt}}^T S_w \Delta u_{\text{opt}} \tag{25}$$

where $\Delta u_{\text{opt}} = u_{\text{opt}} - u_w$. Equivalently,

$$\begin{aligned} L_w(d,n) &= J_w - J(u_{\text{opt}},d) \\ &= -\eta_w^T \Delta u_{\text{opt}} - 0.5 \Delta u_{\text{opt}}^T S_w \Delta u_{\text{opt}} \end{aligned} \tag{26}$$

Furthermore, at the optimal point, the NCO is

$$\eta(u_{\text{opt}},d) = \eta_w + S_w \Delta u_{\text{opt}} = 0$$

Therefore,

$$\Delta u_{\text{opt}} = -S_w^{-1} \eta_w \tag{27}$$

This leads to

$$L_w(d,n) = 0.5 \eta_w^T S_w^{-1} \eta_w \tag{28}$$

Note, a similar result on the loss has been derived in [9], however, for local loss around the nominally optimal point, whilst the result derived in (28) is globally valid.

Although loss derived in (28) can be directly used in (9) for global CV selection, the requirement of S_w at each d and n is prohibitive. However, if CVs are represented as a summation of the NCO and an approximation error as follows,

$$c_w = \eta_w - \epsilon_w \tag{29}$$

then the approximation error, $\epsilon_w = \eta_w$ because $c_w = 0$ is perfectly controlled. Therefore, an upper bound of the global loss can be derived using the approximation error,

$$L_w(d,n) \le 0.5 M \|\epsilon_w\|_2^2 \tag{30}$$

where

$$M = \max_{d \in \mathcal{D}, n \in \mathcal{N}} \bar{\lambda}(S_w) \tag{31}$$

with $\bar{\lambda}(\cdot)$ denoting the maximum eigenvalue of a matrix.

To simplify the optimization problem in (11) further, the continuous operating region specified by $\mathcal{D}$ and $\mathcal{N}$ is discretized in N sampling points, $d_i \in \mathcal{D}$ and $n_i \in \mathcal{N}$ for $i = 1, \ldots, N$. To avoid solving the perfect CV control equation, $\phi(w,y) = 0$, u is also sampled at N points within a feasible range, $\underline{u} \le u_i \le \bar{u}$, accordingly. With these three independent variable samples, the gradient, $\eta_i = \eta(u_i, d_i)$, $y_i = y(u_i, d_i) + n_i$ can be calculated from the process model. Then the following regression problem is to be solved in order to determine the optimal CV parameters,

$$\min_w \frac{1}{2} (\phi(w,y_i) - \eta_i)^T (\phi(w,y_i) - \eta_i) \tag{32}$$

This is a nonlinear least squares problem. The famous Levenberg-Marquardt algorithm [10] is available to solve this problem efficiently. Meanwhile, there are many nonlinear model structures are available in the literature as well, which can be adopted for $\phi(w,y)$, such as the polynomial and Gaussian kernel models. For simplicity, only linear regression is considered in the formulation bellow, for which an analytical solution can be derived.

The general form of linear $\phi(w,y)$ is given as follows.

$$c_w = Hy + b \tag{33}$$

with the parameter vector, $w = \begin{bmatrix} \text{vec}(H)^T & b^T \end{bmatrix}^T$, where $H \in \mathbb{R}^{n_u \times n_y}$, $b \in \mathbb{R}^{n_u}$ and $\text{vec}(\cdot)$ represents a matrix to be arranged in a vector.

Using the linear combination CVs given in (33), n_u CVs can be calculated independently for each CV to approximate one of elements in the gradient vector, η. Therefore, for simplicity, in the following development, it is assumed that $n_u = 1$.

Denote

$$\eta = \begin{bmatrix} \eta_1 & \cdots & \eta_N \end{bmatrix}^T \tag{34}$$

$$Y = \begin{bmatrix} y_1 & \cdots & y_N \\ 1 & \cdots & 1 \end{bmatrix}^T \tag{35}$$

$$w = \begin{bmatrix} H & b \end{bmatrix}^T \tag{36}$$

Then the regression problem (32) is equivalent to a linear regression problem

$$\varepsilon = \min_w \frac{1}{2} (Yw - \eta)^T (Yw - \eta) \tag{37}$$

The least squares solution to the problem can be analytically obtained as

$$w_{\text{opt}} = (Y^T Y)^{-1} Y^T \eta \tag{38}$$

The corresponding minimum total regression cost is

$$\varepsilon = \frac{1}{2} \eta^T (I - Y(Y^T Y)^{-1} Y^T) \eta \tag{39}$$

The corresponding global average loss by adopting this linear combination CV can be bounded by $L_{\text{gav}} \le M\varepsilon$. Note although above solution is derived for linear combinations as CV, it can be easily extended to polynomial form by expanding matrix Y with higher order terms, as illustrated in case studies below.

V. Case Studies

A. Toy example continued

Applying proposed regression method above, the variation ranges for u and d ($u, d \in \begin{bmatrix} -1 & 1 \end{bmatrix}$) are both discretized into 10 parts equally resulting total $N = 11^2 = 121$ sample points. At each sampling point, the measurements and gradient J_u are calculated, then we obtained the matrix Y and vector η. A linear LS regression is simply performed using (38), which results in the following CV

$$c_{w1} = y_1 - 0.9809 y_2 + 0.09809 \tag{40}$$

To calculate the average loss, the control input for c_w is found to be

$$u_{w1} = 2.039 - 2.0389\sqrt{1.0962 - 0.9621 d} \tag{41}$$

Inserting (41) into (12) and (10) to yield the expectation of loss calculated as

$$E[L_{w1}(d)] = 0.00375 \tag{42}$$

The average loss for c_{w1} has been significantly reduced as compared with local method and is only slightly bigger than optimal 0.00278, which is analytically searched in Section III. The convenience of proposed regression method is that it directly determines w via numerical approach, avoiding the requirement of representing input u in terms of d and w, which is inevitable and hard to access in analytical way. To demonstrate the powerful usage of proposed method, a second order polynomial regression is further performed by adding terms y_1y_2, y_1^2 and y_2^2 into Y, the CV is found to be

$$c_{w2} = y_1 - y_2 + 0y_1y_2 + 0.25y_1^2 + 0y_2^2 + 0 \tag{43}$$

The corresponding control input u_{w2} and the expected loss are interestingly found to be $u_{w2} = d$ and $\min_w L_{w2}(d) = 0$, respectively. It means that the process can achieve perfect self-optimizing control under any disturbance! Note, if we specify a quadratic form of $\phi(y, w)$ in the first place and solve it analytically, the solution process will be very complicated and almost prohibitive.

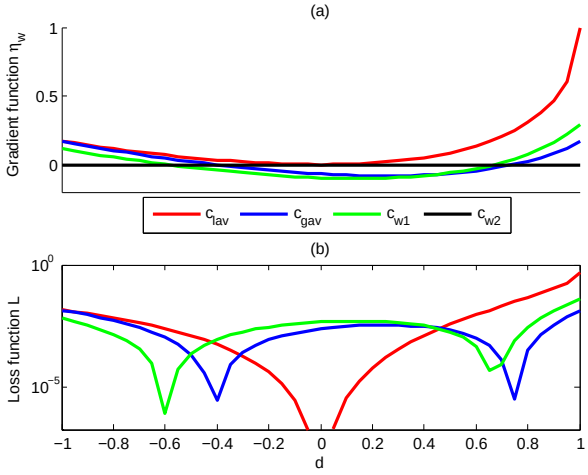

Fig. 2. Comparisons for different CVs for the toy example: (a) gradient function η_w against d; (b) Loss function L against d

Figure 2 (a) and (b) show the loss performances of various CVs when they are perfectly controlled at set-points 0. Compared with c_{lav}, globally optimal c_{gav} is able to steer the gradient η_w closer to 0 and minimize the loss over the entire disturbance range. c_{w1} is suboptimal but its shape is approximately similar to c_{gav}, hence the loss is only slightly bigger. Moreover, c_{w2} achieves perfect self-optimizing control and its curves overlap with desired 0 horizon line in the figures (not shown in semi-logarithmic plot (b)). Although for this problem c_{w2} can also be derived through arrangements for model equations by eliminating u and d, this may be hardly possible for other more complex problems, whereas regression method provides a very simple and efficient alternative, as illustrated in the reactor case study below.

B. Exothermic Reactor

Self-optimizing control for the exothermic reactor has been previously studied by several researchers [3], [9], [11]. The reactant A is fed into a continuous stirred-tank reactor (CSTR) and undergoes a reversible exothermic reaction in the CSTR. The inlet temperature, concentrations of A and product B in the feed are denoted as T_i, C_{Ai} and C_{Bi} respectively, the outlet temperature, concentrations of unreacted A and product B in the outlet stream are denoted as T, C_A and C_B respectively. The schematic of exothermic reactor process is shown in Figure 3.

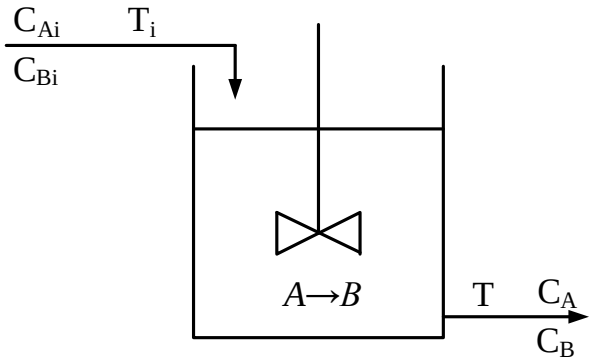

Fig. 3. Exothermic reactor process

The first principle models are composed of differential equations for mass and energy balances

$$\frac{\mathrm{d}C_A}{\mathrm{d}t} = \frac{1}{\tau}(C_{Ai} - C_A) - r \tag{44}$$

$$\frac{\mathrm{d}C_B}{\mathrm{d}t} = \frac{1}{\tau}(C_{Bi} - C_B) + r \tag{45}$$

$$\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{1}{\tau}(T - T_i) + 5r \tag{46}$$

where $\tau = 60$s is the residence time, and r is the rate of reaction which is dependent on process variables

$$r = 5000e^{-\frac{10000}{1.987T}}C_A - 10^5 e^{-\frac{15000}{1.987T}}C_B \tag{47}$$

The classifications for manipulated variable, available measured variables and disturbances are given as

$$u = \begin{bmatrix} T_i \end{bmatrix} \tag{48}$$

$$y = \begin{bmatrix} C_A & C_B & T & T_i \end{bmatrix}^T \tag{49}$$

$$d = \begin{bmatrix} C_{Ai} & C_{Bi} \end{bmatrix}^T \tag{50}$$

The anticipated noises for measured variables are ± 0.01 mol/L for concentrations C_A and C_B, ± 0.5K for temperatures T and T_i. The allowable sets for disturbances are considered as $0.5 \leq C_{Ai} \leq 1.5$ and $0 \leq C_{Bi} \leq 0.5$.

The operational objective of exothermic reactor process is to maximize the economic profit, which is equivalent to minimizing a cost function

$$J = -20090C_B + (0.1657T_i)^2 \tag{51}$$

where the first term of J is the negative profit of product B and the latter represents the cost of heating the input stream. The nominal values for process variables are given in Table 1. The operational degree of freedom for this case is 1, so only 1 CV is to be selected to square the control system.

TABLE I
PROCESS VARIABLES AND NOMINAL VALUES

Variable	Physical description	Nominal value	Unit
C_A	Outlet A concentration	0.498	$\mathrm{mol \cdot L^{-1}}$
C_B	Outlet B concentration	0.502	$\mathrm{mol \cdot L^{-1}}$
T	Outlet steam temperature	426.803	K
T_i	Inlet steam temperature	424.292	K
C_{Ai}	Inlet A concentration	1.0	$\mathrm{mol \cdot L^{-1}}$
C_{Bi}	Inlet B concentration	0	$\mathrm{mol \cdot L^{-1}}$
J	Economic objective	-5149.3	\$

For this example, an analytical CV solution to minimize the globally overall loss is not available. Alternatively, the regression approach is use to select the optimal CV. Samples for regression are collected as follows: the possible variation range of each independent variable (C_{Ai}, C_{Bi} and T_i) is discretized equally into 10 parts, therefore, 11^3 points of data are generated. Each point of data contains four measured variables and dJ/du, which is calculated using input perturbations and finite differences. The variation ranges for disturbances are defined earlier, the range for T_i is considered as $\begin{bmatrix}380\mathrm{K} & 450\mathrm{K}\end{bmatrix}$, which is determined from later observations that the majority of optimum u falls into this interval.

Least square regression is performed straightforward to get a combination model as CV with measurements as predictors. A linear and second order polynomial regression result in the following CVs,

$$c_1 = -772.2 - 184.3y_1 + 152.0y_2 - 7.4y_3 + 9.3y_4 \quad (52)$$

$$\begin{aligned} c_2 = {} & 1131.0 + 324.3y_1 - 1298.8y_2 - 105.5y_3 + 100.3y_4 \\ & + 12.0y_1y_2 - 44.7y_1y_3 + 43.3y_1y_4 + 15.6y_2y_3 \\ & - 12.0y_2y_4 + 81.2y_1^2 - 30.5y_2^2 + 3.4y_4^2 \end{aligned} \quad (53)$$

with an R^2 regression index of 0.9464 and 0.9997, respectively. As a comparison, the methods proposed by Kariwala et al. [4] to minimize average local loss and Alstad et al. [6] using extended null space method are also applied to current example. These CVs are

$$\begin{aligned} c_{\mathrm{Kariwala}} = {} & 0.76y_1 - 0.65y_2 - 6.58 \times 10^{-5}y_3 \\ & - 0.0051y_4 + 2.15 \end{aligned} \quad (54)$$

$$\begin{aligned} c_{\mathrm{Alstad}} = {} & -171.76y_1 + 145.23y_2 + 0.0083y_3 \\ & + 1.15y_4 - 479.18 \end{aligned} \quad (55)$$

A Monte Carlo experiment for 100 set of randomly generated disturbances within expected ranges is conducted and the results are shown in Table 2. The results in Table 2 show that self-optimizing performance can be significantly improved by using proposed method. Compared to c_{Kariwala} and c_{Alstad}, the average losses (11.57 and 10.21) are furthermore effectively reduced by c_1 and c_2 (3.07 and 0.0896) because proposed method minimize the loss globally in the entire operation region.

TABLE II
AVERAGE ECONOMIC LOSSES WITH DIFFERENT COMBINATION CV

CV	Average loss	Maximum loss	Standard deviation
c_1	3.07	15.39	3.26
c_2	0.0896	0.97	0.15
c_{Kariwala}	11.57	52.78	12.11
c_{Alstad}	10.21	71.33	14.76

VI. CONCLUSIONS

This paper presented a formulation for selecting CVs with globally average loss minimization in the context of SOC. A toy example is provided to illustrate the procedure of selecting globally optimal CVs for self-optimizing control. Compared with existing local SOC methods, which are only accurate in small neighborhood around the nominal point, new approach is advantageous that the global loss is minimized in an average sense. To circumvent the difficulty for solving the complicated and maybe non-convex optimization problem, a numerical solution is proposed alternatively to find optimal CVs, which is based on least squares regression to approximate the NCOs. The usage and effectiveness of the numerical method are demonstrated by the toy example and a more realistic exothermic reactor case study. The later shows that the loss over the entire operating range is significantly reduced comparing with the results obtained before using local SOC approaches.

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