The null space method for selecting optimal measurement combinations as controlled variables

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Abstract

The issue in this paper is to select the controlled variables $\mathbf{c}$ as combinations of the measurements $\mathbf{y}$. The objective is to obtain self-optimizing control, which is when we can achieve near-optimal steady-state operation with constant setpoints for the controlled variables, without the need to re-optimize when new disturbances perturb the plant. For sufficiently small disturbances, the null space method yields optimal controlled variables $\mathbf{c} = \mathbf{H}\mathbf{y}$ that are linear combinations of measurements $\mathbf{y}$. The requirement is that we at least have as many measurements as there are unconstrained degrees of freedom, including disturbances, and that the implementation error is neglected. The method is surprisingly simple. From a steady-state model of the plant, the first step is to obtain the optimal sensitivity matrix $\mathbf{F}$ with respect to the disturbances. The optimal matrix $\mathbf{H}$ satisfies $\mathbf{H}\mathbf{F} = 0$, so the next step is to obtain $\mathbf{H}$ in the left null space of $\mathbf{F}$. The method is used to obtain temperature combinations for control of a Petlyuk distillation column.

Keywords: Process control, Control structure selection, Optimizing control, Uncertainty, Temperature control distillation

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1 Introduction

Although not widely acknowledged by control theorists, controlling the right variables is a key element in overcoming uncertainty in operation[1;2]. This applies also when using advanced control (e.g. MPC) or real-time optimization (RTO). This paper focuses

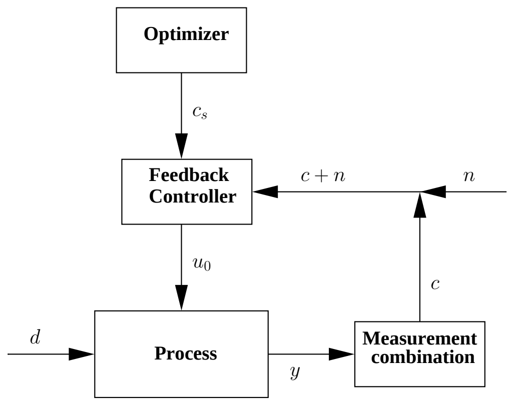

Figure 1: Block diagram of a feedback control structure including an optimizer layer.

on the interaction between the local optimization layer and the feedback control layer, see Figure 1, and more specifically on the selection of the controlled variables **c** that link these layers. Two sub-problems are important here:

1. *Selection of the controlled variables* **c**: This is a structural decision which is made before implementing the control strategy.

2. *Selection of setpoints* $\mathbf{c}_s$: This is a parametric decision which can be done both online and offline.

Here, we focus on the first, structural problem of finding the controlled variables and we will assume constant nominal optimal setpoints. As seen from Figure 1, there are two sources of uncertainty that will make a constant setpoint policy non-optimal:

1. **Disturbances d**: External unmeasured disturbances, including parameter variations.

2. **Implementation error n**: The sum of the effect of the measurement error for **y** and the control error.

Single measurements or functions or combinations of the measurements may be used as controlled variables **c**. The objective is to obtain self-optimizing control[2], which is when we can achieve near-optimal steady-state operation with constant setpoints for the controlled variables, without the need to re-optimize when new disturbances perturb the plant. Use of single measurements is simple and is the preferred choice if the loss is sufficiently small. However, for some applications there may not exist any self-optimizing single measurements, and one may consider measurement combinations.

In this paper, we consider linear combinations, that is, $\mathbf{c} = \mathbf{H}\mathbf{y}$ where $\mathbf{H}$ is a constant matrix.

Ideas related to self-optimizing control have been presented repeatedly in the process control history, but the first quantitative treatment was that of Morari et al.[1]. Skogestad[2] defined the problem more carefully, linked it to previous work, and was the first to include also the implementation error. He mainly considered the case where single measurements are used as controlled variables, that is, $\mathbf{H}$ is a selection matrix where each row has a single 1 and the rest 0's. The loss with a constant setpoint policy for expected disturbances and implementation errors was evaluated using a "brute-force" approach. An important advantage of a brute-force evaluation is that one can also identify controlled variables that may yield infeasability for certain disturbances or implementation errors. This was also considered in more detail by Larsson et al.[3] for the Tennessee-Eastman challenge problem and Govatsmark and Skogestad[4] who suggested to adjust the setpoints to achieve feasibility. However, the computational load of the "brute-force" method can be very large, so local methods based on linearizing the behavior around the steady-state are attractive. Skogestad[2] introduced the approximate maximum gain rule as a simple method for selecting controlled variables. In the multivariable case, the gain is the minimum singular value of the scaled steady-state transfer matrix from $\mathbf{u}$ to $\mathbf{c}$. A similar method was presented by Mahajanam et al.[5]. Halvorsen et al.[6] considered the maximum gain method in more detail and also proposed an exact local method which may be used to obtain the optimal measurement combination $\mathbf{H}$. However, this method is also less attractive computationally and in addition somewhat difficult to use. Hori et al.[7] illustrate the ideas introduces in this paper on indirect control which can be formulated as a subproblem of the null space method presented in this paper.

Related work has been done by Srinivasan[8],[9],[10] on measurement-based optimization to enforce the necessary condition of optimality under uncertainty. The ideas are illustrated on batch processes. Francois et al.[11] extend these ideas and focus on steady-state optimal systems, where a clear distinction is made between enforcing active constraints and requiring the sensitivity of the objective to be zero. Guay and Zhang[12] present related ideas on measurement-based dynamic optimization.

In this paper, the objective is to derive a simple method for selecting the optimal measurement combination matrix $\mathbf{H}$ for the special case with no implementation error. In fact, the method is so simple that the second author (Skogestad) thought it had to be wrong when it was proposed by the first author (Alstad). We have attempted to keep the mathematics as simple as possible. A more detailed comparison with previous results and extensions are presented in a forthcoming publication (see also[13]).

2 Problem formulation

We assume that the operational goal is to use the degrees of freedoms $\mathbf{u}_0$ to minimize the cost J_0 while satisfying equality and inequality constraints. The (original) constrained steady state optimization problem can, for a given disturbance $\mathbf{d}$ be formulated as:

$$\min_{\mathbf{x}_0,\mathbf{u}_0} J_0(\mathbf{x}_0, \mathbf{u}_0, \mathbf{d}) \tag{1}$$

subject to

$$\begin{aligned} \mathbf{f}(\mathbf{x}_0, \mathbf{u}_0, \mathbf{d}) &= 0 \\ \mathbf{g}(\mathbf{x}_0, \mathbf{u}_0, \mathbf{d}) &\leq 0 \\ \mathbf{y} &= \mathbf{f}_y(\mathbf{x}_0, \mathbf{u}_0, \mathbf{d}) \end{aligned} \tag{2}$$

where $\mathbf{x} \in \mathbb{R}^{n_x}$, $\mathbf{u}_0 \in \mathbb{R}^{n_{u_0}}$ and $\mathbf{d} \in \mathbb{R}^{n_d}$ are the states, inputs and disturbances, respectively. $\mathbf{f}$ is the set of equality constraints corresponding to the model equation, $\mathbf{g}$ is the set of inequality constraints which limits the operation, e.g. physical limits on temperature measurements or flow constraints and $\mathbf{y}$ the measurements.

We assume here that we control all active constraints (assumption **A3** below). Thus, we split the original input vector $\mathbf{u}_0$ (degrees of freedom) into:

- $\mathbf{u}'$: vector of degrees of freedom used for controlling the active constraints.
- $\mathbf{u}$: vector of remaining degrees of freedom (with dimension n_u).

Remark. It does not actually matter how the original degrees of freedom $\mathbf{u}_0$ are divided into the new subsets of manipulated variables selected for controlling the active constraints ($\mathbf{u}'$) and the "unconstrained" inputs $\mathbf{u}$, as long as the problem remains well posed. If all the inputs are used for controlling the active constraints, $\mathbf{u}' = \mathbf{u}_0$, then implementation is simple by the use of active constraint control [14;15].

We assume that online information about the system behavior is available through measurements $\mathbf{y}$. The issue in this paper is to find a set of n_u controlled variables $\mathbf{c} = \mathbf{h}(\mathbf{y})$ associated with the "unconstrained" degrees of freedom $\mathbf{u}$. In the measurement vector $\mathbf{y}$, we generally include also the input vector $\mathbf{u}_0$, including the inputs $\mathbf{u}'$ that have been selected to the control active constraints. However, the measurements of the active constraints are not included in $\mathbf{y}$, since they are constant and thus provide no information about the operation.

With the active constraints controlled, we can consider the following *unconstrained* reduced-space optimization problem where the scalar cost function J is to be minimized with respect to the n_u remaining degrees of freedom (inputs) $\mathbf{u}$:

$$\min_{\mathbf{u}} J(\mathbf{u}, \mathbf{d}) \tag{3}$$

Here the equality constraints, including the model equations and active constraints, are implicitly included in J, so J is generally not a simple function of $\mathbf{u}$ and $\mathbf{d}$.

The loss is defined as the difference between the actual cost and the optimal cost [6]

$$L = J(\mathbf{c}, \mathbf{d}) - J(\mathbf{c}^{\mathbf{opt}}(\mathbf{d}), \mathbf{d}) \approx \frac{1}{2}(\mathbf{c} - \mathbf{c}^{opt})^T \mathbf{J}_{cc}(\mathbf{c} - \mathbf{c}^{opt}) \tag{4}$$

where the second-order approximation holds for small deviations from the nominal optimum. The selected controlled variables are assumed to be independent, and the Hessian matrix $\mathbf{J}_{cc}$ is then nonsingular [6]. With a constant setpoint policy, we have $\mathbf{c} = \mathbf{c_s} + \mathbf{n}$ where $\mathbf{n}$ is the implementation error. In this paper, we assume $\mathbf{n} = 0$ (assumption **A4** below) and assume that the setpoint is nominally optimal, $\mathbf{c}_s = \mathbf{c}^{opt}(\mathbf{d}^*)$

where $\mathbf{d}^*$ is the nominal value of the disturbance. Then $\mathbf{c} = \mathbf{c}^{opt}(\mathbf{d}^*)$ and the loss for small deviations from the nominal optimum is

$$L = \frac{1}{2}\left(\mathbf{c}^{opt}(\mathbf{d}^*) - \mathbf{c}^{opt}(\mathbf{d})\right)^T \mathbf{J}_{cc}\left(\mathbf{c}^{opt}(\mathbf{d}^*) - \mathbf{c}^{opt}(\mathbf{d})\right) \tag{5}$$

This gives the following insight (which is not very surprising):

With independent controlled variables $\mathbf{c}$ *and no implementation error, a constant setpoint policy is optimal if* $\mathbf{c}^{\mathrm{opt}}(\mathbf{d})$ *is independent of* $\mathbf{d}$*, i.e.* $\mathbf{c}^{opt}(\mathbf{d}) - \mathbf{c}^{opt}(\mathbf{d}^*) = 0$.

3 Null space method

We consider the unconstrained optimization problem as given by eq. (3), that is, we assume "active constraint control" where all optimally constrained variables are assumed to be kept constant at their optimal values. The goal is to find a linear measurement combination $\mathbf{c} = \mathbf{H}\mathbf{y}$ to be kept at constant setpoints $\mathbf{c}_s$. Here $\mathbf{H}$ is a constant $n_u \times n_y$ matrix and $\mathbf{y}$ is a subset of the available measurements. We make the following assumptions:

A1 Steady-state: We consider only steady-state operation. The justification for this is that the economics of operation is primarily determined by the steady-state. Of course, this assumes that we have a control system in place that can quickly bring the plant to its new steady-state.

A2 Disturbances: Only disturbances that affect the steady-state operation are included.

A3 Active constraint control: We assume that the same active constraints remain active for all values of the disturbances and that we control these constraints.

A4 No implementation error: The implementation error is the sum of the control error and the effect of the measurement error. The assumption of no steady-state control error is satisfied if we use a controller with integral action. It is a more serious assumption to neglect the measurement error, so the method implicitly assumes that the measurements have been carefully selected.

We then have the following result:

Theorem 1 ***Null space method.*** *Assume that we have* n_u *independent unconstrained free variables* $\mathbf{u}$, n_d *independent disturbances* $\mathbf{d}$, n_y *independent measurements* $\mathbf{y}$*, and we want to obtain* $n_c = n_u$ *independent controlled variables* $\mathbf{c}$ *that are linear combinations of the measurements*

$$\mathbf{c} = \mathbf{H}\mathbf{y} \tag{6}$$

Let

$$\mathbf{F} = \frac{\partial \mathbf{y}^{opt}}{\partial \mathbf{d}^T}$$

be the optimal sensitivity matrix evaluated with constant active constraints. If $n_y \geq n_u + n_d$, it is possible to select the matrix **H** *in the left null space of* **F**, $\mathbf{H} \in \mathcal{N}(\mathbf{F}^T)$, *such that we get*

$$\mathbf{HF} = 0$$

With this choice for **H**, *keeping* **c** *constant at its nominal optimal value gives zero loss for sufficiently small disturbance changes* $\Delta\mathbf{d} = \mathbf{d} - \mathbf{d}^*$.

Proof: We first prove that selecting **H** such that $\mathbf{HF} = 0$ gives zero disturbance loss. For small disturbances, the optimal change in the measurements to a change in the disturbances can be written

$$\mathbf{y}^{opt}(\mathbf{d}) - \mathbf{y}^{opt}(\mathbf{d}^*) = \mathbf{F}(\mathbf{d} - \mathbf{d}^*) \tag{7}$$

where

$$\mathbf{F} = \begin{bmatrix} \frac{\partial y_1^{opt}}{\partial d_1} & \cdots & \frac{\partial y_1^{opt}}{\partial d_{n_d}} \\ & \ddots & \\ \frac{\partial y_{n_y}^{opt}}{\partial d_1} & \cdots & \frac{\partial y_{n_y}^{opt}}{\partial d_{n_d}} \end{bmatrix} \tag{8}$$

is the optimal sensitivity matrix evaluated at the nominal point *. From eq. (6) the corresponding optimal change in the controlled variables is $\mathbf{c}^{opt}(\mathbf{d}) - \mathbf{c}_{opt}(\mathbf{d}^*) = \mathbf{H}(\mathbf{y}^{opt}(\mathbf{d}) - \mathbf{y}^{opt}(\mathbf{d}^*)$ and by inserting eq. (7) we get

$$\mathbf{c}^{opt}(\mathbf{d}) - \mathbf{c}^{opt}(\mathbf{d}^*) = \mathbf{HF}(\mathbf{d} - \mathbf{d}^*) \tag{9}$$

From the insight stated at the end of the previous section, the constant setpoint policy is optimal if

$$\mathbf{c}^{opt}(\mathbf{d}) - \mathbf{c}^{opt}(\mathbf{d}^*) = 0 \tag{10}$$

which gives the requirement

$$\mathbf{HF}(\mathbf{d} - \mathbf{d}^*) = 0 \tag{11}$$

This needs to be satisfied for any $(\mathbf{d} - \mathbf{d}^*)$ so we must require that

$$\mathbf{HF} = 0 \tag{12}$$

To satisfy this, we need to select **H** such that $\mathbf{H} \in \mathcal{N}(\mathbf{F}^T)$, and we next need to prove under which conditions this is possible. The rank of the $n_c \times n_y$ matrix **H** is n_u (because $n_y \geq n_c$, $n_c = n_u$ and the controlled variables are independent). The rank of the $n_y \times n_d$ matrix **F** is n_d (because $n_y \geq n_d$ and the disturbances are assumed independent). The fundamental theorem of linear algebra[16] says that the left null space of **F** ($\mathcal{N}(\mathbf{F}^T)$) has rank $n_y - r$ where $r = n_d$ is the rank of **F**. To be able to find a **H** of rank n_u in the left null space of **F** we must then require, $n_y - n_d \geq n_u$ or equivalently $n_y \geq n_u + n_d$. □

Obtaining F. To obtain the optimal sensitivity matrix **F**, one needs a nonlinear steady-state model of the plant. Note that we do not necessarily need an explicit representation of the model equations, as we can find **F** numerically. For example, we may use one of the commercial steady-state process simulators like Aspen™ or Hysys™. In theory, one may even obtain **F** from experiments on a real operating plant, but it seems unlikely that will be sufficiently accurate.

Numerically, the $n_y \times n_d$ matrix **F** may be obtained by perturbing the disturbances **d** and re-solving the optimization problem in eq. (3) with the active constraints constant:

1. At nominal conditions ($\mathbf{d} = \mathbf{d}^*$), use the steady-state model to obtain the nominal optimum $\mathbf{y}^{opt}(\mathbf{d}^*)$ and identify the active constraints (finding the nominal optimum may *not* be an easy task, because the optimization problem is generally non-convex).

2. For each of the n_d disturbances: Make a small perturbation ($d_k = d_K^* + \Delta d_k$) and resolve the optimization with the constant active constraints to obtain $\mathbf{y}^{opt}(\mathbf{d})$ (this is generally an easy task, because it is only a small perturbation to the nominal solution).

3. Let $\Delta \mathbf{y}^{opt} = \mathbf{y}^{opt}(\mathbf{d}) - \mathbf{y}^{opt}(\mathbf{d}^*)$ and obtain $\mathbf{F}$ numerically using (8).

Ganesh and Biegler[17] provide an efficient and rigorous strategy for finding $\mathbf{F}$ based on a reduced Hessian method. In addition, some process simulators have built-in optimizers from which the optimal sensitivity $\mathbf{F}$ may be available.

The next step is to obtain $\mathbf{H}$. Numerically, $\mathbf{H}$ may be obtained from a singular value decomposition of $\mathbf{F}^T$. We have $\mathbf{HF} = 0$ or equivalently $\mathbf{F}^T\mathbf{H}^T = 0$. Thus, selecting $\mathbf{H}^T$ as the input singular vectors of $\mathbf{F}^T$ corresponding to zero singular values in $\mathbf{F}^T$ gives an orthogonal basis.

Example 1 *Consider a simple example with one unconstrained degree of freedom u, $n_u = 1$, and one disturbance d, $n_d = 1$. The cost function to be minimized during operation (for varying d) is*

$$J(u, d) = (u - d)^2$$

Nominally $d^* = 0$. We have available two measurements

$$y_1 = 0.9u + 0.1d$$
$$y_2 = 0.5u - d$$

Since $n_y = 2 = n_u + n_d$ and the two measurements are independent it is possible to find a linear measurement combination

$$\mathbf{c} = \mathbf{Hy} = \begin{bmatrix} h_1 & h_2 \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = h_1 y_1 + h_2 y_2$$

for which a constant setpoint gives zero disturbance loss, at least locally. We first need to obtain the optimal sensitivity matrix $\mathbf{F}$. Optimality is ensured when $\frac{\partial J}{\partial u} = 2(u - d) = 0$ which gives $u^{opt} = d$ and $J^{opt} = 0\ \forall d$. The corresponding optimal outputs are

$$y_1^{opt} = d$$
$$y_2^{opt} = -0.5d$$

and we see that $\mathbf{F}^T = [1\ -0.5]$. From the null space method the optimal matrix $\mathbf{H}$ must satisfy $\mathbf{HF} = 0$, or

$$h_1 f_1 + h_2 f_2 = 0$$

$$h_1 + h_2(-0.5) = 0 \Rightarrow h_1 = 0.5h_2$$

The solution is non-unique. For example, selecting $h_2 = 1$ gives

$$c = 0.5y_1 + y_2$$

Keeping the controlled variable **c** *at its nominally optimal setpoint $c_s = c^{opt}(d^*) = 0$, gives zero disturbance loss, as is easily verified. Generally, the loss will be zero only locally, i.e. for small changes in d, but for this example the cost function is quadratic with linear model equations, and the loss will be zero for any magnitude of the disturbance d.*

4 Discussion

4.1 Measurement selection

One weakness of the null space method is that it does not consider the measurement error, or more generally the implementation error. If we have extra measurements, that is, $n_y > n_u + n_d$, then we have extra degrees of freedom in selecting **H** that should be used to reduce the sensitivity to measurement error. A simple approach is to select a subset of the "best" measurements such that we get $n_y = n_u + n_d$, but which should these measurements be? This is outside the scope of this paper, and is treated in more detail a forthcoming publication on the extended null space method (see also [13]), but let us provide some results. Let the linear model be

$$\Delta\mathbf{y} = \mathbf{G}^y\Delta\mathbf{u} + \mathbf{G}_d^y\Delta\mathbf{d} = \tilde{\mathbf{G}}^y\begin{bmatrix}\Delta\mathbf{u}\\ \Delta\mathbf{d}\end{bmatrix} \tag{13}$$

where **y** has been scaled with respect to the expected measurement error, and **u** and **d** have been scaled such that they have similar effects on the cost. It can then be shown that a reasonable approach is to maximize the minimum singular value of the matrix $\tilde{\mathbf{G}}^y = \begin{bmatrix}\mathbf{G}^y & \mathbf{G}_d^y\end{bmatrix}$ from the combined inputs and disturbances to the selected measurements. To understand why this is reasonable, we may imagine using the measurements to back-calculate the inputs and disturbances. For the case with $n_y = n_u + n_d$, $\tilde{\mathbf{G}}^y$ is invertible and we get

$$\begin{bmatrix}\Delta\mathbf{u}\\ \Delta\mathbf{d}\end{bmatrix} = [\tilde{\mathbf{G}}^y]^{-1}\Delta\mathbf{y} \tag{14}$$

In order to avoid sensitivity to measurement errors in **y** we want the norm of $[\tilde{\mathbf{G}}^y]^{-1}$ to be small which is equivalent to wanting a large minimum singular value, $\underline{\sigma}(\tilde{\mathbf{G}}^y)$. From (14) we also see why it is reasonable to require $n_y \geq n_u + n_d$ in the null space method, because this is the requirement for being able to uniquely determine from the measurements all independent variables (inputs and disturbances).

4.2 Freedom in selecting H

Even for the case $n_y = n_u + n_d$, there are an infinite number of matrices **H** that satisfy $\mathbf{HF} = 0$. This stems from the freedom of selecting basis vectors for the null space [16]. Let $\mathbf{H}_0$ be one such matrix, i.e. $\mathbf{H}_0\mathbf{F} = 0$. For example, $\mathbf{H}_0$ may consist of the one set of basis vectors that span the null space of $\mathbf{F}^T$. Then $\mathbf{H} = \mathbf{C}\mathbf{H}_0$ also satisfies $\mathbf{HF} = 0$ provided the $n_c \times n_c$ matrix $\mathbf{C}$ is non-singular.

Actually, the degrees of freedom in selecting $\mathbf{C}$ (and $\mathbf{H}$) are the same as the degrees of freedom that are used in steady-state decoupling (or similar) in control. The linear model for the selected controlled variables can be written

$$\Delta\mathbf{c} = \mathbf{H}\Delta\mathbf{y} = \mathbf{H}\mathbf{G}^y\Delta\mathbf{u} + \mathbf{H}\mathbf{G}^y_d\Delta\mathbf{d} = \mathbf{G}\Delta\mathbf{u} + \mathbf{G}_d\Delta\mathbf{d} \tag{15}$$

and the degrees of freedom in the matrix $\mathbf{C}$ may be used to affect $\mathbf{G} = \mathbf{H}\mathbf{G}^y$ and $\mathbf{G}_d = \mathbf{H}\mathbf{G}^y_d$. For example, it is possible to select $\mathbf{H}$ such that $\mathbf{G} = \mathbf{I}$, and we have a decoupled steady-state response from $\mathbf{u}$ to $\mathbf{c}$.

4.3 Disturbance elimination

The required number of measurements in the null space method, $n_y \geq n_u + n_d$, may be large if we have many disturbances (n_d large). In practical applications, it is therefore desirable to reduce the number of disturbances. Unfortunately, there does not seems to be any simple rigorous procedure for eliminating unimportant disturbances, although some approaches are discussed in Chapter 5 in Alstad[13]. It is obvious that we may eliminate disturbances d_i that satisfy both of the following conditions:

1. No steady-state effect on the measurements ($\mathbf{y}$ is independent of d_i, i.e., $\mathbf{G}^y_{d_i} = 0$), *and*
2. No steady-state effect on the optimal operation ($\mathbf{u}^{opt}$ is independent of d_i).

It could be argued that we may eliminate all "unobservable" disturbances that satisfy condition 1, because we have no way of detecting them and thus correcting for them. However, such disturbances may affect the optimal operation and result in large losses, so an analysis based on neglecting them may be highly misleading. To achieve acceptable operation in such cases, we need to obtain additional measurements, for example, of the disturbance itself. One example would be a price change as is discussed in more detail below. Also, we cannot eliminate all disturbance that have no effect on optimal operation and thus satisfy condition 2. This is because the disturbance may effect a measurement, and controlling this measurement will then result in a loss.

In practice, with too few measurements, one may eliminate some disturbances and obtain the controlled variables $\mathbf{c} = \mathbf{H}\mathbf{y}$ using the null space method, but one should afterwards analyze the loss with all disturbances included. Alternatively, one may be able to obtain the optimal combination numerically using the exact local method of Halvorsen et al.[6] or the extended null space method presented in a forthcoming publication.

4.4 Physical interpretation

The proposed null space method yields controlled variables that are linear combinations of the available measurements. A disadvantage is that the physical interpretation of what we control is usually lost. This is by no means a fundamental limitation, since in principle we can control any signal from the process as long as they are independent. Thus, if all measurements are regarded as signals, the concept of controlling a combination of signals may be easier to grasp. If possible, one can choose to combine measurements of one type, for instance only temperatures (e.g. in a distillation column) or only mass flows. In any case, we can scale variables such that the resulting measurements are dimensionless, which is common in practice.

4.5 Change in active constraints

A new set of optimal controlled variables (**H**) needs to be found for each set of active constraints. If the active constraints change, this needs to be identified and some logic is involved in order to switch to a new set of controlled variables. Thus, for a process with a small operating window, where the active constraints shift with the disturbances, other methods may be better suited for optimizing control, e.g. real-time optimization (RTO) combined with Model predictive control (MPC). Alternatively, we could use the ideas of Arkun and Stephanopoulos[15] on how to handle varying active constraints.

4.6 Non-observable disturbances and price changes

Self-optimizing control is based on using feedback to detect disturbances and optimally adjust the inputs so as to achieve near-optimal operation. Thus, one must require that the disturbances are observable (visible) in the measurements $\mathbf{y}$. One example of a "disturbance" that is not visible in the measurements is prices. However, prices p_i do enter in the objective function, because typically $J = \sum_i p_i x_i$, and price changes will change the optimal point of operation.

To handle price changes (or more generally disturbances that are not observable in the measurements $\mathbf{y}$), one must assume that the price (disturbances) is known (measured). Price changes can then be handled in two ways:

1. Adjust the setpoints in a feedforward manner. Then, for a price change $\Delta\mathbf{p}$ we have that
$$\mathbf{c}_s = \mathbf{c}_s(p^*) + \mathbf{H}\mathbf{F}_p\Delta\mathbf{p} \tag{16}$$
where $\mathbf{F}_p = \left(\frac{\mathrm{d}\mathbf{y}^{opt}}{\mathrm{d}\mathbf{p}^T}\right)$ is the optimal sensitivity from the prices to the measurements.
2. Include the prices as extra measurements in y and use the regular procedure of selecting self-optimizing control variables as above.

The first approach is probably the simplest and most transparent[18].

4.7 Local optimality and other limitations

The proposed nullspace method is optimal only locally. It is globally optimal in cases where the sensitivity matrix $\mathbf{F}$ does not depend on the operating point, for example, for a system with a quadratic cost objective and linear model equations. Nevertheless, based on several case studies this does not seem to be an important limitation in most practical cases. More serious limitations are that 1) implementation errors are not explicitly handled (except through the selection of which measurements to use), 2) the nominal operating point is assumed to be optimal (i.e., the optimal setpoints for $\mathbf{c}$ need to be obtained), and 3) the optimal active constraints are assumed not to change.

4.8 Controllability

All derivations here are based on steady-state models, and we must later check that the candidate structure has acceptable controllability. If not, we may go back and look for other measurements to use in the combination.

5 Petlyuk distillation case study

5.1 Introduction

The Petlyuk distillation column is an appealing alternative for the separation of ternary mixtures. Compared with the traditional configuration of two columns in series, typical savings in the order of 30% are reported in *both* energy and capital costs [19]. However, the savings in energy may be difficult to achieve in practice, and the goal here is to suggest simple control policies. We are looking for a "self-optimizing" control structure which, despite of external disturbances and measurements errors, gives near-optimal operation with constant setpoints.

The Petlyuk column has six sections and may be implemented as a "divided wall" column as illustrated in Figure 2. The boilup and reflux streams are split at the dividing wall with split fractions $R_V = V_2/V_6$ and $R_L = L_1/L_3$, respectively. With a given feed and pressure, the Petlyuk column has five steady-state degrees of freedom. For example, these may be selected as

$$\mathbf{u}_0^T = \begin{bmatrix} L & V & S & R_L & R_V \end{bmatrix} \tag{17}$$

corresponding to the reflux, boilup, side-stream flow, liquid split and vapor split, respectively.

Assume that the feed consists of three key components A, B and C with mole fractions $\mathbf{z}^T = [z_A\ z_B\ z_C]$ with mole flow rate F and liquid fraction q. The light component A dominates in the distillate stream (D), component B dominates in the side-stream (S) while the heavy component C dominates in the bottom stream (B). We consider a case study with a relative volatility of 3 between the key components and 8 theoretical stages in each of the six sections. Key data are given in Table 1 and further details are found in Chapter 8 in Alstad [13].

We assume that the operational objective is to use the five degrees of freedom to minimize the energy usage, $J = V$, while maintaining the following three product specifications ("active constraints"):

1. Distillate purity ($x_{A,D}$)
2. Bottom purity ($x_{C,B}$)
3. Side-stream purity ($x_{B,S}$)

where $x_{i,j}$ is mole fraction of component "i" in stream "j". Minimizing the energy (V) with respect to the remaining two degrees of freedom ($n_u = 2$ gives an unconstrained nominal optimum with

$$\mathbf{u_0}^{opt}(\mathbf{d}^*)^T = [L^*\ V^*\ S^*\ R_L^*\ R_V^*] = \begin{bmatrix} 0.7618 & 0.5811 & 0.3227 & 0.3792 & 0.5123 \end{bmatrix}$$

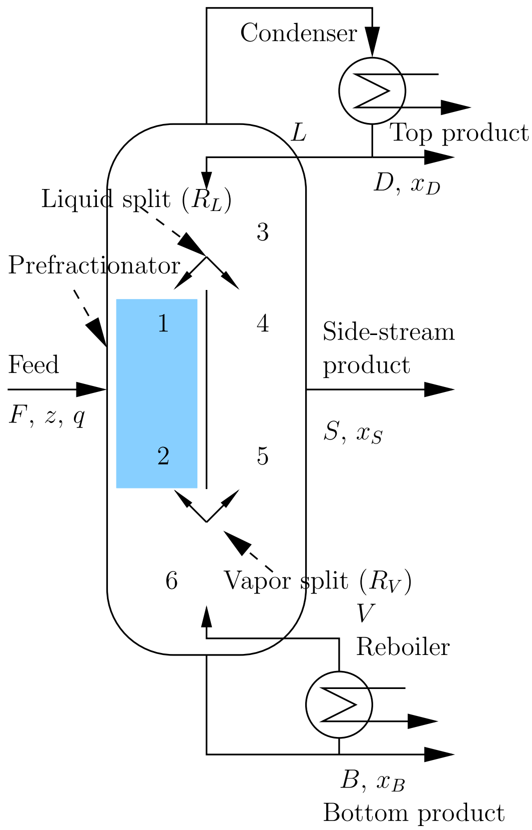

Figure 2: The Petlyuk distillation column implemented in a single shell ("divided wall column").

Table 1: Data for the Petlyuk simulation case

Physical data	
Relative volatilities	$\alpha^T = [9\ 3\ 1]$
# stages section	$N_T = 8$
Boiling point *A*, *B* and *C* [*K*]	$\mathbf{T}_B^T = [299.3\ 342.15\ 399.3]$
Feed	
Flow	$F^* = 1$
Composition	$\mathbf{z}^{*T} = [1/3\ 1/3\ 1/3]$
Liquid fraction	$q^* = 0.477$
Product compositions	
Distillate	$x_{A,D}^{0^*} = 0.97$
Side-stream	$x_{B,S}^{0^*} = 0.97$
Bottom	$x_{C,B}^{0^*} = 0.97$
Disturbances	
Feed flow	$F = F^* \pm 0.1$
Feed composition	$z_A = z_A^* \pm 0.1$
	$z_B = z_B^* \pm 0.1$
Liquid fraction	$q = q^* \pm 0.1$
Product specification	$x_{A,D}^0 = x_{A,D}^{0^*} \pm 0.01$
	$x_{C,B}^0 = x_{C,B}^{0^*} \pm 0.01$
	$x_{B,S}^0 = x_{B,S}^{0^*} \pm 0.01$
Measurement/implementation errors	
Temperatures	0.5 K (absolute)
Flows	2.5% (relative)
R_L, R_V	0.025 absolute

The minimum boilup (V_{min}) with an infinite number of stages is $V_{min}^{\infty} = 0.5438$, so the nominal optimal boilup of 0.5811 is approximately 6% higher than the theoretical minimum.

Since the objective is to minimize the boilup, which also is an input, one may mistakenly believe that one can use an open-loop approach, where the optimal value for the boilup is calculated and implemented in the column, $V = V^{opt}$. However, Halvorsen and Skogestad [20] point out that such an approach is impossible (or at least very difficult):

1. Operation is infeasible for $V < V^{opt}$, so we need to ensure that $V \geq V^{opt}$.
2. The optimal value of V varies with respect to disturbances and may be hard to find, requiring a detailed model and a direct measurement of the disturbances (or a very accurate estimate) in order to be viable. This is unrealistic in most cases.
3. Measurement or estimation of V may be difficult to achieve (measuring vapor flow), thus it may be sensitive to measurement error when trying to implement the optimal V.

Thus, the approach here is to use self-optimizing control. As candidate measurements ($\mathbf{y}$) we include all flows (ratioed to the feed) as well as the temperature on all stages. This gives about 60 measurements. The main component compositions in each product stream are also measured, but since they are active constraints (and thus are constant) they are not useful for self-optimizing control and are not included in $\mathbf{y}$.

Alternative 1: Two degrees of freedom. We first consider using the two available unconstrained degrees of freedom to control (and fix) two measurement combinations. The two degrees of freedom could for example be R_L and R_V (but the specific choice does not actually matter). The assumed disturbance vector is (these are found to be the most important disturbances from the one listed in Table 1).

$$\mathbf{d}_{tdf}^T = \begin{bmatrix} z_A & z_B & q & n_{x_{B,S}} \end{bmatrix} \tag{18}$$

where the subscript *tdf* denotes that the are two degrees of freedom. The last entry represents the composition offset for the sidestream product. The feedrate F is not included because we have choosen to use only intensive variables when forming the controlled variables (with a constant column efficiency, a feedrate change is automatically compensated for at steady state by fixing intensive variables).

To use the nullspace method, we need from Theorem 1 to combine $n_u + n_d = 2 + 4 = 6$ measurements. To select the best sub-set of 6 out of the about 60 candidate measurements, we use the measurement selction approach mentioned in the discussion section. This results in the following six temperature measurements

$$\mathbf{y}_{tdf}^T = \begin{bmatrix} T_{37} & T_{11} & T_{43} & T_{25} & T_4 & T_9 \end{bmatrix} \tag{19}$$

The location of the selected measurements is shown in Figure 3. Note that the majority of measurements are located in the bottom part of the column while only two measurements are located above the feed point. The sensitivity matrix $\mathbf{F}$ was obtained numerically by perturbing each of the four disturbances and reoptimizing. The null space method in Theorem 1 gives the optimal matrix $\mathbf{H}$ corresponding to the following

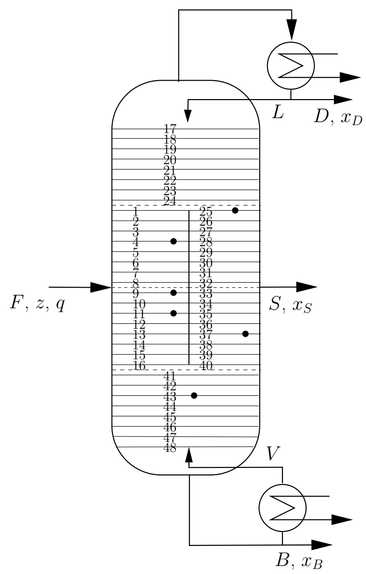

Figure 3: Physical location of the best subset of measurements for alternative 1.

measurement combinations (controlled variables):

$$c_{tdf,1} = -0.472T_{37} + 0.312T_{11} + 0.113T_{43} - 0.457T_{25} + 0.561T_4 - 0.378T_9 \quad (20)$$

$$c_{tdf,2} = 0.185T_{37} + 0.376T_{11} - 0.667T_{43} - 0.524T_{25} - 0.154T_4 + 0.285T_9 \quad (21)$$

Alternative 2: One degree of freedom. We have until now assumed that the vapor split R_V is a degree of freedom during operation (available for manipulation), but most likely this is not possible in practice. It is therefore interesting to consider the case where R_V is fixed. In fixing R_V, we add the implementation error of controlling R_V to the disturbance vector and get

$$\mathbf{d}_{odf}^T = \begin{bmatrix} z_A & z_B & q & n_{x_{B,S}} & n_{R_V} \end{bmatrix} \quad (22)$$

The corresponding minimum number of measurements needed for the nullspace method is $n_u + n_d = 1 + 5 = 6$. The following subset of measurements was obtained

$$\mathbf{y}_{odf}^T = \begin{bmatrix} T_{37} & T_{10} & T_{43} & T_{27} & T_5 & T_{12} \end{bmatrix} \quad (23)$$

which is very similar to the tdf-case. The optimal measurement combination from the nullspace method is

$$c_{odf} = -0.388T_{37} - 0.658T_{10} + 0.192T_{43} - 0.0471T_{27} + 0.448T_5 + 0.421T_{12} \quad (24)$$

Loss evaluation using non-linear model. The two above control structures are compared with two alternative control structures, see Table 2. Alternative 3 in Table 2 is an control structure proposed by Halvorsen and Skogestad [20] ($c_{DT_S} = (T_4 - T_{28}) + (T_{12} -$

Table 2: Alternative control structures

Alt.	c_1	c_2	c_3	c_4	c_5	
1	$x_{A,D}$	$x_{B,S}$	$x_{C,B}$	c^1_{tdf}	c^2_{tdf}	Null space method, use R_V and R_L
2	$x_{A,D}$	$x_{B,S}$	$x_{C,B}$	R_V	c_{odf}	Null space method, fix R_V
3	$x_{A,D}$	$x_{B,S}$	$x_{C,B}$	R_V	DT_S	Fix DT_S and R_V
4	$x_{A,D}$	$x_{B,S}$	$x_{C,B}$	R_V	R_L	Constant splits R_V and R_L

T_{36}), is a measure of the temperature gradient over the dividing wall), while alternative 4 is the "open loop" approach.

The nonlinear losses for the alternative control structures for different realistic magnitude of the disturbances and measurement errors are given in Table 3.

The conclusion is that the self-optimizing properties are excellent for both alternatives 1 and 2. When fixing two measurement combinations in alternative 1, the loss in energy usage (V) is less than 0.02% for the disturbances considered above and about 0.2% for a disturbance in bottom composition (which was not considered when deriving c_{tdf}). The losses with respect to implementation errors are also very small. When fixing R_V and c_{odf} (alternative 2), the loss is about 10 times higher for the disturbances considered above, but it is still only about 0.2% and thus insignificant from a practical point of view. Since the loss is so small, the strategy of fixing R_V and c_{odf} is clearly preferred for practical implementations. The loss for the other two control structures are higher, with a maximum disturbance loss of 11 % for alternative 3 and 95 % for alternative 4. Alstad[13] also considered alternatives where R_V and a single temperature was fixed. The best was to fix a temperature just below the sidestream with a maximum disturbance loss of about 1.4 %.

In Alstad[13] nonlinear closed-loop dynamic simulations are shown. which confirm the practical implementation of this strategy.

Table 3: Percentage loss (L) for all disturbances. ("−" denotes negative perturbation, "+" denotes positive perturbation from the nominal value). The last two columns (L_n) give maximum loss and average loss for the implementation errors.

	Loss [%]							
Alt.	F_-	F_+	z_{A-}	z_{A+}	z_{B-}	z_{B+}	q_{l-}	q_{l+}
1	0.0	0.0	0.0171	0.0207	0.0166	0.0111	0.0001	0.0000
2	0.0	0.0	0.0037	0.1340	0.2247	0.1666	0.1876	0.1084
3	0.0	0.0	5.0840	11.8810	0.3469	0.8295	1.0441	1.1740
4	0.0	0.0	46.7037	6.3019	95.1660	9.8256	32.4629	6.0578

	Loss [%]							
Alt.	$x^0_{A,D+}$	$x^0_{A,D-}$	$x^0_{C,B+}$	$x^0_{C,B-}$	$x^0_{B,S+}$	$x^0_{B,S-}$	L_n^{max}	L_n^{avg}
1	0.0025	0.0095	0.0639	0.2082	0.0002	0.0007	0.0213	0.0117
2	0.0040	0.0110	0.0060	0.0174	0.0004	0.0004	0.0847	0.0206
3	0.0074	0.0207	0.0033	0.0034	0.0025	0.0075	0.2108	0.0475
4	0.0262	0.0253	0.0245	0.0311	0.2579	1.0198	9.3142	3.6254

6 Conclusion

This paper has introduced the null space method for selecting controlled variables $\mathbf{c}$. We consider a constant setpoint policy, where the controlled variables are kept at constant setpoints $\mathbf{c}_s$. We propose to select self-optimizing controlled variables as linear combinations $\mathbf{c} = \mathbf{H}\mathbf{y}$ of a subset of the available measurements $\mathbf{y}$. With no implementation error, it is locally optimal to select $\mathbf{H}$ such that $\mathbf{HF} = 0$, where $\mathbf{F} = (\mathrm{d}\mathbf{y}^{opt}/\mathrm{d}\mathbf{d}^T)$ is the optimal sensitivity with respect to disturbance $\mathbf{d}$. However, ignoring the implementation error is a serious shortcoming for some applications. To partly compensate for this, it is important to use measurement $\mathbf{y}$ that are independent and not sensitive to measurement error. Another shortcoming is that a new set of controlled variables (for the unconstrained degrees of freedom) needs to be found for each possible set of active constraints. The global properties of the proposed variable combination $\mathbf{c} = \mathbf{H}\mathbf{y}$ needs to evaluated by computing the loss for expected disturbances and implementation errors using the nonlinear model, and a controllability analysis should also be performed before implementation. The method has been illustrated on a Petlyuk distillation example where we find that the null space method yields controlled variables with very small losses.

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