Robust operation by controlling the right variable combination

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Abstract

This paper consider how to best *implement* the optimal operation policy in the presence of uncertainty (disturbances and implementation errors) by selecting the right set of controlled variables c to be kept at constant setpoints c_s. More specific, we focus on how to select controlled variables that are linear combinations of the available measurements with good self-optimizing properties. A new method is proposed, that from a linear point of view give controlled variables with perfect self-optimizing control. This is achieved by calculating the change in optimal value for the measurements, $\Delta y_{opt} = F\Delta d$ and to select controlled variables that are linear combinations of the measurements, $\Delta c_{opt} = H\Delta y_{opt} = HF\Delta d$, such that $HF = 0$. It is shown that the number of measurements needed is greater or equal to the number of inputs and disturbances. This secure, from a linear point of view, perfect self-optimizing properties for disturbances if we neglect measurement error. If we have that the number of measurement is greater than the sum of inputs and disturbances we have some freedom in choosing a subset of the measurements. Based on this, a strategy for selecting the necessary measurements, to reduce the effect of the implementation error, is proposed. To illustrate the method several examples are included.

1 Introduction

Although not widely acknowledged, controlling the right variables is a key element in overcoming uncertainty in operation. Control systems often consist of several layers in a hierarchical structure, each operating on a different time scale. Typically, layers include scheduling (weeks), site-wide optimization (day), local optimization (hours), supervisory/predictive control (minutes) and regulatory control (seconds). The layers are interconnected through the controlled variables c; see Figure 1.

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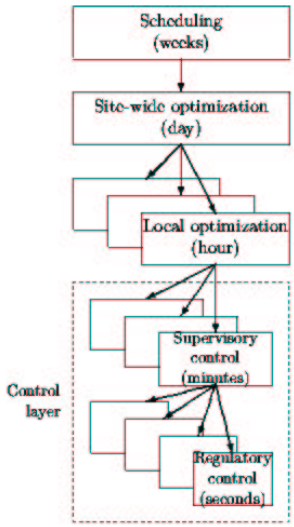

Figure 1: Typical control hierarchy in a chemical plant.

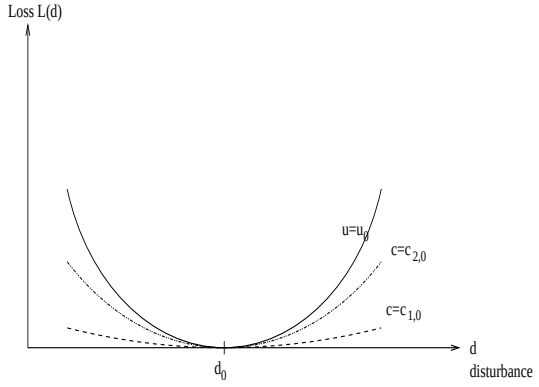

Figure 2: Loss as a function of disturbance for open and closed loop with to different controlled variables c_1 and c_2.

This paper focus on the interaction between the local optimization layer and the feedback control layer, by finding candidate controlled variables with good self-optimizing properties. Self-optimizing control follows the idea of Morari et al. (1980) where one want to find controlled variables that, under the influence of disturbances and implementation errors, operates near optimal when kept at constant setpoints. The term disturbance include both process disturbances and modeling errors.

Optimal operation for a given disturbance (d) can be found by solving the following problem.

$$\min_u J(x,u,d) \tag{1}$$

s.t

$$f(x,u,d) = 0 \tag{2}$$

$$g(x,u,d) \leq 0 \tag{3}$$

$$x \in \mathcal{X}, u \in \mathcal{U}, d \in \mathcal{D}$$

where f is the process model, g is the inequality constraints, u is the independent variables (inputs), d is the disturbances in which we cannot affect and x the states. The solution of (1) give the optimal input $u_{opt}(d)$ and states $x_{opt}(d)$, so the the optimal measurements $y_{opt}(d)$ can be calculated with respect to d. Uncertainty can be classifies as either **signal uncertainty** (measurement noise and disturbances) and **model uncertainty** (parametric and structural model uncertainty). Morari et al. (1980) use a slightly different classification, in which he classifies disturbances as either dominant or insignificant based on the economic impact (change in J_{opt}) and propose to neglect the disturbances with small economic effect. This is partially true, in the sense that the disturbance affect both the economics and the feasibility region of the system. While a disturbance may have little effect on the economics, it may greatly influence the feasibility region for a control structure making it necessary to include it in the analysis. There are two classes of problems that can result by solving (1)

- *Constrained*: The optimal solution lies at active constraints for all expected disturbances.
- *Unconstrained* (the focus of this paper): One or more of the optimization degrees of freedom are unconstrained for all or some expected disturbances.

For constrained problems, we usually select the active constraints as controlled variables (Maarleveld & Rijnsdorp 1970), and implementation is easy. The second class, which is the focus of this paper, we consider the selection of the controlled variables for the remaining n degrees of freedom. From a mathematical point of view, the optimal controller is the one with full information, that based on all available measurements, estimate the disturbances and then calculates the optimal change in the input. In practice, a optimizing controller will not be used due to the complexity of modeling, so a decentralized structure is common in practice. We will show here, that by only controlling the right variable, we are able to operate with an acceptable loss, by keeping the controlled variable at constant setpoints.

Self-optimizing control (Skogestad 2000*a*)*is when an acceptable loss can be achieved using constant setpoints for the controlled variables (without the need to re-optimize when disturbances occur).*

The term self-optimizing control was introduced by Skogestad (2000*a*) and the central issue when searching for the self-optimizing control structure is to decide how to best *implement* the optimal policy in the presence of uncertainty. This is done by selecting the right set of controlled variables c to be kept at constant setpoints c_s. The goal is to minimize the loss, $L = J(c_s + n, d) - J_{opt}(d)$, with a constant setpoint strategy, where the loss is the difference between the value of the objective using a constant setpoint policy and the value of the true optimal objective. From a steady-state perspective with no uncertainty, the only requirement to the selected control structure is that the selected controlled variables form a independent set, it does not matter what variables we select to control. The presence of disturbances make the selection of controlled variable an important task. An illustration is given in Figure 2 where the loss for open loop and two closed loop structures is given with respect to disturbance. Keeping the variables at the nominal optimum, we see that the open-loop structure has the highest loss. Of the two closed loop structures we see that controlling variable c_1 at the nominal value follow the optimal path and give (almost) no loss For a review of self-optimizing control see Skogestad (2000*b*).

Finding the optimal self-optimizing control structure may be formulated by the following minimax problem.

$$\min_{h,u} \left[\max_{d \in \mathcal{D} n \in \mathcal{N}} J(d, c_s, c) \right] \tag{4}$$

s.t.

$$f(x, u, d) = 0 \tag{5}$$

$$g(x, u, d) \leq 0 \tag{6}$$

$$c = h(y) \tag{7}$$

$$c(x,u,d) = c_s + n \qquad (8)$$
$$x \in \mathcal{X}, u \in \mathcal{U}, d \in \mathcal{D}$$

where n is the implementation error. So how do we select h? Due to the binary variables, the optimization problem grows combinatorially and is generally non-convex. From this it is obvious that there is a need for simpler methods to select controlled variables with good self-optimizing properties. Mahajanam et al. (2001) propose a "short-cut" method for evaluating the self-optimizing properties of controlled variables, while Skogestad et al. (1998) propose a method based on a Taylor series approximation of the loss function. Morud (1995) showed that, for a simple Continuous Stirred Tank Reactor (CSTR) example, where one wants to maximize the product composition, by selecting the right linear combinations of the available measurements, the resulting controlled variable had perfect self-optimizing properties from a linear point of view. The analysis did not consider implementation error and the linear combination was found by searching in all possible of the measurements. While this method may apply on small systems, for larger system the method becomes computationally expensive. The objective of this paper is to provide you with a much simpler method.

2 Proposed method for selecting controlled variables as linear combinations of measurements

The overall objective is to find a set of controlled variables c which yields self-optimizing control, that is, we want to obtain near-optimal operation when c is kept at constant setpoints c_s, in spite of disturbances d and implementation errors n. Actually, as shown in this section, if we neglect the implementation error in controlling c (e.g caused by poor control or measurement error), then it is possible from a linear point of view to find a linear combination of the available measurements with zero loss ("perfect self-optimizing control").
Generally, the measured variables y are a function of the independent variables (degrees of freedom) u and disturbances d (as well as the internal states x)

$$y = f_y(u,d) \qquad (9)$$

In most cases the set y also includes the independent variables u. The controlled variables c are to be selected as combinations of the measured variables,

$$c = h(y) \qquad (10)$$

where the generally non-linear function h is free to choose, except that we assume controlled variables are independent and that the number of controlled variables (c's) equals the number of degrees of freedom (u's).We will here consider the case where the function $h(y)$ is linear. We then have that

$$\Delta c = H \Delta y \qquad (11)$$

where the matrix H is free to choose. We assume that the operation is nominally optimal, that is, we have $c_s = c_{opt}(d^*)$ where d^* is the nominal disturbance. We assume

that there is no implementation error ($n = 0$), which implies that we will have $c = c_s$ (constant) for all disturbances d.
This constant setpoint policy will be optimal (with zero loss) provided the optimal value of $c(d)$ remains constant, that is, is $c_{opt}(d)$ is independent of d. This simple insight may be used to find the optimal linear combination (i.e. find the optimal choice for the matrix H).
We consider small changes (disturbances), then the change in the optimal value of the measurements is then given by

$$\Delta y_{opt} = y_{opt,d} - y_{opt,d^*} = F(d - d^*) = F\Delta d \tag{12}$$

where $F = \frac{dy_{opt}}{d\,d}$ may be obtained numerically by solving the optimization problem (1) for small changes in the disturbance variables d, and from this obtain $u_{opt}(d)$ as well as $y_{opt}(d)$. From (11) the corresponding change in the optimal value of c is

$$\Delta c_{opt} = H\Delta y_{opt} \tag{13}$$

We will now require that

$$\Delta c_{opt} = 0 \tag{14}$$

and from this requirement we get that

$$\Delta c_{opt} = HF\Delta d = 0 \tag{15}$$

This need to be satisfied for any Δd so we must have that

$$HF = 0 \tag{16}$$

For this to be true, we have that Hshould be in the left null space of F ($H \in \mathcal{N}(F^T)$). Assume that we have n unconstrained degrees of freedom (the length of vectors u and c are n), we use m independent measurements (see below) when forming c, and we have k independent disturbances. We than have that F is a $m \times k$ matrix and H is a $n \times m$ matrix. The fundamental theorem of linear algebra (Strang 1988) give that $\mathcal{N}(F^T)$, the left null space of F has dimension m-r, where r is the rank of F ($r = Rank(F)$). Since the disturbances are assumed to be independent, we have that $Rank(F) = r = k$ and since $H \in \mathcal{N}(F^T)$ we have that $dim(H) = m - k$. We need as many controlled variables as inputs which give that $dim(H) = n$(so that the number of basis vectors for the left null space is n).

$$m - n = k \Leftrightarrow m = n + k \tag{17}$$

so that

$$\#y = \#d + \#\ u. \tag{18}$$

e.g. the minimum number of measurements needed is equal to the number of inputs plus the number of disturbances.

Theorem 2.1 . ***Self-optimizing control by combination of measurements*** *Assume we have n unconstrained independent variables u, k independent disturbances*

d, and m measurements y, of which $n + k$ are independent. The measurements are combined linearly into n controlled variables

$$\Delta c = H\Delta y \tag{19}$$

If H is selected such that HF=0 where $F = \frac{dy_{opt}}{d\,d}$, then keeping c constant at its nominal optimal value gives zero loss when there are disturbances d, The matrix H is generally not unique.

Summarized, the main idea is to select the selection matrix H such that

$$\mathbf{\Delta c_{opt} = H\Delta y_{opt} = HF\Delta y = 0} \tag{20}$$

by requiring that $H \in \mathcal{N}(F^T)$ using $m = n + k$ measurements. Below we will address the question of how to select which measurement to use.

3 Comparison with previous results

Skogestad & Postlethwaite (1996) derived the following four requirements for a good candidate controlled variables:

1. Its optimal value $c_{opt}(d)$ is insensitive to disturbances.
2. It should be easy to measure and control accurately.
3. The variable c should be sensitive to changes in inputs.
4. The selected variables should be independent.

Skogestad (2000*a*) presents two approaches for selecting controlled variables for self-optimizing control based on a Taylor series approximation of the loss function.:

1. **Approach 1**. Minimum singular value rule. Select variables that maximize the minimum singular value of the appropriately scaled steady-state gain matrix G from inputs (u) to the selected controlled variables (c).
2. **Approach 2**. Exact "brute-force" linear method.

A short description of both methods are included here for reference.

3.1 Approach 1: Minimum Singular Value Approach

Skogestad & Postlethwaite (1996) derived a very useful second-order expansion of the loss function around the nominal optimum for a given disturbance d:

$$L(u,d) = \frac{1}{2}(u - u_{opt}(d))^T J_{uu}(u - u_{opt}(d)) = \frac{1}{2}(e_u)^T J_{uu} e_u = \frac{1}{2}\|z\|_2^2 \tag{21}$$

where

$$z = J_{uu}^{1/2} e_u \tag{22}$$

For a given disturbance d, the corresponding deviation in the controlled variable is:

$$e_c = c - c_{opt}(d) = G(u - u_{opt}(d)) \tag{23}$$

which gives $u - u_{opt}(d) = G^{-1}(c - c_{opt}(d))$ assuming that G is invertible. The loss function then becomes:

$$L(u,d) = \frac{1}{2}[G^{-1}(c - c_{opt}(d))^T J_{uu}(G^{-1}(c - c_{opt}(d)))] \tag{24}$$

If we assume that each controlled variable has been scaled properly $\|c - c_{opt}(d)\|_2 = 1$ and that each "base case" variable u is scaled such that a unit change in the input has the same effect on the cost function J, then the resulting worst case loss may be evaluated by the singular value:

$$\max_{\|e_c\|_2 \leq 1} L = \max_{\|e_c\|_2 \leq 1} \frac{1}{2}\|z\|_2^2 = \frac{1}{2}(\overline{\sigma}(J_{uu}^{1/2}G^{-1})^2 = \frac{\alpha}{2}\frac{1}{\underline{\sigma}(G)^2} \tag{25}$$

where $\alpha = \overline{\sigma}(J_{uu})^2$ and $\underline{\sigma}(G)$ is the minimum singular value of the steady state gain matrix G from c to u. From equation (25) we see that in order to minimize the loss we should maximize $\underline{\sigma}(G)$.

3.2 Approach 2: Exact local method

This section summaries the most important results of (Skogestad et al. 1998) for what we here call the "exact local" method. They showed that change in the input when using a constant setpoint policy is:

$$e_u = u - u_d(d) = (J_{uu}^{-1^*}J_{du}^* - G^{-1}G_d)(d - d^*) + G^{-1}n \tag{26}$$

where * indicates the nominal optimal point, $J_{du}^* = (\frac{\partial^2 J}{\partial u \partial d})^*$ and n is the implementation error. Upon substitution of equation (26) into equation (21) we get:

$$L = \frac{1}{2}\|z\|_2^2 \tag{27}$$

where

$$z = J_{uu}^{1/2}[(J_{uu}^{-1^*}J_{du}^* - G^{-1}G_d)(d - d^*) + G^{-1}n] \tag{28}$$

By proper scaling and assuming that $\| \begin{pmatrix} d \\ n \end{pmatrix} \|_2 \leq 1$, see Figure 4, the worst-case loss is:

$$L = \frac{\overline{\sigma}(M)^2}{2} \tag{29}$$

where

$$M = [M_d \; M_n] \tag{30}$$

$$M_d = J_{uu}^{1/2}(J_{uu}^{-1^*}J_{du}^* - G^{-1}G_d)W_d \tag{31}$$

$$M_n = J_{uu}^{1/2}G^{-1}W_n \tag{32}$$

where W_d and W_n are positive diagonal matrices representing the expected magnitudes of the disturbances and implementation errors respectively. This method require that, for each *candidate set* we calculate the singular value of the matrix M.

Figure 3: Worst case disturbance, in 2-dimensional space.

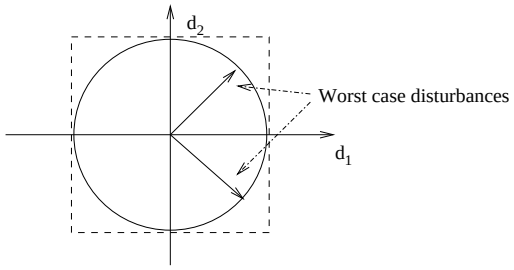

Figure 4: Worst case disturbance, in 2-dimensional space.

3.3 Best combinations of measurements

Skogestad et al. (1998) propose a method, based on approach 2 in Section (3.2), to find the best linear combination of measurements, $\Delta c = H_y y_m + H_u u = Hy$ where $H = [H_y \; H_u]$ and $y = [y_m \; u]$, in that the matrices H_y and H_u are free to choose. G and G_d in the equations (27) to (32) are:

$$G = H_u + H_y G_m^y \tag{33}$$

$$G_d = H_y G_d^y \tag{34}$$

$$W_n = H\,diag[W_{ny}, W_{nu}] \tag{35}$$

where $\Delta y = G^y \Delta u + G_d^y \Delta d$. The method require that one solves the optimization problem:

$$\min_{H_u, H_y} L = \min_{H_u, H_y} \frac{1}{2} \|z\|_2^2 \tag{36}$$

While exact, the optimization may in practice be very difficult due to the non-convexity of the problem. The "exact method" optimization tries simultaneously to minimize the effect of the disturbances (31) and the implementation error (32), by selecting the right variable combination.

3.4 Comparison with the exact local method

The linearized models in the nominal point are.

$$\Delta y = G^y \Delta u + G_d^y \Delta d \tag{37}$$

where $G_y = (\partial f_y / \partial u)^{*T}$ and $G_d^y = (\partial f_y / \partial d)^{*T}$ (in general we assume that it is possible to measure u). If we assume that the nominal point is optimal we have for the optimal input

$$y_{opt}(d) - y_{opt}(d^*) = G^y (u_{opt}(d) - u_{opt}^*) + G_d^y (d - d^*) \tag{38}$$

Skogestad et al. (1998) derived a first-order accurate approximation of the optimal input

$$u_{opt}(d) - u_{opt}(d^*) = -J_{uu}^{*-1} J_{du}^* (d - d^*) \tag{39}$$

and a first order accurate expression for the optimal output change is:

$$\Delta y_{opt} = y_{opt}(d) - y_{opt}(d^*) = \left[-G^y J_{uu}^{*-1} J_{du}^* + G_d^y \right] (d - d^*) \tag{40}$$

and since we would like to have $\Delta c = H\Delta y$ it follows that

$$\Delta c_{opt} = H\Delta y_{opt} = H\left[-G_y J_{uu}^{-1*} J_{du}^* + G_d^y\right](d - d^*) = \left[-GJ_{uu}^{-1*} J_{du}^* + G_d\right](d - d^*) \quad (41)$$

where we have introduced $G = HG_y$, $G_d = HG_d^y$. We now go back to (30) and consider the case with no implementation error ($n = 0$). Then from (31) the loss is zero if $M_d = 0$, which is equal to requiring

$$(J_{uu}^{-1^*} J_{du}^* - G^{-1} G_d) = 0 \quad (42)$$

or

$$GJ_{uu}^{-1^*} J_{du}^* - G_d = 0 \quad (43)$$

and by substituting this into (41) we have re derived that the required $\Delta c_{opt} = H\Delta y_{opt} = 0$ in (14) results in zero loss when there is no implementation error ($n = 0$). Note also from this derivation that $F = -G^y J_{uu}^{-1} J_{du} + G_d^y$, but it is probably easier to obtain Fdirectly from the non-linear model.

4 A simple two-step method considering disturbances and implementation error.

The method outlined in Section 2 did not consider implementation error. The only requirement is that the number of measurements are larger or equal to the number of disturbances and inputs. From (30) we know that the loss is $L = \overline{\sigma}(M)^2/2$ where $M = [M_d\ M_n]$. We have derived a simple procedure for finding a set of candidate variables c ($c = Hy$) such that $M_d = 0$, but M_n may still be large. However, as indicated earlier the matrix H that yield $M_d = 0$ is not unique, so we have some freedom in selecting H such that M_n remains small. It is possible to solve the problem exactly by numerically seeking the matrix H that minimize $\overline{\sigma}(M)$ (Skogestad et al. 2002).
Moreover, we here suggest a much simpler approach, which is to select from all the available measurements, a subset of n+k measurements, which are independent in the sense that they give independent information of the ninputs (u) and k disturbances (d). In addition, we scale the measurements relative to their measurement noise and the inputs and disturbances relative to their range and expected disturbance respectively. More precisely we have that $\Delta y = [G^{y\prime}\ G_d^{y\prime}][\Delta u'\ \Delta d']^T = \tilde{G}\tilde{u}$ and we look for measurements that maximize $\underline{\sigma}(\tilde{G})$ different from zero. From (32) we see that we would like measurements that maximize G, in order to minimize the implementation error. In addition we also want the disturbances to be observable from the measurements, so we should also like that G_d^y is non-singular. In addition, we need F to be non-singular based on the observation that in order for $\Delta c = HF\Delta d$ to be zero H must be in the null space of F.
Assume that u and d are independent, such that G^y and G_d^y has full rank equal to n and k respectively. Then $\tilde{G} = [G^y\ G_d^y]$ has full rank $(n+k)$, which implies that $G^y A + G_d^y$ is non-singular for all A (since G_d is non-singular). Since $\Delta u_{opt}(d) = A\Delta d = -J_{uu}^{-1} J_{du}\Delta d$, we have that F is non-singular as wanted. By finding measurement combinations such that $\tilde{G}$ is non-singular we have shown that F is non-singular. We summarize the preceding in the following procedure:

Details of procedure

Assume that $m \geq n + k$.

1. **Nominal Optimum**. Solve the optimization problem in (1) for the nominal disturbance d^*. This give the solution $(x^*, y^*) = (x_{opt}(d^*), y_{opt}(d^*))$.

2. **Linearization**. Linearize the process model (e.g by a central difference method) in the nominal optimal point. This give $G^y$and G_d^y.

3. **Scaling** Scale each measurement y_i, each input u_j and each disturbance d_k by a scaling factor:

$$y_i' = \frac{y_i}{y_{i,scl}},\ u_j' = \frac{u_j}{u_{j,scl}},\ d_k' = \frac{d_k}{d_{k,scl}} \tag{44}$$

   The scaling factors for the measurement are the corresponding implementation error ($y_{i,scl} = |n_i|$), for each input its allowed range ($u_{j,scl} = u_{j,max}$) and for the disturbance the expected disturbances. This give the scaling matrices $W_n = diag(y_{i,scl})$, $W_u = diag(u_{j,scl})$ and $W_d = diag(d_{k,scl})$

4. **Selection of measurements**. If $m > n+k$ we select measurements as follows:

   (a) **Combined process model**. Calculate the scaled process model $\Delta y' = G_y' \Delta u' + G_d^{y'} \Delta d' = W_n^{-1} G^y W_u \Delta u' + W_n^{-1} G_d^y W_d \Delta d'$ and make a new process matrix $\Delta y = \tilde{G}\tilde{u} = [G^{y'}\ G_d^{y'}][\Delta u'\ \Delta d']^T$

   (b) **Selection of first measurement**. For the first measurement calculate the row norm $\|\tilde{G}_i\|_2$ for all rows i and sort the measurements by decreasing row norm. Select the first measurement which have the highest row norm and add the corresponding process matrix in a selection process matrix $\tilde{G}_s = max_i \|\tilde{G}_i\|_2$

   (c) **Selection of the additional measurements**. Until $m = n + k$ add all remaining measurements to the already selected measurements one-by-one ($\tilde{G}_{s,j+1,i} = [\tilde{G}_{s,j}\ \tilde{G}_i]^T$ for all i and calculate the minimum singular value for all the combinations. Select the new measurement which has the highest minimum singular value and add to the selection process matrix.

5. **Null space of F.**

   (a) Calculate $\Delta y_{opt} = y_{m,opt}(d) - y_{m,opt}(d^*) = F\Delta d$ directly from the nonlinear model or by (40).

   (b) Calculate the null space $\mathcal{N}(F^T)$, such that the resulting basis for the null space is orthogonal.

6. **Selection of controlled variables**

   (a) Select H such that $H \in \mathcal{N}(F^T)$ and such that the rows of H form a orthogonal basis. This ensure that $\Delta c_{opt} = H\Delta y_{opt} = 0$

This selection guarantees that F is never singular. This requirement is conservative, since u and d are not independent, and we really need that F is non-singular in that space.

5 Examples

This section contain three examples to illustrate the proposed method. Case A is a simple "toy example", case B is a CSTR with a chemical reaction, while case C analyze a divided wall (Petlyuk) distillation column. In the following examples we use the notation c_{LC} for the controlled variables that are linear combinations of the available measurements as described above.

5.1 Case A: Toy Example

The simple toy example is from (Skogestad et al. 1998)[1]. Let $J = (u-d)^2$ where nominally $d^* = 0$ We always have $J_{opt} = 0$ corresponding to $u_{opt}(d) = d$. Assume we have the available measurements:

$$y_1 = 0.1(u-d) \qquad y_2 = 20u \qquad y_3 = 10u - 5d \qquad y_4 = u \tag{45}$$

We further assume that the system is scaled such that $|d| \leq 1$ and $|n_i| \leq 1$. We have the following model $y = G_y' u' + G_d^{y'} d'$ where;

$$G^{y'} = \begin{bmatrix} 0.1 \\ 20 \\ 10 \\ 1 \end{bmatrix} \qquad G_d^{y'} = \begin{bmatrix} -0.1 \\ 0 \\ -5 \\ 0 \end{bmatrix} \tag{46}$$

The exact worst case loss are[2] $L_1 = 100$, $L_2 = 1.1025$, $L_3 = 0.36$ and $L_4 = 4$. For the best combination of the measurements with $J_{uu} = 2$ and $J_{du} = -2$. We have that the nominal optimum for $d^* = 0$ is $y_1^* = y_2^* = y_3^* = 0$. The Hessian matrix is: $\mathcal{H}^* = \begin{bmatrix} J_{uu}^* & J_{ud}^* \\ J_{du}^* & J_{dd}^* \end{bmatrix} = \begin{bmatrix} 2 & -2 \\ -2 & 2 \end{bmatrix}$ and we need $m = n + k = 1 + 1 = 2$ measurements, resulting in using measurement y_2 and y_3. We have that $F = [20\ 5]$and $\mathcal{N}([20\ 5]^T) = [-0.2425\ 0.9701]$. We then select $c_{LC} = H_y[y_2\ y_3]^T = [-0.2425\ 0.9701]\ [y_2\ y_3]^T$. Table 1 give the worst case loss for different controlled variables. From Table 1 we see that we

Table 1: Loss for the different controlled variables

Rank	c	L
1	c_{LC}	0.0425
2	y_3	0.26
3	y_2	1.0025
4	y_4	2
5	y_1	100

get the lowest loss with $c_{LC} = H[y_2\ y_3]^T$ and it reduce the loss by a factor of 6 compared to the second best controlled variable. If we neglected the implementation error, the

[1] The loss is calculated by (29)

[2] As showed in (Skogestad et al. 1998) we have for measurement 3 that $u = (c_3 + 5d)/10$ and with $c_3 = c_{3s} + n_3$ we get $L_3 = J_3 = (u-d)^2 = (0.1n_3 + 0.5d - d)^2$.

loss for $c =_{Lc}$is zero. Skogestad et al. (2002) show that by using (36) and optimize the optimal controlled variable (also including the input) give a loss of $L = 0.0405$, which is a slight improvement compared to the combined variable found here. While simple, this example show that choosing the right variable to control is of great importance to overcome uncertainty in operation.

5.2 Case B: CSTR with chemical reaction

To further illustrate the method, we examine a continuous stirred reactor (CSTR) (Economou et al. 1986).

The process consists of an ideal continuous stirred tank reactor, see Figure 5, where the reversible exothermic reaction

$$A \rightleftharpoons B \tag{47}$$

with the reaction rate expression on the form:

$$r = k_1 C_A - k_2 C_B \qquad k_1 = C_1 e^{\frac{-E_1}{RT}} \qquad k_2 = C_2 e^{\frac{-E_2}{RT}} \tag{48}$$

where $k_1 = C_1 e^{\frac{-E_1}{RT}}$ and $k_2 = C_2 e^{\frac{-E_2}{RT}}$. The process model for the system is:
Mass balances

$$\frac{dC_A}{dt} = \frac{1}{\tau}(C_{A,i} - C_A) - r \quad \tau = \frac{M}{F} \tag{49}$$

$$\frac{dC_B}{dt} = \frac{1}{\tau}(C_{B,i} - C_B) + r \tag{50}$$

Energy balance

$$\frac{dT}{dt} = \frac{1}{\tau}(T_i - T) + \frac{-\Delta H_{rx}}{\rho C_p} r \tag{51}$$

Reaction: $A \rightleftharpoons B$

Table 2: Data for the CSTR case

Parameter	Value	Units
F	1	$holdup\ min^{-1}$
C_1	5000	s^{-1}
C_2	10^6	s^{-1}
C_p	1000	$cal\ kg^{-1}K^{-1}$
E_1	10^4	$cal\ mole^{-1}$
E_2	15000	$cal\ mole^{-1}$
R	1.987	$cal\ mole^{-1}\ K^{-1}$
T_i	input	$-$
$C_{A,i}$	1	$mole\ L^{-1}$
$C_{B,i}$	0	$mole\ L^{-1}L$
$-\Delta H_{rx}$	5000	$cal\ mole^{-1}$
ρ	1	$kg\ L^{-1}$
τ	1	min

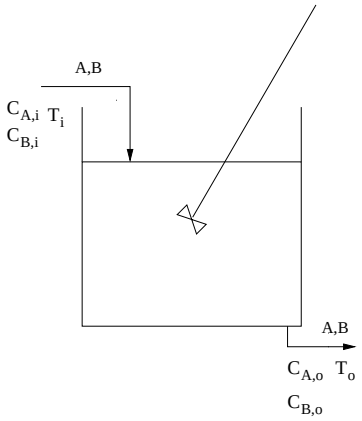

Figure 5: Figure of the CSTR-case

The operating objective is to maximize the mole fraction of the product $x_B = \frac{C_A}{C_A + C_B}$, so:

$$J(u, x, d) = x_B \tag{52}$$

Table 3: Maximum loss for different controlled variables with and without measurement error for the CSTR-case

	$\mathbf{n_{C_A,C_B}=0, n_{T,T_i}=0}$		$\mathbf{n_{C_A,C_B}=0.01, n_{T,T_i}=0.2}$	
c	**Rank**	**Loss**	**Rank**	**Loss**
c_{LC}	1	0.0031	1	0.0049
T_i	2	0.022	2	0.023
T	3	0.024	3	0.025
C_A	$infeas$	–	$infeas$	–
C_B	$infeas$	–	$infeas$	–

where the input is $u = T_i$, $x = [C_A\ C_B\ T]^T$, the disturbances are $d = [C_{A,i}\ C_{B,i}\ F]^T$ and the available measurements are $y = [C_A\ C_B\ T\ T_i]$. We assume that size of the disturbances are $C_{A,i} \in C_A^* \pm 0.3$, $C_{B,i} \in C_B^* + 0.3$ and $F \in F^* \pm 0.3$ where * denotes the nominal disturbance. In this example we assume that the worst case loss correspond to the combined worst case disturbance and implementation error in each direction The nominal optimum is:

$$x = \begin{bmatrix} C_A^* \\ C_B^* \\ T^* \end{bmatrix} = \begin{bmatrix} 0.491 \\ 0.509 \\ 438.4 \end{bmatrix};\ T_i = 435.9 \tag{53}$$

In this case we have that $n + k = m$ so we have to use all the available measurements. Five controlled variables are compared where $[c_1\ c_2\ c_3\ c_4\ c_{LC}]^T = [C_A\ C_B\ T\ T_i\ Hy]$ where $c_{LC} = Hy$ where $H = [0.59\ \ -0.81\ 0.01\ \ -0.02]$ are the combined controlled variable. We have assumed that the measurement error for the different measurements are $n_{C_A,C_B} = 0.01 mole/L$ and $n_{T,T_i} = 0.2K$ for the concentrations and the temperatures respectively. As seen from Table 3 controlling C_{LC} give the lowest loss, while controlling the concentrations give infeasible operation. All the feasible controlled variables have small losses, so there is small earnings in this case for selecting c_{LC}, based on the fact that we need more measurements.

5.3 Case C: The divided wall ("Petlyuk") distillation column

The thermally integrated divided wall ("Petlyuk") arrangement has several advantages compared to the traditionally arrangements. Smith & Triantafyllou (1992) report typical savings in the order of 30% in *both* energy and capital costs compared to traditional arrangements with two columns in series.

The Petlyuk column shown in Figure 6 has at steady state five degrees of freedom, which may be selected as the following inputs $u = [V\ L\ S\ R_l\ R_v]^T$ (boilup, reflux, mid product side-stream flow, liquid split and vapor split). There may be up to 4 product constraints: the top purity ($x_{D,A}$), the bottom purity ($x_{B,C}$), the side-stream purity ($x_{S,B}$) and the ratio of the light and heavy component in the side-stream product ($x_{S,A}/x_{S,C}$). Wolff & Skogestad (1996) have reported discontinuities in the range of feasible operation if all these constraints are optimally active. This is related to the fact that the column sections 4 and 5 are tightly coupled. In this paper we assume that we control one composition in the side-stream namely $x_{S,B}$. The disturbance vector is

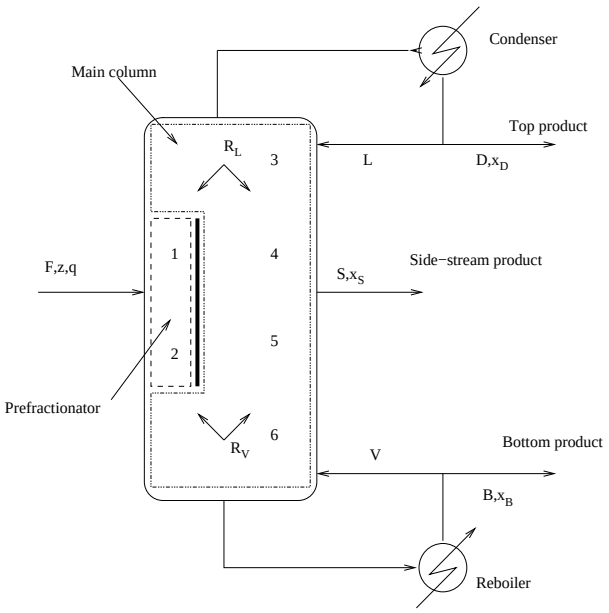

Figure 6: The Petlyuk Distillation column implemented in a single column shell.

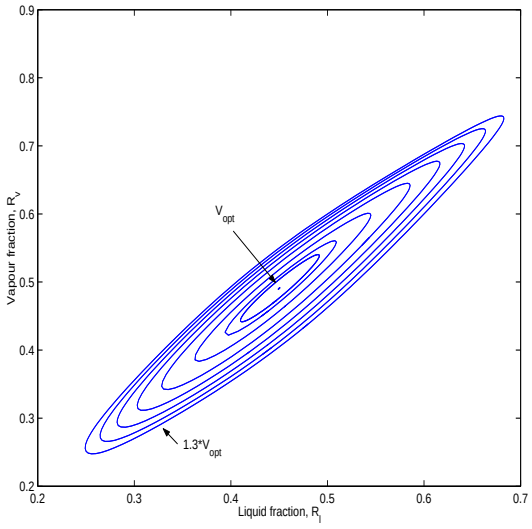

Figure 7: Plot of the contour for the nominal disturbances.

$d = [z_A \ q]$ which correspond to the composition of component A in the feed and the liquid fraction of the feed respectively. The cost function is the reboiler vapor flow

$$J(x, u, d) = V \tag{54}$$

and computations show that the optimally active constraints are the product compositions for the top, bottom and side-stream. Closing these leaves us with two remaining degrees of freedom. Halvorsen & Skogestad (1999) proposes that controlling the DT_S, a measure of the temperature profile symmetry across the dividing wall, has good self-optimizing properties. DT_S is defined as $DT_S = \sum T_{1,i} - T_{4,i} - \sum T_{2,i} - T_{5,i}$, where $T_{j,i}$ is the temperature of tray i in section j. The temperature on each tray is calculated assuming that the contribution of each component with its equilibrium temperature is proportional to its fraction. Based on the observation that the objective function (54) has one "strong" and one "weak" direction, see Figure 7, it should be enough to adjust one input to follow the "weak" direction. So, based on this, Storkaas (1999) choose to fix one input (R_v) and search for all combinations of four temperatures, $c = \pm T_{j1,i1} \pm T_{j2,i2} \pm T_{j3,i3} \pm T_{j4,i4}$ based on the "exact local" method described in Section 3.2. The top four candidates, in addition to the DT_s, for the disturbance vector $d = [F \ z_A \ z_B \ q_l \ x_{D,A,set} \ x_{S,B,set} \ x_{B,C,set} \ R_{v,set}]$[3] were as given in Table 4.

To test the method proposed in this paper, the data in appendix A.1 was used, the number of trays in each of the 6 sections, is 8. The nominal optimization gave the optimal inputs as given in Table 5. For the simulations here, the disturbance vector is assumed to be $d = [z_A \ q] = [z_{A0} \pm 0.1 \ q_0 \pm 0.1]$ and the implementation error for the combined temperature measurement and for R_v is assumed to be $|n| = [T \ R_l] = [0.4 \ 0.05]$, it is assumed that the closed composition loops have zero set-point error. Following the method outlined in Section 4 we have that m=n+k=2+2=4 so we need

[3]Note that this disturbance vector also include set-point error in the composition loops, in addition to a disturbance in component B in the feed

Table 4: The best self-optimizing controlled variables as reported by Storkaas (1999)

Name	c_1	c_2
c_{s1}	R_v	$T_{2,5} - T_{4,4} + T_{4,8} - T_{6,1}$
c_{s2}	R_v	$T_{1,7} - T_{4,3} + T_{5,1} - T_{5,7}$
c_{s3}	R_v	$T_{1,5} - T_{4,5} - T_{5,3} - T_{5,4}$
c_{s4}	R_v	$T_{2,4} - T_{2,8} - T_{4,4} - T_{5,3}$
c_{sDT_S}	R_v	$T_{1,4} + T_{2,4} - T_{4,4} - T_{5,4}$

Table 5: Optimal nominal values for the inputs.

Variable	Value
$R_{l,opt}$	0.4509
$R_{v,opt}$	0.4918
L_{opt}	1.6820
V_{opt}	1.4978
S_{opt}	0.3227

4 measurements. Only temperature measurements on each tray are considered in this analysis and the selection of the measurements give the following selected temperature measurements: $T = [T_{1,6}\ T_{2,1}\ T_{4.2}\ T_{5,7}]^T$. The optimal linear combination is:

$$\mathcal{N}(F) = \begin{bmatrix} -0.322 & -0.700 \\ 0.120 & 0.340 \\ -0.575 & 0.618 \\ 0.74 & -0.120 \end{bmatrix} \tag{55}$$

So we have that $c_{LC,1} = -0.322T_{1,6} + 0.120T_{2,1} - 0.575T_{4.2} + 0.740T_{5,7}$ and $c_{LC,2} = -0.700T_{1,6} + 0.340T_{2,1} + 0.618T_{4.2} - 0.120T_{5,7}$. Since the structure proposed here have two unconstrained degrees of freedom, while the one used by Storkaas (1999) fix R_v, we also make the assumption to fix one input (R_v) and based on this calculate the optimal linear combination of $m = n + k = 3$ measurements[4] $L_{LC,3} = -0.523T_{1,6} + 0.207T_{2,1} + 0.825T_{4.2}$. To compare the different structures the loss was calculated using the non-linear model assuming that the combined disturbance and implementation error is norm bounded. The worst case loss (L_{wc}) and the average loss ($\overline{L}$) for the different control structures are listed in Table 6, where we also have included the loss without implementation error.[5] The rank of the different structures are based on the worst case loss.

Table 6: Loss for the different controlled variables in the Petlyuk Column case

		Implementation error			No implementation error		
c_1	c_2	Rank	L_{wc}	$\overline{L}$	Rank	L_{wc}	$\overline{L}$
$c_{LC,1}$	$c_{LC,2}$	1	0.0047	0.0028	1	0.0005	0.0003
R_v	c_{s3}	2	0.0142	0.0086	4	0.0127	0.0066
R_v	c_{s4}	3	0.0143	0.0084	3	0.0055	0.0029
R_v	$c_{LC,3}$	4	0.0149	0.0068	2	0.0038	0.0011
R_v	c_{s2}	5	0.0173	0.0101	5	0.0158	0.0096
R_v	c_{s1}	6	0.0313	0.0140	6	0.0195	0.0087
R_v	c_{DT_S}	7	0.0674	0.0405	7	0.1131	0.0700

We see that all control structures have good self-optimizing properties, the DT_s has the highest loss. The performance for the control structure that fix one input depends

[4]Note that when calculating F we fix R_v at the nominal optimal point

[5]Note that in both cases, with and without implementation error, we have assumed norm bounded disturbances and implementation error, so in the case of no implementation error the disturbance vector is larger than when we include implementation error, thereby the larger loss for the no implementation case.

of course on the implementation error in R_v. The loss for the control structure $c_{LC,1}$ and $c_{LC,1}$ is negligible, the main contribution is due to the implementation error, and show true self-optimizing properties. The DT_S structure have the highest loss of the structures tested. To try to control a single measurement in the column give infeasible solutions. By trial and error,we searched for single measurements that was feasible. The only feasible temperature measurements is controlling the temperature near the feed (which in large is determined by the feed temperature). Controlling this gave a worst case loss of $L_{T_{1,7}} = 0.26$. If we compare the structures that fix R_v, we see from the table that the structure R_v and $c_{LC,3}$, have a higher worst case loss than some of the structures proposed by Storkaas (1999), which is based on the "exact method" described above. If we look at the average loss in Table 6 we see that controlling R_v and $c_{LC,3}$ have lower average loss than the structures proposed by Storkaas (1999) and is ranked second. Keep in mind that Storkaas (1999) optimized directly on the loss.

6 Concluding remarks

Selecting the right variable to control is of great importance to overcome uncertainty in operation. A new method for selecting controlled variables as linear combinations of the available measurements has been proposed in addition to a method for selecting the necessary measurements. The idea is to find a linear combination of the measurements such that $\Delta c_{opt} = H\Delta y_{opt} = 0$ by using as many measurements as there are unconstrained inputs and disturbances. From a linear point of view, the proposed method guaranty perfect self-optimizing properties if we neglect implementation error. Several examples, both SISO and MIMO, has shown that the proposed method give controlled variables with good self-optimizing properties. The selection of controlled variables has been solely based on steady state models, so in order to complete the analysis, the dynamic robustness and performance properties must be analyzed.

7 Acknowledgments

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A Appendix

A.1 Data for the Petlyuk example

Table A.1 lists the nominal data used for the Petlyuk example:

Parameter/Variable	Value
Relative volality $[\alpha_A\ \alpha_B\ \alpha_C]$	[4 2 1]
Feed composition $[z_A\ z_B\ z_C]$	[1/3 1/3 1/3]
Feed Liquid fraction q	0.477
$y_s = [x_{D,A}\ x_{S,B}\ x_{B,C}]$	[0.97 0.97 0.97]
Feed flow F	1

References

Economou, C., Morari, M. & Palsson, B. (1986), 'Internal model control 5. extension to nonlinear systems', *Ind. Eng. Chem. Process. Des. Dev.* **22**(2), 403–411.

Halvorsen, I. & Skogestad, S. (1999), 'Optimal operation of petlyuk distillation: steady-state behavior', *J. Proc. Control* pp. 407–424.

Maarleveld, A. & Rijnsdorp, J. (1970), 'Constraint control on distillation columns', *Automatica* **6**(1), 51–58.

Mahajanam, R., Zheng, A. & Douglas, J. (2001), 'A shortcut method for controlled variable selection and its application to the butane alkylation process', *Industrial and Engineering Chemistry Research* **40**(14), 3208–3216.

Morari, M., Stephanopoulos, G. & Arkun, Y. (1980), 'Studies in the synthesis of control structures for chemical processes. part i: Formulation of the problem. process decomposition and the classification of the controller task. analysis of the optimizing cotnrol structures', *AIChE Journal* **26**(2), 220–232.

Morud, J. (1995), Studies on the Dynamics and Operation of Integrated Plants, PhD thesis, Norwegian Institute of Technology, Trondheim.

Skogestad, S. (2000*a*), 'Plantwide control: the search for the optimal control structure', *J. Proc. Control* **10**, 487–507.

Skogestad, S. (2000*b*), 'Self-optimizing control: the missing link between steady-state optimization and control', *Comp.Chem.Engng.* **24**, 569–575.

Skogestad, S., Halvorsen, I. & Morud, J. (1998), 'Self-optimizing control: The basic idea and taylor series analysis', *In AIChE Annual Meeting, Miami, FL* .

Skogestad, S., Halvorsen, I. & Morud, J. (2002), 'Self-optimizing control: Local taylor series analysis', *Ind. Chem. Res.* . To be published.

Skogestad, S. & Postlethwaite, I. (1996), 'Multivariable feedback control', *John Wiley & Sons* .

Smith, R. & Triantafyllou, C. (1992), 'The design and operation of fully thermally coupled distillaton columns', *Trans. IChemE.* pp. 118–132.

Storkaas, E. (1999), Optimizing control of a integrated petlyuk distillation column, Master's thesis, Dep. of Chemical Engineering, Norwegian University of Science and Technology. In Norwegian.

Strang, G. (1988), *Linear Algebra ans its Applications*, 3 edn, Harcourt Brace & Company.

Wolff, E. & Skogestad, S. (1996), 'Operation of integrated three-product(petlyuk) distillation columns', *Ind. Eng. Chem. Res* **34**, 2094–2103.