

PROCESS DESIGN AND CONTROL

Optimal Selection of Controlled Variables[†]

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This paper considers the selection of controlled variables for the unconstrained degrees of freedom, such that near-optimal operation is achieved with constant setpoints (“self-optimizing control”). From a second-order Taylor approximation around the optimal point, we derive an exact local method. This may be used to find the optimal linear combination of measurements to use as controlled variables. We also derive the approximate singular value rule, which is very useful for quick screening and elimination of poor candidate variables.

1. Introduction

In this paper we consider optimal operation at steady state. The first step is to quantify the desired operation by defining a scalar cost function. The second step is to optimize the operation by minimizing the cost with respect to the available degrees of freedom. The third step, equally important in our view (but not considered to be an important issue by most people), is the actual *implementation* of the optimal policy in the plant by use of its control system. Obviously, from a purely mathematical point of view, it would be optimal to use a centralized online optimizing controller with a continuous update of its model parameters. However, for a number of reasons, we almost always decompose the control system into several layers, which in a chemical plant typically include scheduling (weeks), site-wide optimization (day), local optimization (hour), supervisory/predictive control (minutes), and regulatory control (seconds). In this paper we consider the interaction between the local optimization layer and the feedback control layer; see Figure 1. The two layers interact through the *controlled variables* c , whereby the optimizer computes their optimal setpoints c_s (typically, updating them about every hour), and the control layer attempts to implement them in practice, i.e., to get $c \approx c_s$. The issue to be considered in this paper is then the following: What variables c should we control? So far, very little theory has been available to analyze this important problem, and the objective of this paper is to study the problem from a local (linear) point of view.

Let us describe the issues in a little more detail. The setpoints c_s for the controlled variables c are kept constant between each update. However, this constant setpoint policy will, for example, because of disturbances d and implementation errors n , result in a loss, $L = J$

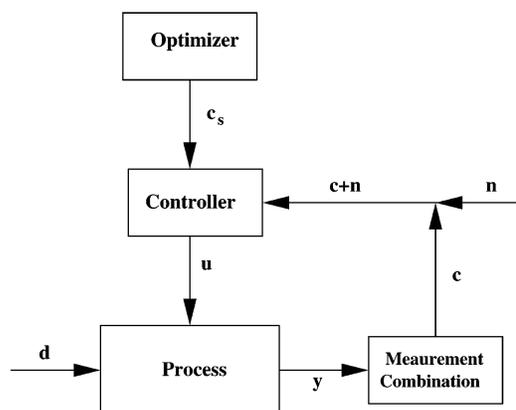


Figure 1. Hierarchical implementation with separate optimization and control layers. Self-optimizing control is when near-optimal operation is achieved with c_s constant.

– J_{opt} , when compared to the truly optimal operation. If this loss is acceptable, then we have a “self-optimizing” control system:

Self-optimizing control¹ is when we can achieve acceptable loss with constant setpoint values for the controlled variables (without the need to reoptimize when disturbances occur).

The term was selected because of its close relation to “self-regulating control”, which is when an acceptable dynamic performance can be achieved with no control (i.e., with constant manipulated variables). Correspondingly, “self-optimizing control” is when an acceptable economic performance can be achieved with no optimization (i.e., with constant setpoints c_s). The term self-optimizing control was used in an early paper by Kalman² to denote what is now called “optimal control”, but the term has hardly been used in this context since then.

We assume in this paper that the optimally active constraints are always enforced (implemented) and consider the implementation of the remaining unconstrained degrees of freedom. It is for such cases that the choice of controlled variables is an important issue, and Skogestad¹ presents three approaches for selecting controlled variables for self-optimizing control:

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Table 1. Summary of Important Notation

u	“base set” for the unconstrained degrees of freedom
d	disturbance variables (slow-varying)
$J(u, d)$	cost function to be minimized
$L = J - J_{\text{opt}}(d)$	loss
$u_{\text{opt}}(d)$	optimal value of u for given d
$e_u = u - u_{\text{opt}}(d)$	deviation from optimal u (that results in a positive loss)
$y = f_y(u, d)$	measured variables
$c = h(y) = f_c(u, d)$	selected controlled variables (function h free to select); $\dim(c) = \dim(u)$
$c_{\text{opt}}(d) = f_c[u_{\text{opt}}(d), d]$	linearized: $\Delta c = \mathbf{H}\Delta y = \mathbf{G}\Delta u + \mathbf{G}_d\Delta d$
$n = c - c_s$	optimal value of c for given d
$v = c_s - c_{\text{opt}}(d)$	implementation error
$e_c = c - c_{\text{opt}}(d) = v + n$	setpoint error
*	deviation from optimal c (resulting in loss)
	nominal operating point (normally assumed optimal)

1. Select variables c that satisfy certain properties that are derived below. The properties are useful for identifying candidate controlled variables but do not provide a quantitative means for selecting the best variables.

2. *Minimum singular value rule*: Select variables that maximize the minimum singular value of the appropriately scaled steady-state gain matrix \mathbf{G}' from inputs (u) to the selected controlled variables (c). This rule is derived below. It is not exact but very simple and often works surprisingly well. It is especially useful for eliminating poor candidates.

3. Exact method based on “brute-force” evaluation of the loss with alternative sets of controlled variables kept at their setpoints.

The last method is normally very expensive numerically. However, in this paper we derive an exact *local* method with a much smaller numerical load. Importantly, this local method may also be used to find the optimal measurement combination.

The reader is referred to ref 1 for references to related work on the selection of controlled variables. Of the earlier work, Morari et al.³ came closest to the ideas presented in this paper. Morari et al.³ considered a local second-order expansion of the cost but did not consider the expansion of the loss in terms of $e_c = c(d) - c_{\text{opt}}(d)$ (with a “moving” disturbance d), which is a key element in this paper. They also did not consider the implementation error.

Although our background is in process control and we make some references to this area, the issue of selecting controlled variables and the idea of self-optimizing control have applicability in most other fields of control, including biological systems.

2. Optimal Operation

2.1. Mathematical Formulation. The most important notation is summarized in Table 1. For simplicity, we do not in this paper include time as a variable; that is, we assume that the cost can be evaluated using a pseudo-steady-state assumption.³ We assume that the optimal operation of the system can be quantified in terms of a scalar cost function (performance index) J_0 , which is to be minimized with respect to the available degrees of freedom $u_0 \in R^{n_0}$

$$\min_{u_0} J_0(x, u_0, d) \quad (1)$$

subject to the constraints

$$g_1(x, u_0, d) = 0; \quad g_2(x, u_0, d) \leq 0 \quad (2)$$

Here $d \in R^{n_d}$ represents all of the disturbances, including exogenous changes that affect the system (e.g., a change in the feed), changes in the model (typically represented by changes in the function g_1), changes in the specifications (constraints), and changes in the parameters (prices) that enter in the cost function and the constraints. $x \in R^{n_x}$ represents the internal variables (states). The equality constraints ($g_1 = 0$) include the model equations, which give the relationship between the independent variables (u_0 and d) and the dependent variables (x). The system must generally satisfy several inequality constraints ($g_2 \leq 0$); for example, we usually require that selected variables are positive. The cost function J_0 is in many cases a simple linear function of the independent variables with prices as parameters. In many cases it is more natural to formulate the optimization problem as a maximization of the profit P , which may be formulated as a minimization problem by selecting $J_0 = -P$.

In most cases some of the inequality constraints are active (i.e., $g_2 = 0$) at the optimal solution. Implementation to achieve this is usually simple: We adjust the corresponding number of degrees of freedom u_0 such that these active constraints are satisfied (the possible errors in enforcing the constraints should be included as disturbances). In some cases this consumes all of the available degrees of freedom. For example, if the original problem is linear (a linear cost function with linear constraints g_1 and g_2), then it is well-known that from linear programming theory that there will be no remaining unconstrained variables. For nonlinear problems (e.g., g_1 is a nonlinear function), the optimal solution may be unconstrained, and such problems are the focus of this paper.

Because our considerations in this paper are of local nature, we assume that the set of active inequality constraints does not change with changing disturbances, and we consider the problem in reduced space in terms of the remaining unconstrained degrees of freedom (which we henceforth call u). We divide the original independent variables $u_0 = \{u', u\}$ in the “constrained” variables u' (used to satisfy the active constraints $g_2 = 0$) and the remaining unconstrained variables u . The value of u' is then a function of the remaining independent variables (u and d). Similarly, the states x are determined by the value of the remaining independent variables. Thus, by solving the model equations ($g_1 = 0$, and for the active constraints $g_2 = 0$), we may formally write $x = x(u, d)$ and $u' = u'(u, d)$ and we may formally write the cost as a function of u and d : $J = J_0(x, u_0, d) = J_0[x(u, d), \{u'(u, d), u\}, d] = J(u, d)$. The *remaining uncon-*

strained problem in reduced space then becomes

$$\min_u J(u, d) \quad (3)$$

where $u \in R^{n_u}$ represents the remaining unconstrained degrees of freedom. J is not generally a simple function in the variables u and d but rather a functional. This is the problem studied in this paper. For any value of the disturbances d , we can then solve the (remaining) unconstrained optimization problem (3) and obtain $u_{\text{opt}}(d)$, for which

$$\min_u J(u, d) = J[u_{\text{opt}}(d), d] \stackrel{\text{def}}{=} J_{\text{opt}}(d)$$

The solution of such problems has been studied extensively and is not the issue of this paper. In this paper the concern is implementation and how to handle variations in d in a simple manner.

2.2. Implementation of Optimal Operation: Obvious Approaches. In the following, we let d^* denote the nominal value of the disturbances. Let us first assume that the disturbance variables are constant, i.e., $d = d^*$. In this case implementation is simple: We keep u constant at $u_s = u_{\text{opt}}(d^*)$ (here u_s is the “setpoint” or desired value for u), and we will have optimal operation. (This assumes that we are able to achieve $u = u_s$, which may not be possible in practice because of an implementation error $n_u = u - u_s$.¹) However, what should we do if d changes? In this case $u_{\text{opt}}(d)$ changes and operation with a fixed value u_s is no longer optimal. Two “obvious” approaches from a mathematical point of view are as follows:

1. If we do not have any information on how the system behaves during actual operation or if it is not possible to adjust u once it has been selected, then the optimal policy is to find the best “average” value u_s for the expected disturbances, which would involve “backing off” from the nominally optimal setpoints by selecting u_s different from $u_{\text{opt}}(d^*)$. The solution to this problem is quite complex and depends on the expected disturbance scenario. For example, we may use stochastic optimization.⁴ In any case, operation may generally be far from optimal for a given disturbance d .

2. In this paper we assume that the unconstrained degrees of freedom u may be adjusted freely. Then, if we have information (measurements y) about the actual operation and we have a model of the system, we may use these measurements to update the estimate of the disturbances d and, based on this, perform a reoptimization to compute a new optimal value $u_{\text{opt}}(d)$, which is subsequently implemented, $u = u_{\text{opt}}(d)$.

Both of these approaches are complex, require a detailed model of the system, and are not likely to be used in practice, except in special cases. Is there any simpler approach that may work?

2.3. Implementation of Optimal Operation: Self-optimizing Control. If we look at how real systems operate, then we see that in most cases a feedback solution is used, whereby the degrees of freedom u are adjusted in order to keep selected controlled variables c at constant values c_s . Here c is a selected subset or combination of the available measurements y ; see Figure 1. Obviously, the idea must be that the optimal value of c , denoted $c_{\text{opt}}(d)$, depends only weakly on the disturbances d , such that keeping c at a constant value c_s indirectly results in near-optimal operation. This basic

idea was formulated more than 20 years ago by Morari et al.,³ who wrote that “we want to find a function c of the process variables which when held constant, leads automatically to the optimal adjustments of the manipulated variables, and with it, the optimal operating conditions. [...] This means that by keeping the function $c(u, d)$ at the setpoint c_s , through the use of the manipulated variables u , for various disturbances d , it follows uniquely that the process is operating at the optimal steady-state.”

Let us summarize how the optimal operation may be implemented in practice:

1. A subset u' of the degrees of freedom u_0 is adjusted in order to satisfy the active constraints $g_2 = 0$ (as given by the optimization).

2. The remaining unconstrained degrees of freedom (u) are adjusted in order to keep selected controlled variables c at constant desired values (setpoints) c_s .

Ideally, it is possible to find a set of controlled variables c such that this results in self-optimizing control where no further optimization is required, but in practice some infrequent update of the setpoints c_s may be required. If the set of active constraints changes, then one may have to change the set of controlled variables c , or at least change their setpoints, because the optimal values are expected to change in a discontinuous manner when the set of active constraints changes.

2.4. Self-optimizing Control: Optimal Controlled Variables. Let us consider in more detail the feedback (self-optimizing) implementation where we attempt to keep the variable(s) $c \in R^{n_c}$ constant at the setpoint c_s . The variables c are selected functions or combinations of the measured variables $y = f_{j0}(x, u_0, d) \in R^{n_y}$. The (candidate) measurements y include all of the information we have of the system behavior, including possible measured values of the disturbances d and independent variables u_0 , and information about changes in cost function parameters (prices) and the specification (values) of the active constraints. We consider the unconstrained problem in reduced space, and by formally eliminating the states using the model equations and active constraints, we may write

$$y = f_j(u, d) \quad (4)$$

The controlled variables c are selected functions of the y 's

$$c = h(y) \quad (5)$$

where the function h is free to choose. Substituting eq 4 into eq 5 gives

$$c = h[f_j(u, d)] = f_c(u, d) \quad (6)$$

We assume that the number of controlled variables c equals the number of independent variables u or more exactly that we, starting from $c = f_c(u, d)$, can derive the inverse relationship

$$u = f_c^{-1}(c, d) \quad (7)$$

where the function f_c^{-1} exists and is unique. The number of included measurements (y 's) must then at least be equal to the number of independent variables (u 's), but preferably it should be larger to be able to correct for disturbances and measurement error.

Examples of possible controlled variables are the difference between two measurements, $h(y) = y_1 - y_2$, the ratio between two inputs, $h(y) = u_1/u_2$ (assuming that the inputs are measured), linear combinations, $h(y) = h_1y_1 + h_2y_2 + h_3u_1 + h_4u_2$, and so on. Provided the variables u can actually be manipulated, an open-loop policy is obtained with $h(y) = u$.

To compare the alternative choices for c , we consider the loss with constant setpoints c_s . The loss L is defined as the difference between the actual value of the cost function obtained with a specific control strategy and the truly optimal value of the cost function, i.e.

$$L = J(c, d) - J_{\text{opt}}(d) \quad (8)$$

In the feedback policy, we adjust u such that $c = c_s + n$, where n is the implementation error. More precisely, the actual value of the controlled variable c will differ from its optimal value $c_{\text{opt}}(d)$ as a result of the presence of the following.

1. Setpoint error:

$$v(d) \stackrel{\text{def}}{=} c_s - c_{\text{opt}}(d) \quad (9)$$

For a nominally optimal system, $v(d^*) = 0$. The (change in) setpoint error is caused by changing disturbances d .

2. Implementation error:

$$n \stackrel{\text{def}}{=} c - c_s \quad (10)$$

The implementation error n is the sum of the measurement error and the control error (Figure 1 is a bit misleading because it (i) only includes the contribution to n from measurement errors and (ii) gives the impression that n is the measurement error in c , whereas in reality n in Figure 1 represents the combined effect on c of the measurement errors for y). The control error is often large if we use an open-loop policy ($c = u$) because the actually implemented value of u differs from u_s . With a closed-loop implementation, the steady-state control error is zero if we use a controller with integral action, so in this case the implementation error n is equal to the measurement error ("noise").

The total error that results in a positive loss is then

$$e_c \stackrel{\text{def}}{=} c - c_{\text{opt}}(d) = v(d) + n \quad (11)$$

Because the disturbances d and implementation errors n are generally assumed to be independent, we have that the two errors $v(d)$ and n are independent. Clearly, we would like to have both $v(d)$ and n small.

The optimal self-optimizing control structure may then be formulated mathematically as the solution to the following problem:

$$\min_h \bar{J}(u, d) \quad (12)$$

subject to

$$y = f_y(u, d) \quad (13)$$

$$h(y) = c_s + n \quad (14)$$

where the measurement combination h must be such that the function $h(f_y)$ is invertible (see above) and \bar{J} is some average value (or norm) of the cost over the sets

of possible disturbances and implementation errors

$$d \in \mathcal{D}, \quad n \in \mathcal{N} \quad (15)$$

In eq 14 it is assumed that the implementation error n is directly on c . This is reasonable if c consists of individual measurements. However, if c consists of measurement combinations, then eq 14 is reasonable only for the control error, which as argued above is zero in most cases. The only contribution to the implementation error then comes from the measurement error for the individual measurements y , so in this case eq 14 should be replaced by

$$h(y + n^y) = c_s \quad (16)$$

Instead of minimizing the average cost \bar{J} in eq 12, we may equivalently minimize the average loss \bar{L} . In this paper, we consider the induced (or worst-case) 2-norm of the loss

$$\bar{L} = \max_{\|f'\|_2 \leq 1} L \quad (17)$$

where (i) $f' = e'_c$ is the weighted control error (when deriving the minimum singular rule) and (ii) $f' = \begin{pmatrix} d \\ n^y \end{pmatrix}$ is the vector of weighted disturbances and implementation errors (for the exact local method).

3. Local Taylor Series Analysis

In the rest of this paper, all of our considerations are of local nature, and as discussed above, we assume that the set of active inequality constraints does not change with the disturbances.³

3.1. Linearized Models. The controlled variables (outputs) c are related to the inputs and disturbances by the relationship $c = f_c(u, d)$ in eq 6. For small deviations from the nominal point (denoted with an asterisk), we may use a linearized relationship between the unconstrained degrees of freedom u and any candidate set of controlled variables c . The linearized model in reduced space becomes

$$\Delta c = \mathbf{G} \Delta u + \mathbf{G}_d \Delta d \quad (18)$$

where $\Delta u = u - u^*$, $\Delta d = d - d^*$, $\Delta c = c - c^*$, $\mathbf{G} = (\partial f_c / \partial u)^{*T}$, and $\mathbf{G}_d = (\partial f_c / \partial d)^{*T}$. Similarly, a linearization of the relationship $y = f_y(u, d)$ in eq 4 yields

$$\Delta y = \mathbf{G}^y \Delta u + \mathbf{G}_d^y \Delta d \quad (19)$$

where $\mathbf{G}^y = (\partial f_y / \partial u)^{*T}$ and $\mathbf{G}_d^y = (\partial f_y / \partial d)^{*T}$, and linearization of $c = h(y)$ in eq 5 yields

$$\Delta c = \mathbf{H} \Delta y \quad (20)$$

where the matrix $\mathbf{H} = (\partial h / \partial y)^T$ is free to choose. Combining these equations yields

$$\mathbf{G} = \mathbf{H} \mathbf{G}^y; \quad \mathbf{G}_d = \mathbf{H} \mathbf{G}_d^y \quad (21)$$

From a linear point of view, the issue of selecting controlled variables is then to find the optimal choice for the matrix \mathbf{H} .

3.2. Expansion of the Cost Function (around the Fixed Nominal Point). We assume that the cost function J is smooth, or more precisely twice dif-

ferentiable, at the operating point we are considering (for more detailed conditions, see the assumptions for the implicit function theorem, as stated in ref 5).

A second-order Taylor series expansion of the cost function about the nominal point (u^* , d^*) then gives

$$J(u, d) = J^* + J_u^{*T}(u - u^*) + J_d^{*T}(d - d^*) + \frac{1}{2}(u - u^*)^T J_{uu}^*(u - u^*) + \frac{1}{2}(d - d^*)^T J_{dd}^*(d - d^*) + (d - d^*)^T J_{du}^*(u - u^*) + \mathcal{O}^3 \quad (22)$$

where

$$J^* = J(u^*, d^*), \quad J_u^* = \left(\frac{\partial J}{\partial u} \right)^*, \quad J_d^* = \left(\frac{\partial J}{\partial d} \right)^*, \\ J_{uu}^* = \left(\frac{\partial^2 J}{\partial u^2} \right)^*, \quad J_{dd}^* = \left(\frac{\partial^2 J}{\partial d^2} \right)^*, \quad J_{du}^* = \left(\frac{\partial^2 J}{\partial d \partial u} \right)^*$$

We can write the expansion in eq 22 more compactly as

$$J(u, d) = J^* + (J_u^* J_d^{*T})^T \begin{pmatrix} \Delta u \\ \Delta d \end{pmatrix} + \frac{1}{2} \begin{pmatrix} \Delta u \\ \Delta d \end{pmatrix}^T \mathcal{H}^* \begin{pmatrix} \Delta u \\ \Delta d \end{pmatrix} \quad (23)$$

where \mathcal{H}^* is the Hessian matrix of J with respect to $\begin{pmatrix} \Delta u \\ \Delta d \end{pmatrix}^T$

$$\mathcal{H}^* = \begin{pmatrix} J_{uu}^* & J_{ud}^* \\ J_{du}^* & J_{dd}^* \end{pmatrix}$$

The Hessian matrix is always symmetric, so J_{uu}^* and J_{dd}^* are symmetric and $J_{ud}^* = J_{du}^{*T}$.

If the nominal point is optimal (so J is at a minimum), then the following apply:

1. $J_u^* = 0$ because the gradient with respect to the independent variables must be zero at the optimum.

2. $\Delta u^T J_{uu}^* \Delta u$ is positive for any nonzero vector Δu , i.e., J_{uu}^* is positive definite: $J_{uu}^* > 0$ (if the minimum is a saddle, then $\Delta u^T J_{uu}^* \Delta u$ is zero in some direction and J_{uu}^* is positive semidefinite; i.e., $J_{uu}^* \geq 0$).

3.3. Optimal Input as a Function of d . We assume here that the nominal operating point (u^* , d^*) is optimal so $u^* = u_{\text{opt}}(d^*)$, and the gradient must be zero

$$J_u^* = \left(\frac{\partial J}{\partial u} \right)^* = 0$$

Next, consider a disturbance and input change so that the new operating point is (u, d) with the new gradient

$$J_u = \frac{\partial J}{\partial u}$$

A first-order expansion of the gradient gives

$$J_u = J_u^* + J_{uu}^*(u - u^*) + J_{ud}^{*T}(d - d^*)$$

We assume that we change the input so that also the new operating point is optimal, i.e., $u = u_{\text{opt}}(d)$. Then also the new gradient is zero, i.e., $J_u = 0$, and we get

$$0 = J_{uu}^*[u_{\text{opt}}(d) - u_{\text{opt}}(d^*)] + J_{ud}^{*T}(d - d^*) \quad (24)$$

and introducing $\Delta u_{\text{opt}} = u_{\text{opt}}(d) - u_{\text{opt}}(d^*)$ and $\Delta d = d -$

d^* , we derive a first-order accurate approximation of the sensitivity in the optimal input to disturbances

$$\Delta u_{\text{opt}} = -J_{uu}^{*-1} J_{ud}^* \Delta d \quad (25)$$

If we consider the original optimization problem (1) with the state variables included, then the sensitivity can be evaluated as shown in ref 5.

We may also express the setpoint error $v(d) = c_s - c_{\text{opt}}(d)$ directly in terms of the disturbance. From the linearized model in eq 18, we have $\Delta c_{\text{opt}} = \mathbf{G} \Delta u_{\text{opt}} + \mathbf{G}_d \Delta d$, and assuming the setpoints are nominally optimal, $c_s = c_{\text{opt}}(d^*)$, eq 25 gives a first-order accurate approximation of the setpoint error

$$v(d) = c_{\text{opt}}(d^*) - c_{\text{opt}}(d) = -\Delta c_{\text{opt}} = (\mathbf{G} J_{uu}^{*-1} J_{du}^* - \mathbf{G}_d) \Delta d \quad (26)$$

3.4. Expansion of the Loss Function (around the Moving Optimal Point). Above, we expanded the *cost function* at the *nominal* point (u^* , d^*), and this required a term for the deviation of the disturbance from its nominal value, $\Delta d = d - d^*$. Here, we instead expand the *loss function* at the *optimal* point [$u_{\text{opt}}(d)$, d] for each given disturbance d ; that is, the point about which we expand moves with the disturbance, and no term $d - d^*$ is needed. For a given disturbance d , a second-order Taylor expansion of the cost function $J(u, d)$ about the optimal point gives

$$J(u, d) \approx J[u_{\text{opt}}(d), d] + J_u^T [u - u_{\text{opt}}(d)] + \frac{1}{2} [u - u_{\text{opt}}(d)]^T J_{uu} [u - u_{\text{opt}}(d)] \quad (27)$$

where

$$J_u = \left(\frac{\partial J}{\partial u} \right)^{\text{opt}} = 0$$

$$J_{uu} = \left(\frac{\partial^2 J}{\partial u^2} \right)^{\text{opt}}$$

The loss function is defined as

$$L(u, d) = J(u, d) - J[u_{\text{opt}}(d), d]$$

and we derive the following very useful second-order expansion of the loss function⁶

$$L(u, d) = \frac{1}{2} [u - u_{\text{opt}}(d)]^T J_{uu} [u - u_{\text{opt}}(d)] = \frac{1}{2} e_u^T J_{uu} e_u \quad (28)$$

This expression quantifies how a (sufficiently small) input deviation $e_u \stackrel{\text{def}}{=} u - u_{\text{opt}}(d)$ affects the loss. From eq 18 we have, for a given disturbance d , that the corresponding deviation in the controlled variables c is $c - c_{\text{opt}}(d) = \mathbf{G}[u - u_{\text{opt}}(d)]$. Here \mathbf{G} is assumed to be invertible (see eq 7), and using eq 11, we derive

$$e_u = \mathbf{G}^{-1} [v(d) + n] \quad (29)$$

where v is the setpoint error and n the implementation error for c . Note that eqs 28 and 29 do not require that the setpoints c_s are nominally optimal.

For the case where the setpoints c_s are nominally optimal, $c_s = c_{\text{opt}}(d^*)$, substitution of eq 26 into eq 29 gives

$$e_u = (J_{uu}^*{}^{-1} J_{ud}^* - \mathbf{G}^{-1} \mathbf{G}_d)(d - d^*) + \mathbf{G}^{-1} n \quad (30)$$

and we find that the loss $L = (1/2)e_u^T J_{uu}^* e_u$ may be expressed as a function of d and n .

Remarks:

1. As an alternative to eq 28, we can express the loss in terms of $e_c \stackrel{\text{def}}{=} c - c_{\text{opt}}(d) = v(d) + n$:

$$L = \frac{1}{2} e_c^T J_{cc} e_c \quad (31)$$

where $J_{cc} = (\mathbf{G}^{-1})^T J_{uu} \mathbf{G}^{-1}$.

2. In eqs 28 and 31, the disturbance d enters implicitly through the errors e_u and e_c .

3. The Hessian matrix J_{uu} is independent of the choice of controlled variables c .

4. Note that J_{uu} in eq 27 is evaluated at the point $(u_{\text{opt}}(d), d)$, which is different from the nominal point (u^*, d^*) considered in eq 22. However, if the nominal point is optimal and the disturbance change is small ($\Delta d = d - d^*$ is small), then $J_{uu} \approx J_{uu}^*$.

4. Selection of Controlled Variables: Simple Methods

4.1. Requirements for Controlled Variables. To minimize the loss $L = (1/2)e_u^T J_{uu} e_u$, we want a small input error e_u . From $e_u = \mathbf{G}^{-1}[v(d) + n]$ in eq 29, we then derive the following **four requirements for a good candidate controlled c variable**.⁶

Requirement 1. Its optimal value is insensitive to disturbances (so that the setpoint error v is small).

Requirement 2. It is easy to measure and control accurately (so that the implementation error n is small).

Requirement 3. Its value is sensitive to changes in the manipulated variables u ; that is, the gain \mathbf{G} from u to c is large (so that the norm of \mathbf{G}^{-1} is small). (Equivalently, from eq 31 $J_{cc} = (\mathbf{G}^{-1})^T J_{uu} \mathbf{G}^{-1}$ should be small; that is, the optimum should be “flat” with respect to the variable c .)

Requirement 4. For cases with two or more controlled variables, the selected variables are not closely correlated (such that \mathbf{G} is not close to singular, resulting in a large \mathbf{G}^{-1}).

All four requirements need be satisfied. *In short, these requirements tell us that we should select variables c for which their variation in the optimal value and the implementation error is small compared to their adjustable range (the range c may be reached by varying u) (ref 6, p 408).*

Note that requirement 1 says that its *optimal value* should be insensitive to disturbances and *not* that its *value* should be insensitive to disturbances. Actually, we usually want its value to be sensitive to disturbances so that we can detect them (and thus correct for them).

4.2. Minimum Singular Value Rule. From eqs 28 and 29, we have that

$$L = \frac{1}{2} e_u^T J_{uu} e_u = \frac{1}{2} \|z\|_2^2 \quad (32)$$

where

$$z = J_{uu}^{1/2} e_u = J_{uu}^{1/2} \mathbf{G}^{-1} e_c \quad (33)$$

where $e_c = c - c_{\text{opt}}(d) = v + n$, $J_{uu}^{1/2} J_{uu}^{1/2} = J_{uu}$, and $\|z\|_2$ denotes the 2-norm of the vector. We assume that each controlled variable c_i is scaled such that the sum of its optimal range (v_i) and its implementation error (n_i) is unity and that for combined errors the 2-norm is less than 1; i.e., $\|e_c\|_2 = \|c - c_{\text{opt}}\|_2 = 1$. We also assume that each “base variable” u is scaled such that a unit change in each input has the same effect on the cost function J (such that the Hessian $J_{uu} = (\partial^2 J / \partial u^2)$ is a scalar times unitary matrix; i.e., $J_{uu} = \alpha U$). We use primes ‘ to show that the variables u and y have been scaled, and \mathbf{G}' denotes the scaled steady-state gain matrix from u' to c' . Then the resulting worst-case loss is

$$\max_{\|e_c\|_2 \leq 1} L = \max_{\|e_c\|_2 \leq 1} \frac{1}{2} \|z\|_2^2 = \frac{1}{2} [\bar{\sigma}(J_{uu}^{1/2} \mathbf{G}'^{-1})]^2 = \frac{1}{2} [\bar{\sigma}(\alpha^{1/2} \mathbf{G}'^{-1})]^2 = \frac{\alpha}{2} \frac{1}{\underline{\sigma}(\mathbf{G}')^2} \quad (34)$$

where the constant $\alpha = \bar{\sigma}(J_{uu})$ is independent of the choice of c and $\underline{\sigma}(\mathbf{G}')$ denotes the minimum singular value of the matrix \mathbf{G}' from u' to c' . The second equality follows because $\bar{\sigma}$ is the induced 2-norm of a matrix. The third equality holds provided J_{uu} is unitary. The last equality follows because $\bar{\sigma}(\mathbf{G}'^{-1}) = 1/\underline{\sigma}(\mathbf{G}')$.

Thus, to minimize the loss L , we should maximize $\underline{\sigma}(\mathbf{G}')$ and we have derived the following rule:

Assume that the base variables u are selected and scaled such that they all have a similar effect on the cost (or, more precisely, such that $J_{uu} = \alpha U$ where U is a unitary matrix), assume that we have scaled each candidate controlled variable c such that the expected variation in $c' - c'_{\text{opt}}$ is of magnitude 1 (including the effect of both disturbances and control error), and let \mathbf{G}' denote the resulting scaled gain matrix from u' to y' ($\Delta y' = \mathbf{G}' \Delta u'$). Then select controlled variables c that maximize the minimum singular value of \mathbf{G}' , $\underline{\sigma}(\mathbf{G}')$.

The expression (34) generally overestimates the value of the worst-case loss. This is because of the following two *limitations* with the singular value rule when applied to multivariable systems (with more than one controlled variable):

1. We have assumed that it is possible to scale the inputs such that $J_{uu} = (\partial^2 J / \partial u^2)^{\text{opt}}$ is a constant times unitary matrix. If this is not the case, then one should search for another set of “base case” inputs. This may not always be possible.

2. More seriously, we have assumed that any output deviation $e_c = c' - c'_{\text{opt}}$ satisfying $\|e_c\|_2 \leq 1$ is allowed, including the “worst-case” combination corresponding to $\underline{\sigma}(\mathbf{G}')$. For this to be true, we must assume that the variations $c_i - c_{i,\text{opt}}$ for the each variable c_i are independent. This generally holds for the implementation error n_i but not for the setpoint error v_i because their optimal values as a function of d are generally correlated.

Some comments on the singular value rule:

1. Interestingly, we note that this rule does not depend on the actual expression for the objective function J , but it does enter indirectly through the variation of c_{opt} with d , which enters into the scaling. A more detailed procedure with scaling is given in the appendix.

2. Because of the limitation 2, we must be a bit careful about eliminating candidate controlled variables with a small value of $\underline{\sigma}(\mathbf{G}')$ (at least for cases where the setpoint error v is larger than the implementation error n). However, we generally have that $u - u_{\text{opt}} = \mathbf{G}^{-1}(v +$

n), where from the identity $\bar{\sigma}(\mathbf{G}^{-1}) = 1/\underline{\sigma}(\mathbf{G})$ a small value of $\underline{\sigma}(\mathbf{G})$ implies that \mathbf{G}^{-1} is large in some direction. Furthermore, as just noted, the implementation errors n_i are generally independent, so any combination (direction) in n is allowed. It then follows that if we scale the outputs c with respect to the implementation errors only, i.e., select $c_{\text{scl},i} = |n_i|$ (see the appendix), to obtain the scaled matrix \mathbf{G}'' , then we may safely eliminate candidate controlled variables with a small value of $\underline{\sigma}(\mathbf{G}'')$ because these will be sensitive to implementation errors.

3. The minimum singular value rule applies also to the case with “back-off” because we do not assume optimal nominal setpoints. We thus find that we should *not* use back-off for variables that correspond to large directions of \mathbf{G}^{-1} (small directions of \mathbf{G}) because then $\mathbf{G}^{-1}v$, and thus the loss L , is large.

4. In this paper we use the minimum singular value rule to select controlled variables (outputs). The minimum singular value $\underline{\sigma}(\mathbf{G}'')$ can also be used as a tool for selecting manipulated input variables (inputs),⁷ but this is actually an unrelated condition which requires a different scaling of the variables.

5. Selection of Controlled Variables: Exact Local Method

In this section we assume that the setpoints are nominally optimal,

$$c_s = c_{\text{opt}}(d^*)$$

Upon substitution of eq 30 into eq 28, we can write the loss as

$$L = \frac{1}{2} \|z\|_2^2 \quad (35)$$

where

$$z = J_{uu}^{-1/2} [(J_{uu}^{-1} J_{ud} - \mathbf{G}^{-1} \mathbf{G}_d)(d - d^*) + \mathbf{G}^{-1} n] \quad (36)$$

First, let the elements in the positive diagonal matrix \mathbf{W}_d represent the expected magnitudes of the individual disturbances. Second, let the elements in the positive diagonal matrix \mathbf{W}_n^y represent the magnitude of the implementation error (measurement noise) associated with each of the candidate measurements y . Recall that the controlled variables c are selected functions of the measurements y , which we linearly write as $\Delta c = \mathbf{H} \Delta y$. The expected magnitudes of the disturbances and implementation errors are then

$$d - d^* = \mathbf{W}_d d$$

$$n = \mathbf{H} \mathbf{W}_n^y n^y = \mathbf{W}_n n^y$$

where d and n^y are normalized to have magnitudes of less than 1. More precisely, we will assume that the *combined* disturbances and implementation errors are 2-norm-bounded (see the discussion section for a justification on why to use the 2-norm).

$$\|f'\|_2 \leq 1; \quad f' \stackrel{\text{def}}{=} \begin{pmatrix} d \\ n^y \end{pmatrix} \quad (37)$$

Under these assumptions, the worst-case loss is

$$\max_{\|f'\|_2 \leq 1} L = \bar{\sigma}(\mathbf{M})^2/2 \quad (38)$$

where

$$\mathbf{M} = (\mathbf{M}_d \mathbf{M}_n) \quad (39)$$

$$\mathbf{M}_d = J_{uu}^{-1/2} (J_{uu}^{-1} J_{ud} - \mathbf{G}^{-1} \mathbf{G}_d) \mathbf{W}_d \quad (40)$$

$$\mathbf{M}_n = J_{uu}^{-1/2} \mathbf{G}^{-1} \mathbf{W}_n \quad (41)$$

and the dependency of \mathbf{M} on the measurement combination matrix \mathbf{H} enters through the matrices

$$\mathbf{G} = \mathbf{H} \mathbf{G}^y; \quad \mathbf{G}_d = \mathbf{H} \mathbf{G}_d^y; \quad \mathbf{W}_n = \mathbf{H} \mathbf{W}_n^y \quad (42)$$

The equality in eq 38 follows from the identity $z = \mathbf{M} f'$ and the fact that the induced (worst-case) 2-norm of a matrix is equal to its maximum singular value. Minimization of the loss L for any (worst-case) combination of disturbances and implementation errors is then equivalent to minimizing $\bar{\sigma}(\mathbf{M})$.

Note that this method does not suffer from the two limitations of the singular value rule. In particular, the disturbances d and measurement errors n^y are generally independent variables, so that any combination satisfying the 2-norm bound in eq 37 is allowed (see the discussion section for more on this).

5.1. Procedure for the Exact Evaluation of Loss.

The exact local procedure for analyzing candidate sets of controlled variables c then becomes as follows:

1. Define the optimal operation problem (specify the cost function J).
2. Solve the nominal optimization problem with respect to the degrees of freedom u and find the second-order derivatives of the cost, J_{uu} and J_{ud} .
3. For each candidate set c of controlled variables, obtain the linear model $\Delta c = \mathbf{G} \Delta u + \mathbf{G}_d \Delta d$.
4. Define the uncertainty by obtaining the matrices \mathbf{W}_d and \mathbf{W}_n .
5. For each *candidate set* c , compute the singular value $\bar{\sigma}(\mathbf{M})$ of the matrix \mathbf{M} in eq 39.
6. The set c with the smallest value of $\bar{\sigma}(\mathbf{M})$ minimizes the loss $L = 1/2 \bar{\sigma}(\mathbf{M})^2$.

Some comments are as follows:

1. It is clear from \mathbf{M}_n in eq 41 that \mathbf{G}^{-1} should be small to minimize the effect of implementation errors.
2. Yi and Luyben⁸ suggest to select controlled variables that minimize the input usage in response to disturbances, $(\partial u / \partial d)_c = \mathbf{G}^{-1} \mathbf{G}_d$. However, from \mathbf{M}_d in eq 40 we see that we do not want to make $\mathbf{G}^{-1} \mathbf{G}_d$ zero (unless $J_{uu}^{-1} J_{ud}$ is zero, which it rarely is), so this certainly is not a general rule.

5.2. Optimal Linear Combination of Measurements. Assume that we, from a given a set of candidate measurements y (which generally also includes the variables u_d), want to find the best linear combination to control.

$$\Delta c = \mathbf{H} \Delta y \quad (43)$$

Here the matrix \mathbf{H} is free to choose, except that we make the restriction that the number of controlled variables (c 's) equals the number of independent inputs (u 's). From eq 38 the optimal local measurement combination, in terms of minimizing the loss when there are distur-

bances and implementation errors bounded as in eq 37, is obtained by searching for the matrix \mathbf{H} that minimizes the $\bar{\sigma}(\mathbf{M})$, i.e.

$$\mathbf{H}_{\text{opt}} = \arg \min_{\mathbf{H}} \bar{\sigma}(\mathbf{M}) \quad (44)$$

The optimal matrix \mathbf{H}_{opt} is generally a "full" matrix; that is, it is generally optimal to combine all available measurements y in the controlled variables c .

6. Examples

Example 1. (a) Problem Statement. As a simple example, we consider a scalar unconstrained problem. The cost function is $J = (u - d)^2$, where nominally $d^* = 0$. For this problem we have three candidate measurements

$$y_1 = 0.1(u - d); \quad y_2 = 20u; \quad y_3 = 10u - 5d$$

We assume that unit magnitude of the disturbance and implementation errors (measurement noise); that is, $|d| \leq 1$ and $|n_j^y| \leq 1$.

The question is, what should we select as the controlled variable c [and keep constant at the value $c = c_s + n$, where $c_s = c_{\text{opt}}(d^*)$]? We first consider the use of the three individual measurements $c = y_1$, $c = y_2$, and $c = y_3$. At the end, we will consider the optimal measurement combination.

(b) Optimization. For this problem, we always have $J_{\text{opt}}(d) = 0$ corresponding to $u_{\text{opt}}(d) = d$, $y_{1,\text{opt}}(d) = 0$, $y_{2,\text{opt}}(d) = 20d$, and $y_{3,\text{opt}}(d) = 5d$. For the nominal case with $d^* = 0$, we thus have $u_{\text{opt}}(d^*) = 0$ and $y_{\text{opt}}(d^*) = 0$ for all measurements [i.e., we will use $c_s = c_{\text{opt}}(d^*) = 0$].

(c) Exact Nonlinear Evaluation of Loss. The losses can, for this example, be evaluated analytically, and with the three measurements as controlled variables ($c^1 = y_1$, $c^2 = y_2$, and $c^3 = y_3$; superscript k , e.g., c^k , is used to denote controlled variable set number k), we find that

$$L^1 = (10n_1^y)^2; \quad L^2 = (0.05n_2^y - d)^2; \quad L^3 = (0.1n_3^y - 0.5d)^2$$

[For example, with $c^3 = y_3$, we have $u = (y_3 + 5d)/10$, and with $c^3 = c^{3s} + n^3 = n_3^y$, we get $J^3 = (u - d)^2 = (0.1n_3^y + 0.5d - d)^2$.] With $|d| \leq 1$ and $|n_j^y| \leq 1$, the worst-case values of the losses (with $|d| = 1$ and $|n_j^y| = 1$) are $L^1 = 100$, $L^2 = 1.05^2 = 1.1025$, and $L^3 = 0.6^2 = 0.36$, and we find that $c = y_3$ is the best overall choice for self-optimizing control and $c = y_1$ is the worst. (However, with no implementation error, y_1 would be the best, and with no disturbances, y_2 would be the best.)

We will now compare this result with the linear methods derived in this paper.

(d) Linearized Models. The linearized models for the three choices of controlled variables

$$c^1 = y_1: \quad \mathbf{G}^1 = 0.1, \mathbf{G}_d^1 = -0.1$$

$$c^2 = y_2: \quad \mathbf{G}^2 = 20, \mathbf{G}_d^2 = 0$$

$$c^3 = y_3: \quad \mathbf{G}^3 = 10, \mathbf{G}_d^3 = -5$$

We have $J_u = 2(u - d)$, $J_d = -2(u - d)$, $J_{uu} = 2$, and $J_{ud} = -2$, and at the nominal operating point, we have

(where we as before omit the superscript asterisk to simplify notation).

$$J_u = 0, \quad J_d = 0, \quad J_{uu} = 2, \quad J_{ud} = -2$$

1. Singular Value Rule. For the three choices of controlled variables, we have without scaling $\underline{\sigma}(\mathbf{G}^1) = 0.1$, $\underline{\sigma}(\mathbf{G}^2) = 20$, and $\underline{\sigma}(\mathbf{G}^3) = 10$. This would indicate that $\bar{c}^2 = y_2$ is the best choice, but this is only correct with no disturbances. The reason for the error is that we have not scaled the controlled variables properly; in particular, we have not taken into account the effect of the disturbances on the magnitude of $c - c_{\text{opt}}(d)$.

Let us now follow the singular value procedure given in the appendix. We use method B because the Hessian matrix is available.

1. Scale each input u_j such that a unit deviation in each input from its optimal value has the same effect on the cost function J :

$$\mathbf{D}_u = u_{\text{scl}} = 1/\sqrt{J_{uu}} = 1/\sqrt{2}$$

2. For each candidate controlled variable, obtain its maximum setpoint error $v_{\text{max},i}$ due to variation in disturbances:

$$v_i = c_{i,\text{opt}}(d^*) - c_{i,\text{opt}}(d) = [\mathbf{G}J_{uu}^{-1}J_{ud} - \mathbf{G}_d]_i(d_{\text{max}} - d^*)$$

Here, $d_{\text{max}} - d^* = 1$, and for $c = y_1$, we get

$$v^1 = 0.1 \frac{1}{2}(-2) - (-0.1) = 0$$

and, similarly, $v^2 = -20$ and $v^3 = 5$.

3. For each candidate controlled variable c^k , it is given that the implementation error is $n^k = 1$.

4. Scale each candidate controlled variable such that the sum of the magnitudes of v_i [subscript i , e.g., v_i , refers to element number i in the vector (although the vector v here happens to be a scalar)] and the implementation error n_i is 1; that is, use $c_{\text{scl},i} = |v_i| + |n_i|$. We get

$$\mathbf{D}_c^1 = c_{\text{scl}}^1 = 0 + 1 = 1$$

$$\mathbf{D}_c^2 = c_{\text{scl}}^2 = 20 + 1 = 21$$

$$\mathbf{D}_c^3 = c_{\text{scl}}^3 = 5 + 1 = 6$$

5. Obtain from eq 50 the scaled gain matrix, $\mathbf{G}' = \mathbf{D}_c^{-1}\mathbf{G}\mathbf{D}_u$, and from eq 34 the worst-case losses:

$$c^1 = y_1: \quad \mathbf{G}' = \frac{1}{1}0.1/\sqrt{2} = 0.071; \quad L^1 = \frac{1}{2|\mathbf{G}'|^2} = 100$$

$$c^2 = y_2: \quad \mathbf{G}' = \frac{1}{21}20/\sqrt{2} = 0.67; \quad L^2 = \frac{1}{2|\mathbf{G}'|^2} = 1.1025$$

$$c^3 = y_3: \quad \mathbf{G}' = \frac{1}{6}10/\sqrt{2} = 1.18; \quad L^3 = \frac{1}{2|\mathbf{G}'|^2} = 0.360$$

6. Select as candidates those sets of controlled variables that correspond to a large value of the minimum singular value $\underline{\sigma}(\mathbf{G}')$. For a scalar G , $\underline{\sigma}(G) = |G|$, and the singular value rule tells us (as expected) that y_3 is the best choice for the controlled variable, followed by y_2 and

y_1 . We note from the computed losses that, for this scalar case, the singular value rule gives identically the same results as the "exact" procedure, but this will not generally be the case when we have more than one unconstrained degree of freedom (such that c is a vector).

2. Exact Local Method. Minimization of the loss L for any (worst-case) 2-norm combination of disturbances and implementation errors is equivalent to minimizing $\bar{\sigma}(\mathbf{M})$ in eqs 39–41 where we in this case have $\mathbf{W}_d = 1$ and $\mathbf{W}_n = 1$. We find for $c^1 = y_1$:

$$M_d = J_{uu}^{-1/2} (J_{uu}^{-1} J_{ud} - \mathbf{G}^{-1} \mathbf{G}_d) \mathbf{W}_d = \sqrt{2} 2^{-1} (-2) - 0.1^{-1} (-0.1) \times 1 = 0$$

$$M_n = J_{uu}^{1/2} \mathbf{G}^{-1} \mathbf{W}_n = \sqrt{2} 0.1^{-1} \times 1 = 10\sqrt{2}$$

which gives

$$L^1 = \frac{\bar{\sigma}(\mathbf{M})^2}{2} = \frac{1}{2} [\bar{\sigma}(0 \quad 10\sqrt{2})]^2 = 100$$

Similarly, we find with $c^2 = y_2$ and $c^3 = y_3$:

$$L^2 = \frac{\bar{\sigma}(\mathbf{M})^2}{2} = \frac{1}{2} [\bar{\sigma}(-\sqrt{2} \quad \sqrt{2}/20)]^2 = 1.0025$$

$$L^3 = \frac{\bar{\sigma}(\mathbf{M})^2}{2} = \frac{1}{2} [\bar{\sigma}(-\sqrt{2}/2 \quad \sqrt{2}/10)]^2 = 0.26$$

The reason for the slight difference from the exact nonlinear results presented initially ($L^1 = 100$, $L^2 = 1.1025$, and $L^3 = 0.36$) is not due to nonlinearity but the fact that we in the nonlinear evaluation allowed d and n individually to be less than 1, whereas we in the local method assumed that the combined 2-norm of d and n is less than 1. [For example, in the nonlinear evaluation the worst case was $|d| = 1$ and $|n| = 1$, which has a combined 2-norm of $\| \begin{pmatrix} 1 \\ 1 \end{pmatrix} \|_2 = 1.414$, which is not allowed in the exact local method where the combined 2-norm must be less than 1.] As argued in the discussion section, the use of the combined 2-norm is usually more reasonable from a practical point of view.

3. Optimal Combination of Measurements. Above, we considered control of the individual measurements y_1 , y_2 , and y_3 . We now want the best linear combination $c = \mathbf{H}y$ of all candidate measurements

$$\mathbf{y} = (y_1 \ y_2 \ y_3 \ u)^T$$

We have here included also the input u as a candidate measurement, with an assumed unit implementation error, $n^u = 1$. We then have

$$\mathbf{W}_n^y = I$$

where \mathbf{W}_n^y is a 4×4 matrix. Furthermore, we have as before $J_{uu} = 2$, $J_{ud} = -2$, $\mathbf{W}_d = 1$, and

$$\mathbf{G}^y = (0.1 \ 20 \ 10 \ 1)^T$$

$$\mathbf{G}_d^y = (-0.1 \ 0 \ -5 \ 0)^T$$

We want to find the optimal matrix $\mathbf{H} = (h_1 \ h_2 \ h_3 \ h_4)$ by minimizing $\bar{\sigma}(\mathbf{M})$ as given in eq 44. Numerical

optimization yields $\mathbf{H}_{\text{opt}} = (0.02094 \ -0.23296 \ 0.97797 \ -0.01164)$; that is, the optimal combination of the three measurements and the manipulated input u is

$$c = 0.02094y_1 - 0.23296y_2 + 0.97797y_3 - 0.01164u$$

We note, as expected, that the most important contribution to c comes from the variable y_3 . The loss is $L = 0.04055$, so it is reduced by a factor of 6 compared to the previously best case ($L = 0.26$) with $c = y_3$. The reason for this large reduction is because we are able to reduce the magnitude of M_d in eq 40 to almost zero. It should also be noted that in the optimal matrix \mathbf{H} we have $h_2/h_4 = 20$, which is not surprising because this is the ratio between the effective noise level for these otherwise identical variables (recall that $y_2 = 20u$ and $y_4 = u$).

Example 2. The purpose of this example is to illustrate the limitations of the minimum singular value rule for the case with two or more independent variables u .

We consider a problem with two independent variables, $u = (u_1 \ u_2)^T$, and one disturbance d of unit magnitude. The cost function is

$$J = (x_1 - x_2)^2 + (x_1 - d)^2$$

where the states depend linearly on u and d

$$x = \mathbf{G}^x u + \mathbf{G}_d^x d$$

with

$$\mathbf{G}^x = \begin{pmatrix} 11 & 10 \\ 10 & 9 \end{pmatrix}; \quad \mathbf{G}_d^x = \begin{pmatrix} 10 \\ 10 \end{pmatrix}$$

At the optimal point, we have $x_1 = x_2 = d$ and $J_{\text{opt}}(d) = 0$. At the nominal point, we have $d^* = 0$, which gives $u = 0$ and $x = 0$, and we find

$$J_{uu} = \begin{pmatrix} 244 & 222 \\ 222 & 202 \end{pmatrix}, \quad J_{ud} = \begin{pmatrix} 198 \\ 180 \end{pmatrix}$$

We assume that the states are measured ($y_1 = x_1$ and $y_2 = x_2$) and assume an implementation (measurement) error of magnitude 1 on each candidate measurement, $\mathbf{y} = (y_1 \ y_2 \ u_1 \ u_2)^T$. We consider three candidate sets for the controlled variables:

$$c^1 = (y_1 \ y_2)^T, \quad c^2 = (y_1 \ u_1)^T, \quad c^3 = (u_1 \ u_2)^T$$

(the latter is an "open-loop" policy). The unscaled gain matrices for three sets are

$$\mathbf{G}^1 = \begin{pmatrix} 11 & 10 \\ 10 & 9 \end{pmatrix}, \quad \mathbf{G}^2 = \begin{pmatrix} 11 & 10 \\ 1 & 0 \end{pmatrix}, \quad \mathbf{G}^3 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

Applying the scaling procedure in the appendix (method B) gives the following scaled gain matrices:

$$\mathbf{G}^{1s} = \begin{pmatrix} 0.352 & 0.352 \\ 0.320 & 0.317 \end{pmatrix}, \quad \mathbf{G}^{2s} = \begin{pmatrix} 0.352 & 0.352 \\ 0.0064 & 0 \end{pmatrix}, \\ \mathbf{G}^{3s} = \begin{pmatrix} 0.0064 & 0 \\ 0 & 0.0070 \end{pmatrix}$$

with minimum singular values

$$\underline{\sigma}(\mathbf{G}^1) = 0.0017, \quad \underline{\sigma}(\mathbf{G}^2) = 0.0045, \quad \underline{\sigma}(\mathbf{G}^3) = 0.0064$$

We want to maximize the minimum singular value, so from this it seems that the open-loop policy ($c^3 = u$) is the best. However, computing the losses using the exact local method in eq 38 gives

$$L^1 = 3, \quad L^2 = 2.7, \quad L^3 = 303$$

and we find that the open-loop policy is clearly the worst with a very large loss of 303, whereas the two other policies have a loss of 3 and 2.7, respectively. This is close to the optimal because a numerical search for the optimal combination of all four measurements gave a loss of $L = 1.999$ and

$$\mathbf{H}_{\text{opt}} = \begin{pmatrix} 0.913 & 0.085 & 0.887 & 0.274 \\ 0.469 & 0.743 & 1.223 & -0.118 \end{pmatrix}$$

The minimum singular value rule therefore gives the wrong order. In addition, the losses L computed based on the minimum singular values using eq 34 are a factor 100 or more too high.

This example was constructed with an almost singular matrix \mathbf{G}^x , and the reason the minimum singular value rule fails in this case is that the optimal values of all of the variables (y_1, y_2, u_1, u_2) are strongly correlated, such that the assumption of independent variations in $c - c_{\text{opt}}$ does not hold.

If we consider the same example, but with $\mathbf{G}^x = \begin{pmatrix} 11 & -10 \\ 10 & 9 \end{pmatrix}$, which is not ill-conditioned, then we find that the minimum singular value rule works well. In this case the minimum singular values of the scaled gain matrices are

$$\underline{\sigma}(\mathbf{G}^1) = 0.22, \quad \underline{\sigma}(\mathbf{G}^2) = 0.015, \quad \underline{\sigma}(\mathbf{G}^3) = 0.031$$

(indicating that controlled variable c^1 is clearly the best), and this compares nicely with the exact losses computed from eq 38

$$L^1 = 3, \quad L^2 = 761, \quad L^3 = 535$$

from which we see that c^1 gives by far the lowest loss.

7. Discussion

7.1. "Ideal" Choice of Controlled Variables. If we for the moment disregard the implementation error n , then the ideal choice of controlled variables would be to have $v(d) = c_s - c_{\text{opt}}(d) = 0$ for any value of d . Here $c_s = c^*$ is constant, so to achieve this, we need the optimal value of the controlled variable to be independent of the disturbance.

From a linear point of view, it is clear from eq 26 that an example of an "ideal" controlled variable is one that achieves $\mathbf{G} = J_{uu}$ and $\mathbf{G}_d = J_{ud}$.

More generally, an ideal controlled variable would be a direct measurement of the gradient of the cost function with respect to the input (because it is optimal for any disturbance to have this gradient zero and we could directly specify its setpoint at zero). In particular, the controlled variable

$$c = f_c(u, d) = \alpha_1 \frac{\partial J(u, d)}{\partial u} + \alpha_0 = \alpha_1 J_u + \alpha_0 \quad (45)$$

where α_0 and α_1 are constants, is ideal in terms of

having $c_{\text{opt}}(d)$ independent of d . In general, the realization of the ideal variable assumes that we can measure all of the independent variables, including the disturbances d .

In example 1, we have $J_u = 2(u - d)$, so when the implementation error is disregarded, an ideal controlled variable for this case would be $c = \alpha_1(u - d) + \alpha_2$. In general, however, the implementation error n may be a very important factor in practical cases, and the ideal controlled variable may not be the best after all [as confirmed by example 1 where $c = y_1 = 0.1(u - d)$ actually came out as the poorest controlled variable].

7.2. Use of 2-Norm for Noise and Disturbances. Instead of the 2-norm in eq 37, we could have used the vector infinity norm, $\|(\frac{d}{n})\|_{\infty} \leq 1$, which would have

allowed for the extreme case with all variables simultaneously at their worst-case values ($|d_k| = 1$ and $|n_i| = 1$). However, two reasons for using the 2-norm in eq 37 are as follows:

1. From eq 35 the loss is given by the 2-norm of the vector \mathbf{z} , and it is therefore mathematically convenient to use the 2-norm also for the disturbance and noise.

2. With the 2-norm, it is *not* possible to have all of the individual disturbance and noise variables simultaneously at their worst-case values ($|d_k| = 1$ and $|n_i| = 1$). We argue that this is reasonable from a physical point of view because it is unlikely that this extreme worst case occurs in practice.

For example, for the case with three variables, the following three variable combinations have 2-norm equal to 1:

$$\left\| \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \right\|_2 = 1; \quad \left\| \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \right\|_2 = 1; \quad \left\| \begin{pmatrix} 1/\sqrt{3} \\ 1/\sqrt{3} \\ 1/\sqrt{3} \end{pmatrix} \right\|_2 = 1$$

We note that we can have only one variable at a time equal to 1, and if all three variables are equal in magnitude, then their maximum value is $1/\sqrt{3} = 0.577$.

This property of the vector 2-norm is also reasonable from a statistical point of view, from which we expect that the use of many independent measurements reduces the variance. For example, assume that we have p independent measurements y_i of the same variable y , and we take their average $\bar{y} = (1/p)\sum_{i=1}^p y_i$. The noise (implementation error) on each individual measurement y_i is n_i ; i.e., $y_i = y + n_i$, and we assume that the noise satisfies $\|\mathbf{n}\|_2 \leq 1$, where \mathbf{n} is vector of the individual noises n_i . We assume that the true variable is equal to zero ($y = 0$). We then have $y_i = n_i$, and $\bar{y} = (1/p)\sum_{i=1}^p y_i = (1/p)(\mathbf{1} \cdot \mathbf{n})$, where $\mathbf{1} = (1 \ 1 \ \dots \ 1)$ is a row vector of length p and \mathbf{n} is a column vector of the individual noises. The worst-case value of the measured average is then

$$|\bar{y}| = \frac{1}{p} \max_{\|\mathbf{n}\|_2 \leq 1} (\mathbf{1} \cdot \mathbf{n}) = \frac{1}{p} \bar{\sigma}(\mathbf{1}) = \frac{1}{p} \sqrt{p} = 1/\sqrt{p}$$

(the first equality is the definition of the average, and the second equality follows from the definition of the maximum singular value). That is, the worst-case average is reduced as we increase the number p of measurements, and, importantly, this reduction goes as $1/\sqrt{p}$, which is equal to the (estimated) reduction in statistical variance when we have p measurements (samples) with the same mean. This agreement with

statistics further justifies the use of the vector 2-norm to bound \mathbf{n} (on the other hand, if we used the vector infinity-norm, then we would not get any benefit of adding extra measurements, which is unreasonable).

7.3. Relationship to Indirect and Partial Control. Consider a problem which from the outset is a setpoint problem; that is, the objective is to keep the "primary" controlled variables y_1 at their setpoints y_{1s} . This may be written in the form considered in this paper by defining

$$J = \frac{1}{2}(y_1 - y_{1s})^T(y_1 - y_{1s}) = \frac{1}{2}e_1^T e_1 \quad (46)$$

To make the problem interesting, we assume that the ideal choice $c = y_1$ cannot be used because direct control of y_1 is difficult or impossible. Instead, the idea is to use *indirect control*, where we, by controlling a set of "secondary" variables c , indirectly achieve good control of y_1 . The linear models relating the variables are

$$\Delta y_1 = \mathbf{G}_1 \Delta u + \mathbf{G}_{d1} \Delta d \quad (47)$$

$$\Delta c = \mathbf{G} \Delta u + \mathbf{G}_d \Delta d \quad (48)$$

where $\Delta u = u - u^*$, etc. We assume that the nominal operating point (u^* , d^*) is optimal; i.e., $y_1^* = y_{1s}$. Differentiation gives

$$J_u = (\mathbf{G}_1 \Delta u + \mathbf{G}_{d1} \Delta d)^T \mathbf{G}_1, \quad J_{uu} = \mathbf{G}_1^T \mathbf{G}_1, \\ J_{ud} = \mathbf{G}_1^T \mathbf{G}_{d1}$$

and we can compute the matrix \mathbf{M} in the exact method (39) and search for the optimal measurement combination. Note, in particular, that the term $(J_{uu}^{-1} J_{ud} - \mathbf{G}^{-1} \mathbf{G}_d)$ in \mathbf{M}_d is equal to $(\mathbf{G}_1^T \mathbf{G}_{d1} - \mathbf{G}^{-1} \mathbf{G}_d)$ where $\mathbf{G}_1^\dagger = (\mathbf{G}_1^T \mathbf{G}_1)^{-1} \mathbf{G}_1^T$ is the pseudoinverse (left inverse) of \mathbf{G}_1 . From this, it is clear that $M_d = 0$ for the ideal ("uninteresting") case with $c = y_1$ (as expected). The goal of indirect control is to search for other ("interesting") choices for the controlled variables c (measurement combinations) with \mathbf{M}_d small or even zero.

Additional insight about indirect control is obtained by solving eq 48 with respect to Δu to obtain

$$\Delta u = \mathbf{G}^{-1} \Delta c - \mathbf{G}^{-1} \mathbf{G}_d \Delta d$$

Substituting into eq 47 then yields

$$\Delta y_1 = \underbrace{\mathbf{G}_1 \mathbf{G}^{-1}}_{P_c} \Delta c + \underbrace{(\mathbf{G}_{d1} - \mathbf{G}_1 \mathbf{G}^{-1} \mathbf{G}_d)}_{P_d} \Delta d \quad (49)$$

where the P s are called the partial control gains.⁶ P_d gives the effect of disturbances on the primary outputs y_1 with closed-loop ("partial") control of the variables c , and P_c gives the effect of the control error. To minimize J , we want Δy_1 small, and eq 49 shows that we should select controlled variables c such that the "partial gains" P_c and P_d are small. This simple approach has been used on a distillation case study.⁹ Here we find that we cannot use temperature measurements at the end of the column because of sensitivity to implementation error n (measurement noise) (i.e., P_y is large at the column end), and we cannot use measurements close to the middle of the column because of sensitivity to disturbances (i.e., P_d is large in the middle). The best balance between sensitivity to measurement noise and distur-

bances is found when the measurements are located somewhere between the end and the middle of the column.

8. Conclusion

We have derived an exact and numerically efficient local method for evaluating the loss when controlling the variables c at constant setpoints, by evaluating $\bar{\sigma}(\mathbf{M})$ where \mathbf{M} is given in eq 39. This approach may also be used to numerically search for the optimal linear measurement combination, $\Delta c = \mathbf{H} \Delta y$, to use as controlled variables.

A simpler method is to evaluate the minimum singular value $\sigma(\mathbf{G}')$, of the scaled gain matrix \mathbf{G}' from the "inputs" u to the controlled variables c . For the multi-variable cases, this method is not exact, but it provides a simple method for quickly screening candidate sets of controlled variables. This follows because a small value of $\sigma(\mathbf{G}')$ is always bad because it implies that there is a combination of implementation errors (n) that result in a large loss.

Appendix. Singular Value Rule with Scaling

A procedure for use of the minimum singular value to select controlled variables is summarized below. A key part of this procedure is the scaling, and we let a prime ' denote the scaled model and variables. We have in the original units $\Delta c = \mathbf{G} \Delta u$. We scale each input j and controlled variable i by a scaling factor

$$c'_i = \frac{c_i}{c_{scl,i}}, \quad u'_j = \frac{u_j}{u_{scl,j}}$$

The model in scaled units is then $\Delta c' = \mathbf{G}' \Delta u'$ with

$$\mathbf{G}' = \mathbf{D}_c^{-1} \mathbf{G} \mathbf{D}_u \quad (50)$$

where the diagonal scaling matrices are

$$\mathbf{D}_c = \text{diag}\{c_{scl,i}\}, \quad \mathbf{D}_u = \text{diag}\{u_{scl,j}\} \quad (51)$$

Note that the scaling changes the units, but the problem itself is unchanged. Two methods for generating the scalings are given as follows:

Method A: Direct use of the nonlinear model (this is usually preferred in practice because of its simplicity).

Method B: Use of Hessians and linear model matrices obtained by linearizing the problem.

The procedure is then as follows:

1. Scale each input u_j such that a unit deviation in each input from its optimal value has the same effect on the cost function J :

Method A: For each input, find the change $u_{scl,j}$ that increases the loss L from 0 until 1 (or, more generally, select $u_{scl,j} = \Delta u_j / \sqrt{\Delta L}$).

Method B: Select $u_{scl,j} = 1/\sqrt{[J_{uu}]_{jj}}$ (the inverse of the square root of the corresponding diagonal element of J_{uu}).

2. For each candidate controlled variable, obtain its maximum optimal variation $v_{\max,i}$ due to variation in disturbances:

Method A: From the nonlinear model, compute the optimal parameters (inputs and outputs) for various conditions (disturbances and operating points). (This yields a "lookup" table of optimal parameter values as a function of the operating conditions.) From this,

identify

$$v_i = \max(|c_{s_i} - c_{i_{\text{opt,max}}}|, |c_{s_i} - c_{i_{\text{opt,min}}}|)$$

Method B: Assuming that the setpoints are nominally optimal, i.e., $c_s = c_{\text{opt}}(d^*)$, we have from eq 26

$$v_i = c_{i_{\text{opt}}}(d^*) - c_{i_{\text{opt}}}(d) = [\mathbf{G} \mathbf{J}_{uu}^{-1} \mathbf{J}_{ud} - \mathbf{G}_d]_i (d_{\text{max}} - d^*)$$

where $d_{\text{max}} - d^*$ is a vector consisting of the expected magnitude of each disturbance.

3. For each candidate controlled variable, obtain its expected implementation error n_i (sum of measurement error and control error).

4. Scale the candidate controlled variables such that for each variable i the sum of the magnitudes of v_i and the implementation error n_i is similar, which corresponds to selecting the scaling

$$c_{\text{scl},i} = |v_i| + |n_i|$$

5. Compute the scaling matrices \mathbf{D}_c and \mathbf{D}_u from eq 51 and obtain the matrix $\mathbf{G}' = \mathbf{D}_c^{-1} \mathbf{G} \mathbf{D}_u$ from eq 50.

6. Select as candidates those sets of controlled variables that correspond to a large value of the minimum singular value $\underline{\sigma}(\mathbf{G}')$.

Literature Cited

- (1) Skogestad, S. Plantwide control: the search for the self-optimizing control structure. *J. Process Control* **2000**, *10*, 487–507.
- (2) Kalman, R. E. Design of a self-optimizing control system. *Trans. ASME* **1958**, 468–478.
- (3) Morari, M.; Stephanopoulos, G.; Arkun, Y. Studies in the synthesis of control structures for chemical processes. Part I. *AIChE J.* **1980**, *26* (2), 220–232.
- (4) Birge, J. R.; Louveaux, F. *Introduction to stochastic programming*; Springer: New York, 1997.
- (5) Ganesh, N.; Biegler, L. T. A reduced hessian strategy for sensitivity analysis of optimal flowsheets. *AIChE J.* **1987**, *33*, 282–296.
- (6) Skogestad, S.; Postlethwaite, I. *Multivariable Feedback Control*; John Wiley & Sons: New York, 1996.
- (7) Morari, M. Design of Resilient Processing Plants—III. *Chem. Eng. Sci.* **1983**, *38* (11), 1881–1891.
- (8) Yi, C. K.; Luyben, W. L. Evaluation of plant-wide control structures by steady-state disturbance sensitivity analysis. *Ind. Eng. Chem. Res.* **1995**, *34*, 2393–2405.
- (9) Havre, K. Studies on controllability analysis and control structure design. Ph.D. Thesis, NTNU, Trondheim, Norway. Available from <http://www.chembio.ntnu.no/users/skoge/>, 1998.

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