

Linear Combination of Gradients as Optimal Controlled Variables

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Abstract

In this paper, we show that optimal economic operation can be achieved using feedback control, by controlling the right variables that translate economic objectives into control objectives. We formulate a generic framework for selecting the controlled variables based on the Karsh-Kuhn-Tucker (KKT) conditions, that can be used to select the optimal controlled variables for different operating conditions. The proposed generalized framework is given as a linear combination of cost gradients. Furthermore, we also show that, the proposed linear gradient combination framework can be used to select the economically optimal controlled variables for parallel operating units. The proposed linear gradient combination framework can be used with any gradient estimation scheme. A benchmark Williams-Otto reactor example is used to demonstrate the effectiveness of the proposed CV selection framework.

Keywords: Measurement-based optimization, self-optimizing control, gradient

1. Introduction

One of the challenges that impede practical implementation of traditional real-time optimization is the need to solve numerical optimization problems online. In order to avoid the need to solve numerical optimization problems, there is an increasing interest in a class of methods for real-time optimization, known as “feedback-optimizing control” or “direct-input adaptation”. Here the objective is to indirectly move the optimization into the control layer, thereby converting the optimization problem into a feedback control problem.

The idea of achieving optimal operation using feedback control predates 1980s, where Morari et al. (1980) proposed a “feedback optimizing control” structure that translates the economic objectives into process control objectives. This idea was further studied in detail by Skogestad (2000), where the objective was to find a simple feedback control strategy, with near optimal cost subject to constraints.

When converting the optimization problem into a feedback control problem, one of the most important question that arises is “*What to control?*”. In other words, one has to find appropriate controlled variables that translates the economic objectives into control objectives. Addressing this problem, Skogestad (2000) advocates that it is important to control the constraints tightly that are optimally active. This is known as active constraint control and results in zero loss. In fact, the feedback optimizing control structure presented by Morari et al. (1980) also resulted in active constraint control. If there are

any unconstrained degrees of freedom, Skogestad (2000) advocates that one should find self-optimizing variables, which when kept at a constant setpoint, leads to acceptable loss.

The simplest and the earliest methods to find a self-optimizing CV was using a brute-force method that evaluates the performance loss of different possible candidate CVs (Skogestad, 2000). Since then there has been several developments in methods to select the optimal measurements or linear measurement combinations $\mathbf{c} = \mathbf{H}\mathbf{y}$ as self-optimizing CVs, where \mathbf{H} is known as the optimal selection matrix. Some notable approaches of finding the optimal selection matrix \mathbf{H} include the nullspace method (Alstad and Skogestad, 2007) and the exact local method (Alstad et al., 2009), which are based on linearized models around some nominal operating point.

The main drawback of using a linear measurement combination is that the loss increases as the optimal point moves away from the point of linearization. Using linear measurement combination also involves selecting a subset of all the available measurements that one wants to include in the measurement combination $\mathbf{c} = \mathbf{H}\mathbf{y}$, which may require additional offline analysis and/or process insight.

In this paper, we consider the linear combination of cost gradients as self-optimizing variables instead of linear measurement combination. By using a linear *gradient* combination, we show that one can achieve zero loss even when disturbances occur. To this end, we propose a generalized framework for selecting the self-optimizing variables based on the Karush-Kuhn-Tucker (KKT) conditions that can be used for different operating scenarios.

2. Selection of controlled variables

Consider the steady-state economic optimization problem

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

where $\mathbf{u} \in \mathbb{R}^{n_u}$ denotes the vector of manipulated variables (MV) and $\mathbf{d} \in \mathbb{R}^{n_d}$ denotes the vector of disturbances, $J: \mathbb{R}^{n_u} \times \mathbb{R}^{n_d} \rightarrow \mathbb{R}$ is the scalar cost function and $\mathbf{g}: \mathbb{R}^{n_u} \times \mathbb{R}^{n_d} \rightarrow \mathbb{R}^{n_g}$ denotes the vector of constraints. The Lagrangian of the optimization problem is given by

$$\mathcal{L}(\mathbf{u}, \mathbf{d}) = J(\mathbf{u}, \mathbf{d}) + \boldsymbol{\lambda}^\top \mathbf{g}(\mathbf{u}, \mathbf{d}) \quad (2)$$

where $\boldsymbol{\lambda} \in \mathbb{R}^{n_g}$ is the vector of Lagrangian multipliers for the constraints. The Karush-Kuhn-Tucker conditions for optimality states that the first order necessary conditions are satisfied when

$$\nabla_{\mathbf{u}} \mathcal{L}(\mathbf{u}, \mathbf{d}) = \nabla_{\mathbf{u}} J(\mathbf{u}, \mathbf{d}) + \boldsymbol{\lambda}^\top \nabla_{\mathbf{u}} \mathbf{g}(\mathbf{u}, \mathbf{d}) = 0 \quad (3a)$$

$$\mathbf{g}(\mathbf{u}, \mathbf{d}) \leq 0 \quad (3b)$$

$$\boldsymbol{\lambda}^\top \mathbf{g}(\mathbf{u}, \mathbf{d}) = 0 \quad (3c)$$

$$\boldsymbol{\lambda} \geq 0 \quad (3d)$$

Depending on the disturbances realization, different constraints may be active. By active constraints, we mean a set of constraints $\mathbf{g}_\Delta \subseteq \mathbf{g}$ that are optimally at its limiting value. Let $n_a \leq n_g$ denote the number of active constraints $\mathbf{g}_\Delta(\mathbf{u}, \mathbf{d})$. The complementary

slackness condition (3c) states that, for the active inequality constraints $\mathbf{g}_\Delta(\mathbf{u}, \mathbf{d}) = 0$, the corresponding Lagrange multipliers are positive $\lambda_\Delta > 0$ and for the constraint $\mathbf{g}_\Pi(\mathbf{u}, \mathbf{d}) < 0$ that are not active, the corresponding Lagrange multipliers are zero, $\lambda_\Pi = 0$.

The Lagrangian (2) can be re-written as

$$\mathcal{L}(\mathbf{u}, \mathbf{d}) = J(\mathbf{u}, \mathbf{d}) + [\lambda_\Delta \quad \lambda_\Pi]^\top \begin{bmatrix} \mathbf{g}_\Delta(\mathbf{u}, \mathbf{d}) \\ \mathbf{g}_\Pi(\mathbf{u}, \mathbf{d}) \end{bmatrix} \Rightarrow J(\mathbf{u}, \mathbf{d}) + \lambda_\Delta^\top \mathbf{g}_\Delta(\mathbf{u}, \mathbf{d}) \quad (4)$$

For a system with n_g constraints, we can have at most 2^{n_g} active constraint regions. To convert the optimization problem into a feedback control problem, we need to find optimal controlled variables for each active constraint region.

Active constraint control: As mentioned in Skogestad (2000), if there are any active constraints, we control the active constraints tightly. For each active constraint, we choose an associated CV, usually the constraint itself, i.e. $\text{CV} = \mathbf{g}_\Delta$ which is controlled to its limit. If the number of active constraints is the same as the number of MVs, then active constraint control is sufficient to achieve optimal operation.

Unconstrained degrees of freedom: After controlling the active constraints, we need to find CVs for any remaining $(n_u - n_a)$ unconstrained degrees of freedom. In this case, from (3) and (4), the necessary conditions of optimality is given by

$$\nabla_{\mathbf{u}} \mathcal{L}(\mathbf{u}, \mathbf{d}) = \nabla_{\mathbf{u}} J(\mathbf{u}, \mathbf{d}) + \lambda_\Delta^\top \nabla_{\mathbf{u}} \mathbf{g}_\Delta(\mathbf{u}, \mathbf{d}) = 0 \quad (5)$$

$$\Rightarrow \nabla_{\mathbf{u}} J(\mathbf{u}, \mathbf{d}) = -\lambda_\Delta^\top \nabla_{\mathbf{u}} \mathbf{g}_\Delta(\mathbf{u}, \mathbf{d}) \quad (6)$$

Since λ_Δ is unknown in (6), we can eliminate it by looking into the nullspace of the active constraint gradients $\nabla_{\mathbf{u}} \mathbf{g}_\Delta(\mathbf{u}, \mathbf{d})$. (Jäschke and Skogestad, 2012). \mathbf{N} is defined as the nullspace of $\nabla_{\mathbf{u}} \mathbf{g}_\Delta(\mathbf{u}, \mathbf{d})$ if $\mathbf{N}^\top \nabla_{\mathbf{u}} \mathbf{g}_\Delta(\mathbf{u}, \mathbf{d}) = 0$.

Theorem 1 (Linear combination of gradients as self-optimizing variables). *Given a steady-state optimization problem (1) with $n_a < n_u$ active constraints $\mathbf{g}_\Delta(\mathbf{u}, \mathbf{d})$. Let $\mathbf{N} \in \mathbb{R}^{n_u \times (n_u - n_a)}$ be the nullspace of the active constraint gradients $\nabla_{\mathbf{u}} \mathbf{g}_\Delta(\mathbf{u}, \mathbf{d})$, such that $\mathbf{N}^\top \nabla_{\mathbf{u}} \mathbf{g}_\Delta(\mathbf{u}, \mathbf{d}) = 0$. Then the necessary conditions of optimality can be achieved by controlling the linear combination of the gradients*

$$\mathbf{c} = \mathbf{N}^\top \nabla_{\mathbf{u}} J(\mathbf{u}, \mathbf{d}) \quad (7)$$

to a constant setpoint of zero.

Proof. Pre-multiplying (6) by \mathbf{N}^\top gives

$$\mathbf{N}^\top \nabla_{\mathbf{u}} J(\mathbf{u}, \mathbf{d}) = -\mathbf{N}^\top \nabla_{\mathbf{u}} \mathbf{g}_\Delta(\mathbf{u}, \mathbf{d})^\top \lambda_\Delta \quad (8)$$

Since $\mathbf{N}^\top \nabla_{\mathbf{u}} \mathbf{g}_\Delta(\mathbf{u}, \mathbf{d})^\top = 0$, $\Rightarrow \mathbf{N}^\top \nabla_{\mathbf{u}} J(\mathbf{u}, \mathbf{d}) = 0$ \square

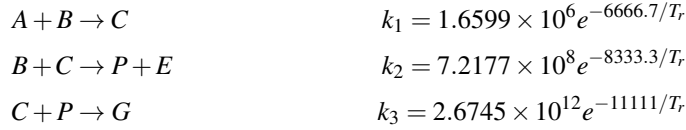
Therefore, controlling $\mathbf{c} = \mathbf{N}^\top \nabla_{\mathbf{u}} J(\mathbf{u}, \mathbf{d}) \in \mathbb{R}^{(n_u - n_a)}$ to a constant setpoint of zero satisfies the necessary condition of optimality (Krishnamoorthy and Skogestad, 2019). Since $n_a < n_u$, Linear independent constraint qualification (LICQ) is satisfied (i.e. $\nabla_{\mathbf{u}} \mathbf{g}_\Delta(\mathbf{u}, \mathbf{d})$ has full row rank) and \mathbf{N} is well defined. If $n_a = 0$ (fully unconstrained case), $\mathbf{N} = I_{n_u \times n_u}$, which means that the n_u self-optimizing CVs are simply the cost gradients $\mathbf{c} =$

$\nabla_{\mathbf{u}}J(\mathbf{u}, \mathbf{d})$. Therefore, for any active constraint region, $(n_u - n_a)$ CVs can be chosen as $\mathbf{c} = \mathbf{N}^T \nabla_{\mathbf{u}}J(\mathbf{u}, \mathbf{d})$ which by construction is of size $(n_u - n_a)$.

The proposed framework also enables us to select the CVs without having to develop reduced models for each active constraint region. One the CVs are chosen from each active constraint region, one can switch between the different active constraint regions using simple logic blocks such as selectors or split-range, as demonstrated by Krishnamoorthy and Skogestad (2019) and Reyes-Lúa et al. (2018). Although the gradients are ideal self-optimizing CVs, they are not readily available measurements. One has to estimate the gradients using the measurements. There are several model-based and model-free gradient estimation algorithms, which are briefly summarized by Srinivasan et al. (2011).

3. Illustrative example: Williams-Otto reactor

Consider the benchmark Williams-Otto reactor example, where the raw materials A and B are converted to useful products P and E through a series of reactions



The feed stream F_A with pure A component is a disturbance to the process and the manipulated variables are the feed stream F_B with pure B component and the reactor temperature T_r . The objective is to maximize the production of valuable products P and E , subject to some purity constraints on G and A in the product stream,

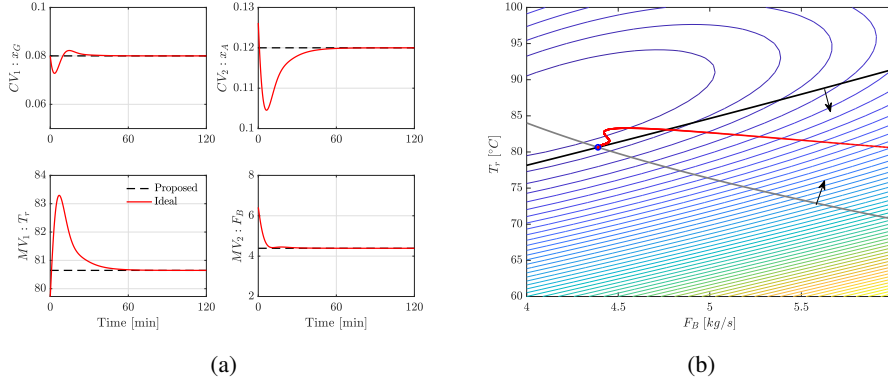
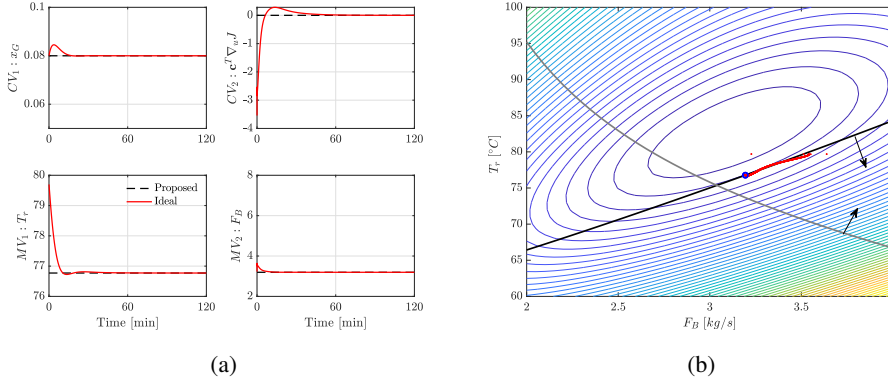
$$\begin{aligned} \min_{T_r, F_B} & -1043.38x_P(F_A + F_B) - 20.92x_E(F_A + F_B) + 79.23F_A + 118.34F_B & (9) \\ \text{s.t.} & x_G \leq 0.08, \quad x_A \leq 0.12 \end{aligned}$$

Since we have two constraints, we can have at most $2^2 = 4$ active constraint regions, namely, 1) x_A and x_G active, 2) only x_G active, 3) only x_A active, and 4) unconstrained. However, the max limit on x_G is so low that x_G will always be active. Therefore, we can eliminate regions 3 and 4, and we only need to choose CVs for regions 1 and 2. In region 1, we simply control the concentration of x_A to its limit of 0.12kg/kg and x_G to its limit of 0.08kg/kg . In region 2, we control x_G to its limit of 0.08kg/kg , and control the linear gradient combination $c := 0.9959\nabla_{F_B}J + 0.0906\nabla_{T_r}J$ to a constant setpoint of zero.

Region 1 ($F_A = 1.8275\text{kg/s}$): - When the disturbance is $F_A = 1.8275\text{kg/s}$, we are operating in region 1, with both the constraints active. This is the simplest case, where optimal operation is achieved using active constraint control.

Region 2 ($F_A = 1.3\text{kg/s}$): - When the disturbance is $F_A = 1.3\text{kg/s}$, we are operating in region 2, with only x_G constraint active. We use the reactor temperature T_r to control this constraint tightly and use F_B to control the linear gradient combination $c := 0.9959\nabla_{F_B}J + 0.0906\nabla_{T_r}J$. In this case, we use a model-based gradient estimation method proposed by Krishnamoorthy et al. (2019). The simulation results are shown in Fig. 2, where it can be seen that the proposed CVs are able to drive the process to its true optimum.

Switching between x_A and c can automatically be achieved using a selector block. Additional results such as, comparison of the proposed approach with the linear measurement


 Figure 1: Region 1: Simulation results using the proposed CVs when $F_A = 1.8275 \text{ kg/s}$.

 Figure 2: Region 2: Simulation results using the proposed CVs when $F_A = 1.3 \text{ kg/s}$.

combination and brute force method, including automatic CV-CV switching between x_A and c using a selector block can be found in the first author's PhD thesis (Krishnamoorthy, 2019, Appendix D).

4. Optimal operation of parallel operating units

In this section, we show how the proposed linear gradient combination framework can be used to choose the CVs for optimal operation of parallel operating units. Often in practice, when a plant capacity expands, this is done by simply adding new units in parallel to the existing units. The parallel units often share common resources such as feed, hot water etc. The different units may have different capacities, different equipment condition and different efficiencies.

Consider the optimal operation of p parallel units each with a cost function $\ell_i(u_i)$ and a given total feed U^{max} . The optimization problem is given as

$$\min_{u_i} J = \sum_{i=1}^p \ell_i(u_i) \quad \text{s.t.} \quad \sum_{i=1}^p u_i - U^{max} = 0 \quad (10)$$

In this case, $\nabla_{\mathbf{u}}\mathbf{g}_{\mathbb{A}} = \mathbf{1}^p$ and $\mathbf{N} \in \mathbb{R}^{(p-1) \times p}$ is chosen such that $\sum_{j=1}^p \eta_{i,j} \nabla_{\mathbf{u}_j} J$ and $\sum_{j=1}^p \eta_{i,j} = 0 \quad \forall i = 1, \dots, p-1$ where $\eta_{i,j}$ is the i and j^{th} element in \mathbf{N} . This implies $\nabla_{\mathbf{u}_i} \ell_i = \nabla_{\mathbf{u}_j} \ell_j$ for all $i \neq j$. That is the optimal operation of parallel units occur when the marginal cost is the same for all the units, which was also proved by Downs and Skogestad (2011) and commonly used in practice.

To illustrate this, consider a process with $p = 3$ parallel units. Using the nullspace of $\nabla_{\mathbf{u}}\mathbf{g}_{\mathbb{A}} = [1, 1, 1]^T$, we get

$$\begin{aligned} c_1 : -0.5774 \nabla_{\mathbf{u}_1} J + 0.7887 \nabla_{\mathbf{u}_2} J - 0.2113 \nabla_{\mathbf{u}_3} J &= 0 \\ c_2 : -0.5774 \nabla_{\mathbf{u}_1} J - 0.2113 \nabla_{\mathbf{u}_2} J + 0.7887 \nabla_{\mathbf{u}_3} J &= 0 \end{aligned}$$

Adding $c_1 + c_2$ yields $-\nabla_{\mathbf{u}_2} J + \nabla_{\mathbf{u}_3} J = 0$. Substituting this in c_1 gives $-0.5774 \nabla_{\mathbf{u}_1} J + 0.5774 \nabla_{\mathbf{u}_2} J = 0$, which results in $\nabla_{\mathbf{u}_1} J = \nabla_{\mathbf{u}_2} J = \nabla_{\mathbf{u}_3} J$. Although this is not a new result and is a well known concept, this re-iterates the general applicability of the proposed linear gradient combination framework.

5. Conclusion

In this paper, we proposed a generalized framework for selecting *what to control* in order to achieve optimal economic operation. An optimization problem can be converted into a feedback control problem by controlling:

- Active constraints $\mathbf{g}_{\mathbb{A}} \rightarrow 0$
- Linear gradient combination $\mathbf{c} = \mathbf{N}^T \nabla_{\mathbf{u}} J \rightarrow 0$ (with $\mathbf{N}^T \nabla_{\mathbf{u}} \mathbf{g}_{\mathbb{A}} = 0$)

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