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Optimal measurement-based cost gradient estimate for feedback real-time optimization

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ABSTRACT

This work presents a simple and efficient way of estimating the steady-state cost gradient J_u based on available uncertain measurements y. The main motivation is to control J_u to zero in order to minimize the economic cost J. For this purpose, it is shown that the optimal cost gradient estimate for unconstrained operation is simply $\hat{J}_u = H(y_m - y^*)$ where H is a constant matrix, y_m is the vector of measurements and y^* is their nominally unconstrained optimal value. The derivation of the optimal H-matrix is based on existing methods for self-optimizing control and therefore the result is exact for a convex quadratic economic cost J with linear constraints and measurements. The optimality holds locally in other cases. For the constrained case, the unconstrained gradient estimate $\hat{J}_u$ should be multiplied by the nullspace of the active constraints and the resulting "reduced gradient" controlled to zero.

1. Introduction

When the aim is to implement a control strategy to achieve optimal steady-state operation, the common industrial approach is to add a real-time optimization (RTO) layer (Engell, 2007) which adjusts the setpoints to the control layer. RTO uses a two-step procedure where first the available measurements are combined with a plant model to derive an estimate of the states (including disturbances), and next, in the optimization step, the nonlinear steady-state plant model is used to find the optimal values of the degrees of freedom (decision variables, here denoted u) that minimize the cost J. Based on the first-order optimality conditions of an unconstrained problem (Nocedal and Wright, 2006), the cost minimization is often based on first obtaining the cost gradient J_u[1] and then finding the optimal u which makes $J_u = 0$. Because of this, there is an intrinsic link between real-time optimization and gradient estimation methods (Krishnamoorthy and Skogestad, 2022).

The success of RTO relies on estimating the disturbances, and traditionally a steady-state model is used in the estimation step, which means that the measurement values to be used should also be at steady state. This imposes practical limitations regarding steady-state detection, especially for large-scale processes (Câmara et al., 2016). To avoid the steady-state wait time for the estimation, Krishnamoorthy et al. (2018) proposed to use a Kalman filter for dynamic state and disturbance estimation, and the model is then linearized around the expected steady-state operating point to give an estimate for the disturbances and the gradient J_u. There, this gradient is driven to zero by feedback control, which can be done using a PI-controller or pure I-controller. This is based on the "trick", also known as "dynamic inversion" (e.g., Lee et al. (2016)), of using feedback control to solve steady-state equations, that is, to find the value of u that makes a function of u (in this case J_u) equal to zero. All these approaches are referred to as "conventional RTO" in this paper.

Conventional RTO uses a steady-state or dynamic model for gradient estimation. An alternative, model-free approach is to directly estimate the cost gradient J_u from plant data by input excitation, and drive the estimated gradient to zero using feedback control, typically an I-controller. This approach is known as extremum-seeking control (ESC) (Tan et al., 2010; Scheinker, 2024). For gradient estimation in ESC, the classical approach is to use a sinusoidal excitation of the inputs combined with a trick of multiplying two sinusoidal signals to obtain a gradient estimate in a simple way (Scheinker, 2024). However, other model-free gradient estimation methods may also be used. This includes finite difference methods (François et al., 2005; Jäschke and Skogestad, 2011), and more generally least-squares regression on other kinds of perturbation data (Hunnekens et al., 2014), as well as machine learning regression methods (Matias and Jäschke, 2019).

In theory, extremum seeking control (which we define to include all model-free gradient estimation methods) is optimal in the sense that it avoids the problem of model-plant mismatch (Tan et al., 2006). It can also deal with constraints with specific formulations (Atta et al., 2019).

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[1] In this paper, the cost gradient $\partial J/\partial u$ is denoted J_u, but it is denoted $\nabla_u J$ in some other works.

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Unfortunately, extremum-seeking control, based on input perturbations to estimate the cost gradient, is of little practical significance for most chemical processes. The reason is that the convergence time is typically at least 100 times larger than the time constant of the process, so as to account for gradient estimation dynamics and convergence to the optimum. And since the time constant for a typical full process (for which we want to minimize the economic cost J) is typically several hours, the convergence time may be in the order of days or even months, which is of course unsuitable for real applications with frequent disturbances. There are also model-free methods that estimate the cost gradient through local dynamic models identified from data (Golden and Ydstie, 1989), but they must be continuously excited to ensure convergence, similarly to ESC.

Of course, there do exist cases where purely model-free approaches, like ESC, may be used alone, and this is when the dynamics (of the controlled plant) are fast and a fast cost measurement J is available. In process control, this may apply to local optimization of part of a process, but not for the full process where the economic cost J has to be computed based on knowing the value of all input and output streams and utilities. In other cases, a combination of these model-free gradient estimation methods and model-based RTO is favored, as it is done in modifier adaptation schemes (Marchetti et al., 2016).

Both conventional RTO and ESC tend to be slow, meaning that operation may be non-optimal for extended times following disturbances. This problem can circumvented by feedback-optimizing control where the aim is to move the optimization into the control layer (Morari et al., 1980), so that the RTO or ESC layer may be eliminated or at least less frequent updates are needed (Jäschke and Skogestad, 2011). Importantly, these approaches are complementary and not competing (Jäschke and Skogestad, 2011). The most important decision for feedback-optimizing control is the proper selection of the controlled variables (CVs), which is the idea of self-optimizing control (Skogestad, 2000).

Another issue with these model-based and model-free optimization schemes is that the gradient estimation and the use of the gradient for control are divided into separate tasks. However, this separation between estimation and control is not generally optimal. In other words, since it is not clearly defined upfront what the gradient J_u will be used for, we cannot expect that the estimated gradient will be optimal for minimizing the cost J. This is also the theme of a recent work (Kashani et al., 2024) which attempts to bridge estimation and control into the same extremum-seeking control scheme. On the other hand, self-optimizing control aims at finding CVs that minimize the cost, that is, the selection of CVs (which may be viewed as the estimation step) is directly linked to their use of minimizing the cost J. In addition, self-optimizing methods are much easier to implement.

Note that the ideal self-optimizing CV is the cost gradient. The present work, which may be viewed as a third approach for estimating the gradient, is based on self-optimizing control theory. The resulting gradient estimate is on the simple form:

$$\hat{J}_u = H(y_m - y^*)$$

where H is a constant matrix derived from self-optimizing theory, y_m is the vector of measurements and y^* is their nominally optimal values. An important advantage of the proposed approach is simplicity, as the resulting gradient estimate is a static linear combination of the available measurements.

Depending on the assumptions, there are three different ways of obtaining H from self-optimizing theory. First, there is the "nullspace method" (Alstad and Skogestad, 2007) for the case with no measurement error and a sufficient number of measurements. Second, for the case with even more measurements and with measurement error, there is the "extended nullspace method" (Alstad et al., 2009). Third, there is the "exact local method" (Alstad et al., 2009), which applies also to cases with few measurements, and which we will show (Theorem 1) gives the optimal gradient estimate. When used for obtaining self-optimizing CVs, the matrix H is not unique, as the expressions include a matrix M_n which is free to choose. However, as we show in this paper, the estimation of the gradient requires the particular choice $M_n = J_{uu}^{-1/2}$, where J_{uu} is the Hessian of the cost J. Actually, it has been known for some time that the "nullspace method" is linked to the cost gradient for the simple case with a sufficient number of noise-free measurements (Jäschke and Skogestad, 2011); and an equivalent result was obtained by Gros et al. (2009) with a neighboring-extremal scheme for gradient estimation assuming output feedback. The main contribution of the present work is to extend this link to the more general case with measurement/implementation error where the H-matrix may be obtained from the "extended nullspace method" and the "exact local method". The latter case is presented in Theorem 1 where we use the notation $H = H^J$ to avoid confusion with other H-matrices.

This paper focuses on estimating the unconstrained gradient, but it can also be applied to constrained optimization, for example, by multiplying it with the nullspace of the constraints to obtain the reduced gradient (Theorem 2). This is illustrated for switching of PID controllers in Examples 1 and 2, where active constraints change during operation. The use of the unconstrained gradient estimate for real-time optimization with changing active constraints is also discussed in more detail in three recent publications (Dirza and Skogestad, 2024; Bernardino and Skogestad, 2024a,b) in the Journal of Process Control (2024). In fact, it was the work with these three papers that motivated the need for a simpler gradient estimator (simpler than a Kalman filter or perturbation-based estimator) which led to results in the present paper. In Bernardino and Skogestad (2024b), the estimate of the reduced gradient is based on the "nullspace method" of self-optimizing control, whereas we in the present paper focus on presenting the more general "exact local method" (Theorem 1).

Note that although the gradient estimation presented in this paper is based on the plant model, this model is used only offline to obtain the H-matrix, so when implemented in combination with a control layer (e.g., using PID or MPC) that drives the estimated gradient to zero, the proposed approach is measurement-based and is believed to provide a fast, simple and efficient alternative to conventional RTO.

The paper is organized as follows. Section 2 presents the mathematical problem considered in this work. Section 3 describes how this problem is related to self-optimizing control. In Section 4 we present the main result of this work which is a simple measurement-based estimate of unconstrained cost gradient (Theorem 1). This is complemented by the analysis of the constrained problem in Section 5 (Theorem 2). An application of these results to real-time optimization using decentralized PID control is shown in Section 6 (Example 1), showing its use with changing active constraints. Real-time optimization of the more realistic Williams–Otto benchmark process is studied in Section 7 (Example 2). Some remarks about the presented results are made in Section 8, and the paper is concluded in Section 9.

2. Problem statement

The steady-state optimization problem considered in this work is of the form:

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

Here, J: $\mathbb{R}^{n_u} \times \mathbb{R}^{n_d} \rightarrow \mathbb{R}$ denotes the objective (cost) function, g: $\mathbb{R}^{n_u} \times \mathbb{R}^{n_d} \rightarrow \mathbb{R}^{n_g}$ the inequality constraints, $u \in \mathbb{R}^{n_u}$ the decision variables (inputs; manipulated variables for steady-state control), and $d \in \mathbb{R}^{n_d}$ the disturbance variables (including model parameters) which are assumed varying and generally unknown in this paper. The available online information about the system is assumed to be the measured variables $y \in \mathbb{R}^{n_y}$ (which usually include u and may include measured disturbances). Any internal states have been formally eliminated from the mathematical formulation in (1).

The optimal input, which is the solution to the problem in Eq. (1), is in the paper denoted $u^{opt}(d)$. It satisfies the following first-order KKT conditions (Nocedal and Wright, 2006):

$$J_u(u^{opt}, d) + g_u(u^{opt}, d)^T \lambda^{opt} = 0 \quad (2a)$$

$$g(u^{opt}, d) \le 0 \quad (2b)$$

$$\lambda^{opt} \ge 0 \quad (2c)$$

$$g(u^{opt}, d)^T \lambda^{opt} = 0 \quad (2d)$$

Here, $J_u(u,d) \in \mathbb{R}^{n_u}$ denotes the gradient of J with respect to u, $g_u(u,d) \in \mathbb{R}^{n_g \times n_u}$ denotes the gradient of g with respect to u, and $\lambda^{opt} \in \mathbb{R}^{n_g}$ denotes the Lagrange multipliers at the optimum. Note that it is the *unconstrained* cost gradient J_u that enters into the first-order optimality conditions.

The cost $J(u,d)$ and the constraints $g(u,d)$ in Eq. (1) can be approximated locally by the following Taylor expansions centered at the nominal point (u^*, d^*):

$$J(u,d) = J^* + \begin{bmatrix} J_u^{*T} & J_d^{*T} \end{bmatrix} \begin{bmatrix} (u-u^*) \\ (d-d^*) \end{bmatrix} + \frac{1}{2} \begin{bmatrix} (u-u^*)^T & (d-d^*)^T \end{bmatrix} \underbrace{\begin{bmatrix} J_{uu} & J_{ud} \\ J_{ud}^T & J_{dd} \end{bmatrix}}_{\mathcal{H}} \begin{bmatrix} (u-u^*) \\ (d-d^*) \end{bmatrix} \quad (3)$$

$$g(u,d) = g^* + \begin{bmatrix} g_u^* & g_d^* \end{bmatrix} \begin{bmatrix} (u-u^*) \\ (d-d^*) \end{bmatrix} \quad (4)$$

where $(u-u^*)$ and $(d-d^*)$ denote, respectively, the inputs and disturbances as their deviation from the nominal point.

The cost expression in Eq. (3) is exact for quadratic problems where the Hessian $\mathcal{H}$ (including J_{uu}) is independent of the operating point. In general, there will be an approximation error if the actual operation moves away from the nominal point. Strictly speaking, the elements in the Hessian matrix $\mathcal{H}$ should have a superscript $*$ (e.g. J_{uu}^*), but this is omitted to simplify notation, and also because it assumed that they remain approximately constant.

The objective of this paper is to find from the available measurements y (which are subject to noise n^y) an optimal estimate of the gradient J_u (which will vary as a function of u and d) for use in real-time optimization. The expected magnitudes of the disturbances and measurement errors are quantified by diagonal weight matrices W_d and W_{n^y}. That is, we assume that:

$$\begin{aligned}(d-d^*) &= W_d d' \\ n^y &= W_{n^y} n^{y\prime}\end{aligned} \quad (5)$$

where the combined generating set of possible d' and $n^{y\prime}$ is unit two-norm bounded, i.e.:

$$\left\| \begin{bmatrix} d' \\ n^{y\prime} \end{bmatrix} \right\|_2 \le 1 \quad (6)$$

Note that we are considering steady-state operation, so n^y represents the static measurement error, that is, the measurement bias. Often, n^y is called measurement noise, but this may be a bit misleading because the average (steady-state) value is not zero, as is usually assumed in stochastic optimal control. For example, $n^y = 0.15$ means that if the actual value is $y = 2.7$, then the measured value is $y_m = y + n^y = 2.85$. Finally, note that the objective of this paper is not to find the "optimal" gradient J_u in itself, but the optimal estimate $\hat{J}_u$ to be used in the first-order optimality condition (2a) to solve the problem in (1).

3. Optimal operation for the unconstrained case: Self-optimizing control

In the following consider the case with no constraints g and assume that the nominal operating point is optimal, that is,

$$u^* = u^{opt}(d^*)$$

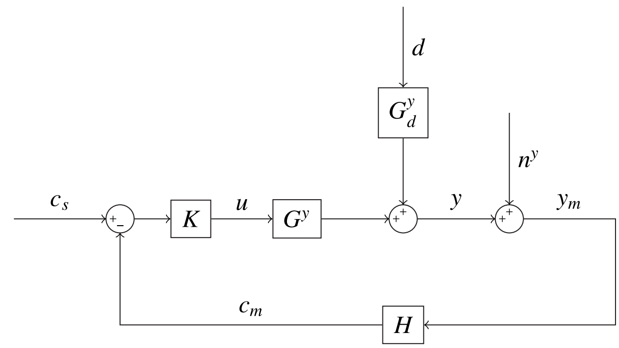


Fig. 1. Block diagram of closed-loop system. When H is selected as proposed in this paper, the input to the controller K is the negative cost gradient, that is, $c_s - H y_m = -\hat{J}_u$ see Eq. (21). This achieves optimal steady-state operation if in addition any active constraints are controlled.

It then follows from the first-order KKT condition (2a) that:

$$J_u^* = 0$$

This assumption is made to simplify the expressions for the loss, and the controlled variables derived here do not depend on this assumption (see chapter 6 in Alstad (2005)).

Following Halvorsen et al. (2003), we can derive from Eq. (3) the economic loss encountered by applying an input u, compared to using the optimal input $u^{opt}(d)$:

$$L = J(u,d) - J^{opt}(d) = \frac{1}{2}(u - u^{opt})^T J_{uu} (u - u^{opt}) = \frac{1}{2}\|z\|_2^2 \quad (7)$$

where $J^{opt}(d) = J(u^{opt}(d), d)$ is the optimal cost for a given d and the loss variable z is defined as:

$$z \triangleq J_{uu}^{1/2}(u - u^{opt}) \quad (8)$$

The idea of self-optimizing control is to achieve optimal operation using feedback control. In this paper, the controlled variables (CVs) c are assumed to be linear combinations of the measured variables, $c = Hy$, and we use a linear steady-state measurement model:

$$y = G^y u + G_d^y d \quad (9)$$

Note that the actual measured value is $y_m = y + n^y$. The setpoints c_s are assumed to be constant; see Fig. 1. To be nominally optimal (with no disturbances or measurement noise), we must choose $c_s = c^* = Hy^*$ where $y^* = y^{opt}(d^*)$. The controller K has integral action, which means that at steady state the control error

$$(c_m - c^*) = H(y_m - y^*)$$

is controlled to a constant value of zero. The controlled variables c should use up all the available degrees of freedom, and therefore $n_c = n_u$. In this paper, H is allowed to be a full matrix, that is, there are no structural limitations on H.

For the expected disturbances and noise in Eq. (6), Alstad et al. (2009) derived the following analytical expression for the optimal H, known as the "exact local method", which minimizes both the worst-case and average loss L in Eq. (7):

$$H = M_n^{-1} J_{uu}^{1/2} \left[G^{yT} \left(\tilde{F}\tilde{F}^T\right)^{-1} G^y \right]^{-1} G^{yT} \left(\tilde{F}\tilde{F}^T\right)^{-1} \quad (10)$$

where

$$\tilde{F} = [FW_d \quad W_{n^y}]$$

$$F = \frac{dy^{opt}}{dd} = G_d^y - G^y J_{uu}^{-1} J_{ud} \quad (11)$$

The solution for H is not unique as the matrix $M_n = J_{uu}^{1/2}(HG^y)^{-1}$ can be freely chosen. The non-uniqueness comes because if $c - c^* = 0$

then so is $D(c - c^*) = 0$ for any non-singular D. In the solution derived in Alstad et al. (2009), the choice is $M_n = I$. The simplest expression for the optimal H results if we select M_n such that $H = G^{yT}\left(\tilde{F}\tilde{F}^T\right)^{-1}$ (Yelchuru and Skogestad, 2012).

However, in the next section, we want to find an estimate for J_u (also when $J_u \neq 0$), and in this case directions matter. For this reason, we will choose:

$$M_n = J_{uu}^{-1/2} \tag{12}$$

and we show below that the optimal estimate for the gradient J_u is then equal to $H^J(y - y^*)$, where according to the exact local method:

$$H^J = J_{uu}\left[G^{yT}\left(\tilde{F}\tilde{F}^T\right)^{-1}G^y\right]^{-1}G^{yT}\left(\tilde{F}\tilde{F}^T\right)^{-1} \tag{13}$$

With different assumptions, other expressions for H may be derived. For the case with a sufficient number of independent measurements ($n_y \geq n_u + n_d$) it is possible to achieve zero disturbance loss for the case with no measurement noise by choosing H such that $HF = 0$ (nullspace method). For the case $n_y = n_u + n_d$, we have the following explicit expression for the nullspace method:

$$H = M_n^{-1}\tilde{J}(\tilde{G}^y)^{-1} \tag{14}$$

where $\tilde{G}^y = [G^y \quad G_d^y]$ and $\tilde{J} = J_{uu}^{1/2}[I \quad J_{uu}^{-1}J_{ud}]$. The generalization to use all measurements ($n_y \geq n_u + n_d$) in a way that also minimizes the effect of measurement noise is known as the extended nullspace method (Alstad et al., 2009) for which we have:

$$H = M_n^{-1}\tilde{J}(W_{n^y}^{-1}\tilde{G}^y)^{\dagger}W_{n^y}^{-1} \tag{15}$$

All these expressions for H can be used for gradient estimation, provided that we choose $M_n = J_{uu}^{-1/2}$, or equivalently $HG^y = J_{uu}$.

4. Optimal gradient estimate for the unconstrained case

We will now use the results from self-optimizing control to derive the optimal gradient estimate, where by "optimal" we mean that controlling the gradient estimate to zero achieves optimal steady-state operation, that is, it minimizes the loss L in Eq. (7) (worst-case or average value) for the expected disturbances and noise as in Eq. (6).

To do this, we want to express the loss variable z from (8) in terms of the gradient J_u. First, note that (Fig. 1):

$$(c - c^{opt}(d)) = HG^y(u - u^{opt})$$

Second, a first-order Taylor expansion of the gradient around the optimal operating point gives:

$$J_u(u,d) = \underbrace{J_u(u^{opt},d)}_{J_u^{opt}(d)} + J_{uu}(u - u^{opt}(d))$$

Inserting the above two expressions into the definition of the loss variable z in (8) gives:

$$z \triangleq J_{uu}^{1/2}(u - u^{opt}) = \underbrace{J_{uu}^{1/2}(HG^y)^{-1}}_{M_n}(c - c^{opt}(d)) = J_{uu}^{-1/2}(J_u - J_u^{opt}(d)) \tag{16}$$

For the unconstrained case, we have $J_u^{opt}(d) = 0$, and this is assumed in the following. We then get $z = J_{uu}^{-1/2}J_u$ and to minimize the norm of z, and thereby the loss in (7), we conclude that we ideally want $J_u = 0$ at steady state. However, as we will see, it is not possible to achieve $J_u = 0$ in practice because of measurement error.

For the choice $M_n = J_{uu}^{-1/2}$ (which we will use in the following), we derive from (16) the following expression for the gradient:

$$J_u = c - c^{opt}(d) = Hy - Hy^{opt}(d)$$

which may be rewritten as:

$$J_u = H(y_m - y^*) - H\underbrace{(y_m - y)}_{n^y} - H(y^{opt}(d) - y^*) \tag{17}$$

where we choose $y^* = y^{opt}(d^*)$ because the nominal point is assumed optimal. Note from (11) that $(y^{opt}(d) - y^*) = F(d - d^*)$ for the unconstrained case. We then have:

$$J_u = H(y_m - y^*) - Hn^y - HF(d - d^*) \tag{18}$$

Note that with a fixed matrix H, the last two terms are unaffected by the input u, that is, unaffected by control.

With no measurement error ($n^y = 0$), the second term in Eq. (18) is zero. If we use the nullspace method to choose H, then $HF = 0$, and also the third term is zero. The optimal control policy, according to self-optimizing control, is then to adjust u such that the first term is zero, for example, to use feedback control to keep the measurement combinations keep $c_m = Hy_m$ at a constant setpoint $c^* = Hy^*$. This gives $J_u = 0$ and the loss is zero.

More generally, with measurement noise and disturbances, we can use the exact local method to choose the H that minimizes the combined effect of the second and third terms in (18). The optimal control policy, similarly to the case without noise, is then to adjust u such that the first term in Eq. (18) is zero. This minimizes the expected norm of z as in (16), and consequently the economic loss L in (7). More importantly, and this is the main result of the paper, the optimal gradient estimate for unconstrained operation, which should be kept at zero at steady state, is simply the first term in (18), that is:

$$\hat{J}_u = H(y_m - y^*) \tag{19}$$

where y_m is the measurement vector, $y^* = y^{opt}(d^*)$ is the nominal optimal value of the measurement y, and H is given by H^J in Eq. (13) (exact local method). This follows from self-optimizing control theory, because choosing $H = H^J$ minimizes the effect of the second and third terms in Eq. (18) (it minimizes both the expected and worst-case loss when d and n^y vary as given in (6)).

Interestingly, since the second and third terms in (18) are generally nonzero (due to measurement noise and disturbances), it follows that optimal operation (in terms of minimizing the economic loss) does not give $J_u = 0$ at steady state. This may seem surprising, but it is expected because one cannot achieve truly optimal steady-state operation (with $J_u = 0$ and zero loss) with unknown disturbances and static measurement bias (nonzero n^y).

In summary, the steady-state loss L in Eq. (7) is minimized when we keep $\hat{J}_u = H^J(y_m - y^*) = 0$, and we have proven the following theorem:

Theorem 1 (*Optimal Unconstrained Gradient Estimate ("exact local method")*). *Consider the static optimization problem in (1) with no active constraints, where the quadratic approximation (3) holds. The available measurements are $y_m = G^y u + G_d^y d + n^y$ (linear approximation) where the unknown disturbances d and static measurement errors n^y are bounded as given in (5) and (6). Consider further that the point (u^*, d^*) is an optimal unconstrained point, such that $J_u(u^*, d^*) = 0$, $u^* = u^{opt}(d^*)$ and $y^* = y^{opt}(d^*)$. The cost gradient J_u is then given in (18) and the estimate $\hat{J}_u = H^J(y_m - y^*)$ with H^J in (13) is an optimal estimate in the sense that adjusting the inputs u to make $\hat{J}_u = 0$ (e.g., by feedback control, see Fig. 1) minimizes both the average and the worst-case value of the economic loss (7).*

If there is no measurement error ($n^y = 0$, that is, $W_{n^y} = 0$) and we have a sufficient number of measurement ($n_y = n_u + n_d$) then instead of using $H = H^J$ from the exact local method, we may use H from the nullspace method (Eq. (14) with $M_n = J_{uu}^{-1/2}$). This gives H in the nullspace of F ($HF = 0$) and achieves zero loss for disturbances (with no measurement error), that is, the last term in (18) is zero. If we have additional measurements ($n_y > n_u + n_d$) then we may use H from the "extended nullspace method" (Eq. (15) with $M_n = J_{uu}^{-1/2}$) which uses the extra measurements to minimize also the second term in (18). However, in general we recommend using $H = H^J$ from the exact local method. It gives the optimal balance between disturbances and measurement error (as it minimizes both the average and worst-case sum of last two terms in (18)) and importantly applies also to the case with fewer measurements ($n_y < n_u + n_d$).

5. Optimal gradient estimate for the constrained case

Now, we focus on the use of the new estimate of the unconstrained cost gradient (Theorem 1) to real-time optimization for the general case with changing active constraints. This is discussed in detail in three recent papers (2024) in the Journal of Process Control (Dirza and Skogestad, 2024; Bernardino and Skogestad, 2024a,b), but we include a summary of the results here so that the reader can appreciate the usefulness of our main result (Theorem 1). The application of the gradient estimate to constrained online optimization is further illustrated in Examples 1 and 2.

We first state the following result for estimating the reduced cost gradient:

Theorem 2 (*Optimal Gradient Estimate in Constrained Case*)**.** *The optimal unconstrained gradient estimate $\hat{J}_u = H^J(y_m - y^*)$ (Theorem 1) is optimal also in the constrained case when used in the first-order KKT conditions (2). This also means that the optimal estimate of the reduced gradient (which should be zero at the optimal point) is ${N_{\mathcal{A}}}^T\hat{J}_u = {N_{\mathcal{A}}}^T H^J(y_m - y^*)$ where $N_{\mathcal{A}}$ is a basis for the nullspace of $g_{u,\mathcal{A}}$, that is, $g_{u,\mathcal{A}}N_{\mathcal{A}} = 0$, and $\mathcal{A}$ represents the set of active constraints.*

The theorem may seem straightforward and require no further proof since J_u in (2a) is the unconstrained gradient, and the gradient estimate $\hat{J}_u$ in (19) is the one that minimizes the loss in the unconstrained case for a given measurement set y. Furthermore, the idea of reduced gradient is well-established, being used in optimization methods (Rosen, 1960; Lasdon et al., 1974) and to solve control problems (Jäschke and Skogestad, 2012; Torrisi et al., 2018). Nevertheless, in Appendix A, we provide a detailed proof that controlling the reduced gradient estimate ${N_{\mathcal{A}}}^T\hat{J}_u$ minimizes the loss for the constrained case.

It is important to note that Eq. (19) is valid when the nominal point (u^*, d^*) is an *optimal unconstrained* reference point. If the reference point has a non-zero gradient, the optimal gradient estimate takes the form (the reader is referred to Appendix B for a derivation of this expression):

$$\hat{J}_u = H(y_m - y^*) + J_u^* \tag{20}$$

where $J_u^* = J_u(u^*, d^*)$ (obtained from the nonlinear model). Note here that both (19) and (20) can be written in the form:

$$\hat{J}_u = H y_m - c_s \tag{21}$$

where c_s is a constant (see Fig. 1).

The simple gradient estimate in (19) and (20) avoids implementing a model-based estimator, for example, a dynamic Kalman filter, and thus greatly simplifies the practical use of feedback-based real-time optimization, which is based on the first-order KKT condition (2a).

The gradient estimate can be used in a wide array of feedback-optimizing control applications. In particular, it may be used in the following approaches for optimal steady-state operation with changes in active constraints:

1. *Primal–dual approaches* (Krishnamoorthy, 2021) based directly on the optimality condition (2a) with a (slow) update of the Lagrange multiplier λ. This may be done using a slow controller K_{dual} which controls the measured constraints by manipulating the dual variables (λ) and with max-selectors for switching active constraints, see Fig. 2 (Dirza et al., 2021; Dirza and Skogestad, 2024).

2. *Region-based control* (Jäschke and Skogestad, 2012; Krishnamoorthy and Skogestad, 2022) where we in each region i control the active constraints and the associated reduced gradient $N_{\mathcal{A},i}^T\hat{J}_u$ to zero, see Fig. 3.

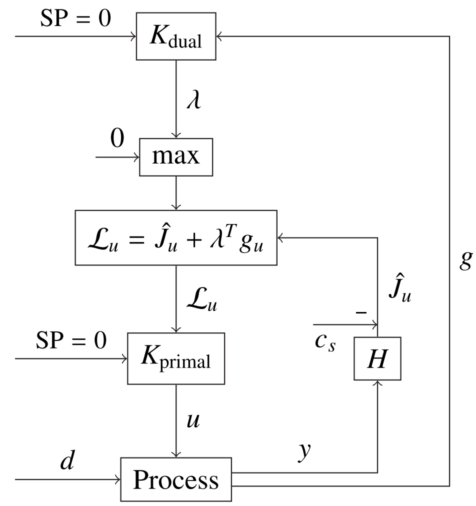


Fig. 2. Primal–dual optimizing control structure using the proposed gradient estimate. The controller K_{dual} is always diagonal (decentralized), whereas the controller K_{primal} may be multivariable or diagonal.

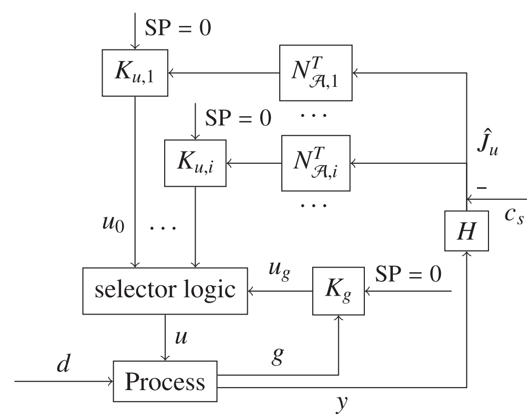


Fig. 3. Region-based optimizing control structure using the proposed gradient estimate. In this scheme, each projection matrix $N_{\mathcal{A},i}$ is linked to a different set of active constraints $\mathcal{A}_i$, and the resulting gradient projection $N_{\mathcal{A},i}^T\hat{J}_u$ is controlled by a different controller $K_{u,i}$ (which in general is multivariable). If $n_u \geq n_g$, a fixed projection matrix can be used for all $\mathcal{A}_i$, and simple max/min-selectors can be used (see Fig. 4).

2 A. Region-based control may be applied to multivariable control, for example, model predictive control, by changing the cost function for designing the controller for each region (Bernardino and Skogestad, 2024b). There, the gradient estimate is also used for constraint switching.

2B. Decentralized region-based control with constraint switching using selectors (Bernardino et al., 2022; Bernardino and Skogestad, 2024a) (Fig. 4). This approach requires at least as many inputs (degrees of freedom) as constraints, that is, $n_u \geq n_g$. An example of its application is given next.

In summary, the cost gradient estimate presented in Eq. (20) (based on Theorem 1) can be used in a wide array of control applications focused on optimal operation, eliminating the need for a dynamic state estimator and thus greatly simplifying implementation.

6. Example 1: Decentralized region-based control

Here, we consider a system with more inputs than constraints ($n_u \geq n_g$) and design a region-based decentralized control structure with

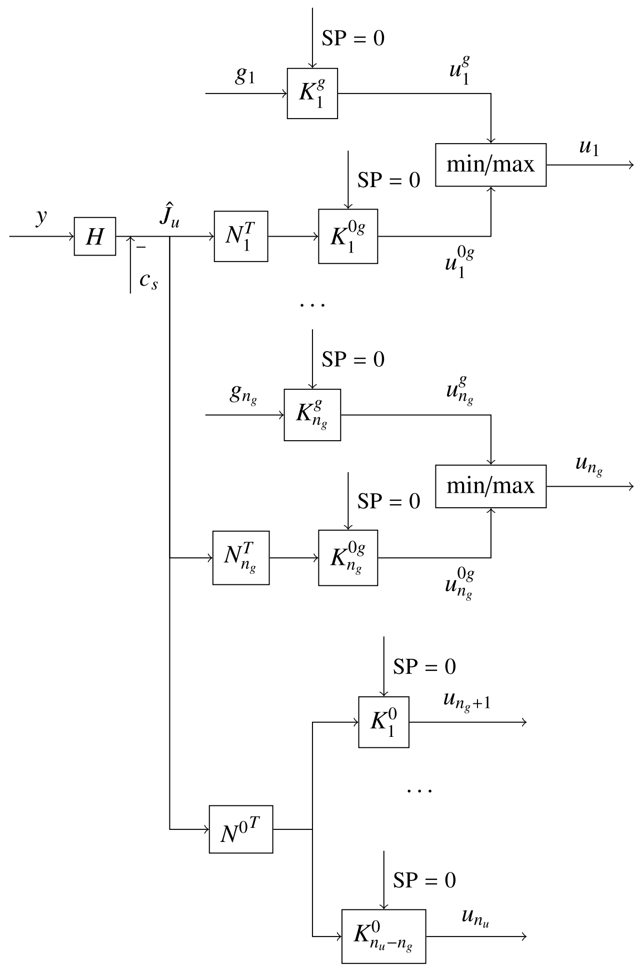


Fig. 4. Decentralized region-based optimizing control structure using the proposed gradient estimate combined with SISO controllers and selectors. This scheme, with projection matrices (N^0 and N_i) computed according to Steps S1 and S2, applies when there are at least as many inputs as constraints (Bernardino and Skogestad, 2024a).

simple min/max-selectors (Fig. 4) that minimizes the loss in all active constraint regions (Bernardino and Skogestad, 2024a). In order to use simple switching, the nullspace associated with the unconstrained gradients (Theorem 2) needs to be selected in accordance with the constraint directions. This is done using the following steps (Bernardino and Skogestad, 2024a):

Step S1. Define N^0 as an orthonormal basis for the nullspace of g_u, such that $g_u N^0 = 0$;

Step S2. Find $W = \begin{bmatrix} g_u \\ N^{0^T} \end{bmatrix}^{-1}$, and define the vectors N_i, $i = 1, \dots, n_g$ as the first n_g normalized columns of W.

Then, controlling the active constraints g_i, for $i \in \mathcal{A}$ and the remaining unconstrained degrees of freedom $N_i^T J_u$, for $i \notin \mathcal{A}$, and $N^{0^T} J_u$ will lead to optimal operation (Bernardino and Skogestad, 2024a). The final simple decentralized control system with min or max selectors can be implemented as shown in Fig. 4 where all controllers (K) are single-input single-output (SISO), for example, PID controllers. The controllers linked to selectors must have anti-windup action, to cancel the integral action when the controllers are inactive.

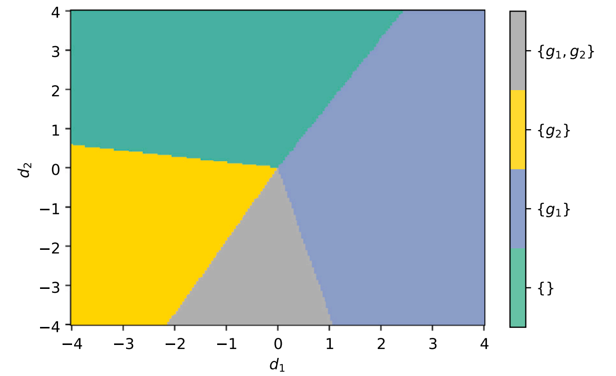


Fig. 5. Optimality regions for Example 1.

As a case study, we consider a linear dynamic system with a quadratic cost function given by:

$$\min_u \quad \frac{1}{2} x^T \begin{bmatrix} 1 & 0 \\ 0 & 10 \end{bmatrix} x + \frac{1}{2} u^T \begin{bmatrix} 1 & -0.1 & -0.2 \\ -0.1 & 0.8 & -0.1 \\ -0.2 & -0.1 & 0.3 \end{bmatrix} u$$
$$\text{s.t.} \quad \begin{cases} g_1 = x_1 - 0.8 x_2 \leq 0 \\ g_2 = u_1 + u_2 + u_3 \leq 0 \end{cases} \tag{22}$$

$$\dot{x} = \begin{bmatrix} -\frac{1}{\tau_1} & 0 \\ 0 & -\frac{1}{\tau_2} \end{bmatrix} x + \begin{bmatrix} \frac{0.2}{\tau_1} & 0 & 0 \\ 0 & \frac{0.2}{\tau_2} & 0 \end{bmatrix} u + \begin{bmatrix} \frac{1}{\tau_1} & 0 \\ 0 & \frac{1}{\tau_2} \end{bmatrix} d \tag{23}$$

with $\tau_1 = 1$ and $\tau_2 = 2$. The set of optimal active constraint regions can be visualized as a function of the two disturbances as shown in Fig. 5. Here, the upper left green region is unconstrained and the lower middle gray region is with all constraints being active (and one unconstrained degree of freedom).

For estimating the cost gradient, the following measurements are available:

$$y = \begin{bmatrix} g_1 \\ g_2 \\ x_1 \\ x_2 \\ u_2 \\ u_3 \end{bmatrix} = \begin{bmatrix} 1 & -0.8 \\ 0 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{bmatrix} x + \begin{bmatrix} 0 & 0 & 0 \\ 1 & 1 & 1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} u \tag{24}$$

Note that both constraints and both states are measured. In addition, we choose to include two of the three inputs. The expected static disturbance and noise magnitudes are $W_d = \text{diag}([4,\ 4])$ and $W_{n^y} = \text{diag}([0,\ 0,\ 1,\ 2,\ 1.5,\ 5])$. The two first zeros in W_{n^y} imply that the constraints have no static measurement error, that is, the constraints can be perfectly controlled. In general, static measurement error for a constraint may be counteracted by using back-off for its setpoint, but this issue is not explored in the case study.

To find the optimal cost gradient estimate using the formulation proposed in this work, we first use (23) with $\dot{x} = 0$ to derive the steady-state relationship:

$$x = \begin{bmatrix} 0.2 & 0 & 0 \\ 0 & 0.2 & 0 \end{bmatrix} u + \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} d \tag{25}$$

This is used to eliminate the states x from the problem (22), resulting in the following steady-state optimization problem:

$$\min_u \quad J = \frac{1}{2} u^T \underbrace{\begin{bmatrix} 1.04 & -0.1 & -0.2 \\ -0.1 & 1.2 & -0.1 \\ -0.2 & -0.1 & 0.3 \end{bmatrix}}_{J_{uu}} u + u^T \underbrace{\begin{bmatrix} 0.2 & 0 \\ 0 & 2 \\ 0 & 0 \end{bmatrix}}_{J_{ud}} d$$
$$\text{s.t.} \quad g = \underbrace{\begin{bmatrix} 0.2 & -0.16 & 0 \\ 1 & 1 & 1 \end{bmatrix}}_{g_u} u + \begin{bmatrix} 1 & -0.8 \\ 0 & 0 \end{bmatrix} d \leq 0 \tag{26}$$

From the matrix g_u, we can find the projections N_i and N^0 to be multiplied with the unconstrained gradient J_u. N^0 is the nullspace of g_u given by:

$$N^0 = \begin{bmatrix}-0.36214 & -0.45268 & 0.81482\end{bmatrix}^T \tag{27}$$

The vectors N_i are the first n_g normalized columns of $W = \begin{bmatrix} g_u \\ N^{0T} \end{bmatrix}^{-1}$, calculated as:

$$W = \begin{bmatrix} 2.8689 & 0.29508 & -0.36214 \\ -2.6639 & 0.36885 & -0.45267 \\ -0.20491 & 0.33607 & 0.81482 \end{bmatrix} \tag{28}$$

$$N_1 = \begin{bmatrix}0.73179 & -0.67952 & -0.052271\end{bmatrix}^T \tag{29}$$

$$N_2 = \begin{bmatrix}0.50902 & 0.63627 & 0.57971\end{bmatrix}^T \tag{30}$$

To estimate the gradient from the measurements, we also need their corresponding steady-state model. Plugging the steady-state expression for the states into (24) leads to:

$$y = \underbrace{\begin{bmatrix} 0.2 & -0.16 & 0 \\ 1 & 1 & 1 \\ 0.2 & 0 & 0 \\ 0 & 0.2 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}}_{G^y} u + \underbrace{\begin{bmatrix} 1 & -0.8 \\ 0 & 0 \\ 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}}_{G^y_d} d \tag{31}$$

The optimal sensitivity is then:

$$F = \frac{d y^{opt}}{dd} = G^y_d - G^y J_{uu}^{-1} J_{ud} = \begin{bmatrix} 0.9599 & -0.5830 \\ -0.4207 & -2.8867 \\ -0.0065 & 0.6479 \\ -0.0324 & -1.7605 \\ -0.1618 & -0.8026 \\ 0.9547 & -0.0647 \end{bmatrix} \tag{32}$$

With this information and the matrices from Eq. (26), we can calculate the measurement combinations H^J from the "exact local method" in Eq. (13), which gives:

$$H^J = \begin{bmatrix} 0.2741 & 0.9842 & 0.1560 & -1.0715 & -1.1842 & 0.0050 \\ -0.1897 & -0.0735 & 1.7813 & 0.8869 & -0.0265 & 0.0570 \\ -0.0180 & -0.1964 & -0.0091 & 0.0953 & 0.4964 & -0.0003 \end{bmatrix} \tag{33}$$

and the estimated gradient is $\hat{J}_u = H^J(y - y^*) = H^J - c_s$. Here, we note that the approximations in (3) and (4) are exact for this example, and therefore H^J does not depend on the nominal point to be considered. However, we still need a reference point to calculate the constant $c_s = H^J y^*$, and for that, we choose an optimal point with $d^* = [0,\ 0]^T$. This gives $c_s = [0,\ 0,\ 0]^T$.

Dynamic simulation results for the closed-loop system with the proposed control structure in Fig. 4 with $H = H^J$ are shown in Fig. 6. The PI controllers tuning are given in Table 1. The simulated disturbances cover all four active constraint regions but we did not include measurement noise. The responses are fairly smooth (see the three input profiles) and there are as expected three changes in active constraints. The gradient estimate with $H = H^J$ is optimal in terms of minimizing the average loss with the expected (assumed) disturbances and noise. However, this means that the gradient estimates (and resulting CVs) are not designed to reject the disturbances completely, as they simultaneously try to reduce the effect of measurement noise. This is the reason why the resulting steady-state inputs u_i (blue lines) do not match exactly the corresponding optimal values (magenta dashed lines). At steady state, the economic loss L resulting from this input mismatch is, however, very small.

Table 1
Proportional and integral gains of controllers for example 1. All controllers have anti-windup with tracking time $\tau_T = 0.01$.

Controller	Parameter	Value
K^g_1	K_c K_I	50 50
K^g_2	K_I	100
K^{0g}_1	K_I	−1.191
K^{0g}_2	K_I	1.528
K^0	K_I	2.761

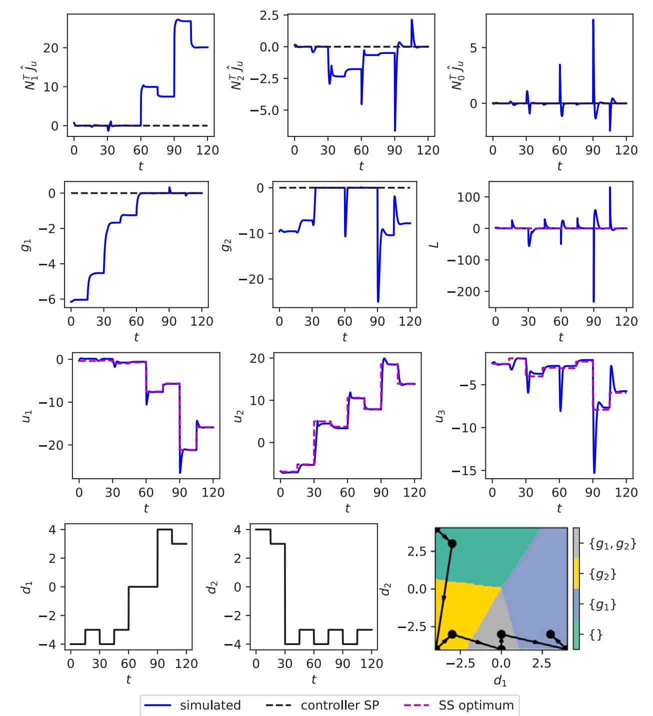
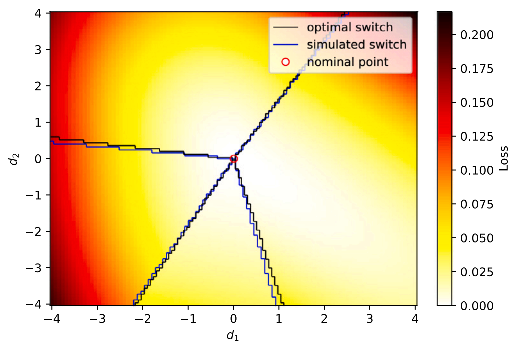


Fig. 6. Dynamic simulation over all active constraint regions using the proposed control structure with $H = H^J$ (exact local method) (Example 1).

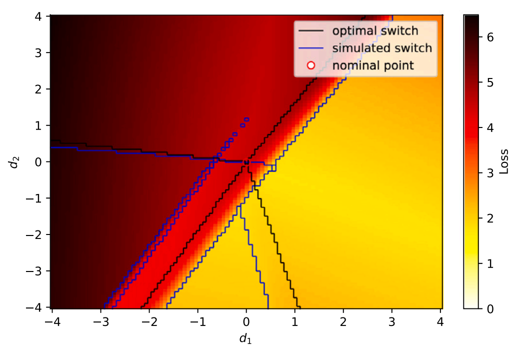
In Fig. 7, we present the steady-state loss obtained in closed loop both without and with static measurement noise (bias). The loss is shown as a heatmap for each disturbance combination. The much larger loss (note the difference in scale) with measurement noise in Fig. 7(b) is for the worst-case measurement error satisfying $n^y = W_{n^y} n^{y\prime}$ with $\|n^{y\prime}\|_2 \leq 1$. The optimal active constraint regions (same as Fig. 5) are shown by black lines whereas the actual operating regions resulting from using the control structure are shown by blue lines. Note that the constraint switching is moved away from the optimal, which is not surprising (see discussion).

Fig. 7(a) shows that the measurement combination $H = H^J$ (which is based on the exact local method of self-optimizing control) does not perfectly reject disturbances, even without measurement error. To achieve zero loss for disturbances, H must be in the nullspace of F. For instance, if we apply the extended nullspace method (15) to this problem (with $M_n = J_{uu}^{-1/2}$), we get:

$$H = \begin{bmatrix} 0.195 & 1 & 0.156 & -1.1 & -1.2 & 0.005 \\ -0.0624 & -0.1 & 1.95 & 0.9 & 0 & 0.0624 \\ 0 & -0.2 & 0 & 0.1 & 0.5 & 0 \end{bmatrix} \tag{34}$$

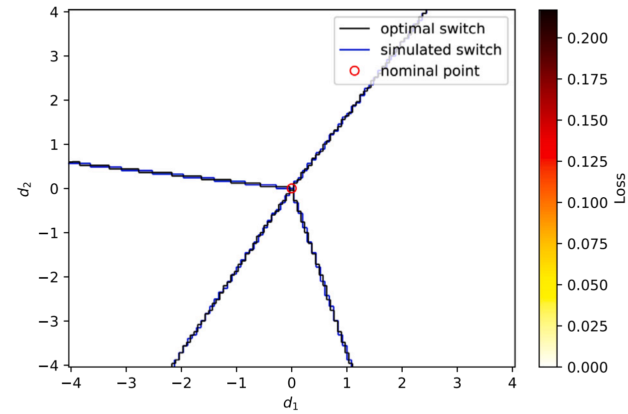


(a) Loss without measurement error ($n^y = 0$). Note from the scale that the loss is very small.

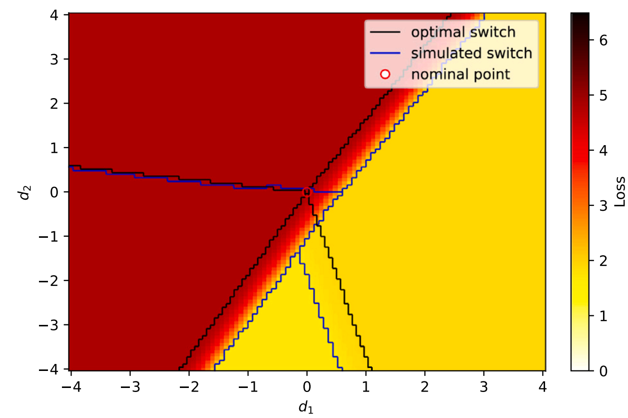


(b) Worst-case loss with measurement error. The new narrow operating region (which starts from point $d = [-2.8, -4]^T$) has both constraints g_1 and g_2 active.

Fig. 7. Steady-state loss for closed-loop operation with $H = H^J$ from the exact local method (Example 1).



(a) Zero loss without measurement error ($n^y = 0$).



(b) Worst-case loss with measurement error.

Fig. 8. Steady-state loss for closed-loop operation with H from the extended nullspace method (Example 1).

With the resulting gradient estimate (and set of CVs), the steady-state closed loop loss for the extended nullspace method (without noise and with the worst-case noise) are presented in Fig. 8. We see that in the case without noise (Fig. 8(a)), the economic loss is exactly zero in all constraint regions. This is expected since the original problem is linear with a quadratic cost. However, we see that the exact local method (H^J) is better at locally rejecting noise (note that the worst-case loss in Fig. 7(b) is smaller around the nominal point), but the extended nullspace method (Fig. 8(b)) handles large disturbances better, as expected.

7. Example 2: Williams-Otto reactor

This case study is a well-known benchmark for process control introduced by Williams and Otto (1960). The reactor is illustrated in Fig. 9.

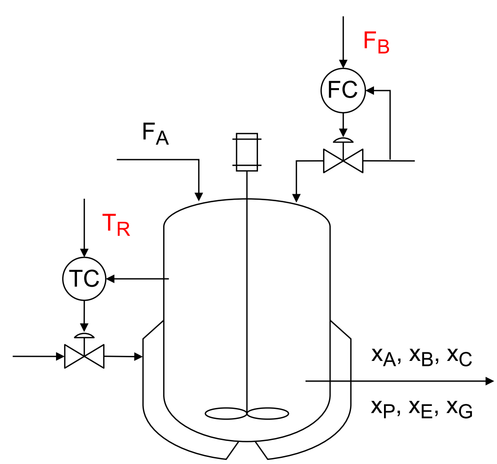


Fig. 9. Schematic representation of Williams–Otto reactor with control inputs in red (Example 2).

The following chemical reactions take place in the system:

$$A + B \xrightarrow{k_1} C \qquad k_1 = k_{0,1} e^{-E_1/T_r}$$
$$C + B \xrightarrow{k_2} P + E \qquad k_2 = k_{0,2} e^{-E_2/T_r}$$
$$P + C \xrightarrow{k_3} G \qquad k_3 = k_{0,3} e^{-E_3/T_r}$$

The component mass balances for the six components give the following set of ODEs:

$$\frac{dx_A}{dt} = \frac{F_A}{W} - \frac{(F_A + F_B)x_A}{W} - k_1 x_A x_B \tag{35a}$$
$$\frac{dx_B}{dt} = \frac{F_B}{W} - \frac{(F_A + F_B)x_B}{W} - k_1 x_A x_B - k_2 x_C x_B \tag{35b}$$
$$\frac{dx_C}{dt} = -\frac{(F_A + F_B)x_C}{W} + 2k_1 x_A x_B - 2k_2 x_C x_B - k_3 x_P x_C \tag{35c}$$
$$\frac{dx_P}{dt} = -\frac{(F_A + F_B)x_P}{W} + k_2 x_C x_B - 0.5 k_3 x_P x_C \tag{35d}$$
$$\frac{dx_E}{dt} = -\frac{(F_A + F_B)x_E}{W} + 2k_2 x_C x_B \tag{35e}$$

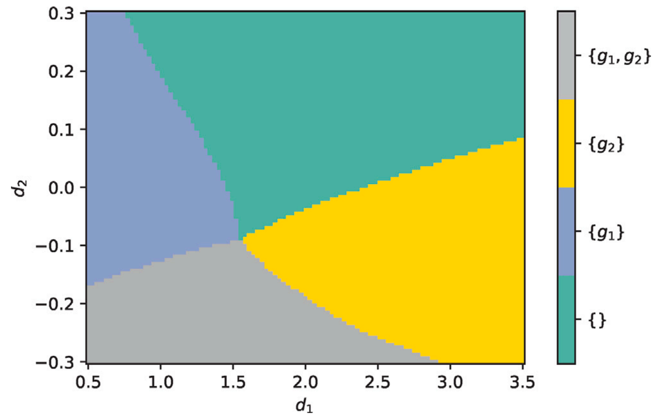


Fig. 10. Active constraint regions as a function of disturbances for example 2.

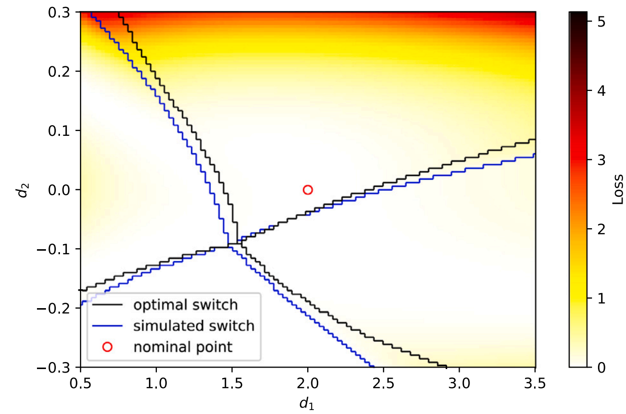


Fig. 11. Steady-state loss for closed-loop operation with $H = H^J$ from the exact local method for example 2.

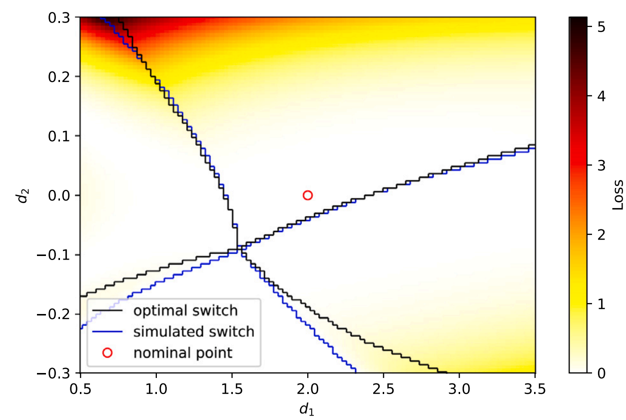


Fig. 12. Steady-state loss for closed-loop operation with H from the extended nullspace method for example 2.

$$\frac{dx_G}{dt} = -\frac{(F_A + F_B)x_G}{W} + 1.5k_3 x_P x_C \tag{35f}$$

The steady-state optimization problem to be considered for this system is:

$$\begin{aligned} \min_u J &= p_A F_A + p_B F_B - (F_A + F_B)\left[p_P(1+\Delta p_P)x_P + p_E x_E\right] \\ \text{s.t.} \quad & g_1 = x_E - 0.30 \le 0 \\ & g_2 = x_A - 0.12 \le 0 \end{aligned} \tag{36}$$

The inputs considered for this example are $u = \begin{bmatrix} F_B & T_r \end{bmatrix}^T$. The active constraint regions of the problem are shown in Fig. 10 as a function of the disturbances $d = \begin{bmatrix} F_A & \Delta p_P \end{bmatrix}^T$. The vector of available measurements is:

$$y = \begin{bmatrix} g_1 & g_2 & x_B & x_C & x_P & x_G & \Delta p_P \end{bmatrix}^T$$

Similarly to the first example, we calculate the optimal measurement combinations to be used for gradient estimation. For that, we approximate Eq. (36) as a quadratic programming (QP) problem around a nominal point, here considered as the optimal point for $d^* = \begin{bmatrix} 2 & 0 \end{bmatrix}^T$. To scale the disturbances and measurement error, W_d was chosen as $W_d = \text{diag}\left(\begin{bmatrix} 1.5 & 0.3 \end{bmatrix}\right)$, and W_{n^y} was chosen as the maximum deviation between the approximate and the true model predictions, which resulted in $W_{n^y} = \text{diag}\left(\begin{bmatrix} 0, 0, 0.076, 0.0089, 0.0056, 0.038, 0 \end{bmatrix}\right)$.

The optimal measurement combinations for the exact local method and the extended nullspace method are, respectively:

$$H^J = \begin{bmatrix} -1388 & 136.5 \\ -508 & -5.5 \\ 6.57153 & -1.71026 \\ 143.648 & -37.3849 \\ 786.6 & -204.715 \\ -51.2488 & 13.3377 \\ -116 & 0.6875 \end{bmatrix}^T \tag{37}$$

$$H = \begin{bmatrix} -1363.26 & 129.003 \\ -511.492 & -4.98053 \\ 8.00163 & -2.08245 \\ 174.909 & -45.5206 \\ 957.78 & -249.265 \\ -62.4016 & 16.2402 \\ -115.267 & 0.428895 \end{bmatrix}^T \tag{38}$$

The steady-state loss obtained in closed loop with the control structure proposed in Fig. 4 and using the exact local method ($H = H^J$) is shown in Fig. 11 as a function of the disturbances. Similarly, the results for using the extended nullspace method are shown in Fig. 12. The economic performance of both methods is reasonable (for comparison, the optimal cost at the nominal point is $J^* = -88.24$). For this example, choosing the exact local method results in a smaller maximum loss, which comes at the expense of having a higher loss than the extended nullspace method for certain disturbance realizations.

8. Discussion

8.1. Local gradient estimation (block-diagonal H)

The matrix H^J in (14) for the optimal gradient estimate is a full matrix. This means that control systems in Figs. 2 and 4 may not be decentralized, even if the controllers K themselves are decentralized. To obtain a decentralized control system, the relationship from y (measurements) to u (inputs) needs to be decoupled. For example, if we have a complex process with many units, then decentralized control implies that only measurements from unit k should be used by the control system to compute the inputs for unit k. To accomplish this, the matrix H needs to be block-diagonal. There exists no analytical solution in this case so the optimal block-diagonal H must be obtained numerically. Depending on the case study, there may be a small or large performance loss compared to using a full H. This problem has been studied in detail by Yelchuru and Skogestad (2012) using mixed-integer quadratic programming (MIQP). However, their objective was to find self-optimizing controlled variables $c = Hy_m + c_s$, so their results need to be modified to estimate instead the gradient, $\hat{J}_u = Hy_m + c_s$.

Finally, note that for the primal–dual optimizing control structure in Fig. 2, the Lagrange multiplier (λ) may introduce a coupling from the measured constraint (g) to the inputs (u) even for cases where the gradient controller (K_{primal}) is diagonal and the gradient estimator (matrix H) is block-diagonal.

8.2. Addition of RTO layer and model mismatch

The optimality of the static gradient estimate is based on a quadratic approximation (3) of the cost, and a linear approximation of the constraints (4) and of the measurement model (9). In general, these assumptions are not satisfied, and in this case, a static real-time optimization layer may be used to provide updates of the constants presented in this work, namely the controller setpoints c_s, the measurement combinations H, and the projection matrices N_i and N^0 (or $N_{\mathcal{A}}$ when generalizing to centralized approaches).

Using the RTO layer to update the setpoints c_s is the simplest and most important, being sufficient to drive the system to optimality in a new operating condition. That is, c_s is optimally updated, while the matrix H and the projection matrices constant can be kept constant. The use of constant matrices implies the self-optimizing properties (related to optimality on a shorter time scale) may degrade somewhat in a new operating point. On the other hand, changing these matrices will affect the control problem and, consequently, the controllers' tuning that should be used. Thus, updating only c_s is recommended in most practical applications.

As an alternative to a model-based RTO layer, an upper data-based layer based on perturbing the process, for example, extremum-seeking control, may be used to update c_s. However, data-based methods are not realistic for most process control applications because the convergence of these methods is too slow to track changing disturbances. Regardless, these methods are complementary to the method discussed in this work, as they are applied on an upper layer.

We remark that these RTO updates address the mismatch between the model used for the design of the gradient estimate and the plant behavior, but the improvement obtained is often small. In fact, for the unconstrained part of the optimization problem, model uncertainty is usually not critical as long as we are reasonably close to the optimum where the cost function is flat. Regardless of this, even though model mismatch is an important challenge for RTO problems to ensure exact plant optimality, it is not the main challenge that hinders its implementation. The main challenges for practical RTO implementation are slow convergence and numerical problems in performing disturbance estimation and optimization for given disturbances and high costs of implementation and maintenance.

8.3. Required model information

The methods for self-optimizing control used to obtain the matrix H for the gradient estimate use model information only offline. Furthermore, they only need model information in the form of the sensitivity matrix F and the gain matrix G^y, both of which can be estimated from plant data or steady-state simulations with relative ease. For estimating the gradient J_u, we additionally require knowledge of the Hessian matrix J_{uu} so that the directions of the unconstrained gradient are retrieved. The Hessian is harder to estimate from measurement information, as it requires more data. In addition, the constraint gradient g_u is needed to find the nullspace matrix for the reduced gradient $N_{\mathcal{A}}^T J_u$, but g_u is easy to estimate from data similarly to G^y. However, if a steady-state model is available for control structure design, all of these matrices can easily be obtained.

8.4. Discussion of example 1

In this work, we illustrate the method with a case study where the formulation is exact, that is, Eqs. (3), (4) and (9) hold. It was shown that the exact local method (13) is not designed to perfectly reject disturbances, that is $\Delta c_{opt} = HF\Delta d \neq 0$, which results in non-zero loss as shown in Fig. 7(a). Therefore, if a new estimate of the disturbances is available, an update of c_s will lead to improved performance around the new operating point, even if the optimal H is unchanged. This is not the case for the extended nullspace method, where we see in Fig. 8(a) that the obtained loss is zero for all disturbance values, which means that the optimal setpoint value is constant, i.e. $\Delta c_{opt} = HF\Delta d = 0$.

We see from Fig. 7 that measurement bias has a comparatively bigger effect on the economic loss than the disturbances in this numerical example, which is worsened the further the disturbances are from their design value. We also see that the measurement bias may trigger control of constraints that are not optimally active, which could be a problem if there were no constraint controllers. This is the reason why the pattern of the operating regions is so different from the optimal in Fig. 7(b). Overall, we see that for the nominal case (Fig. 7(a)), optimal behavior is well captured, with the closed-loop operating regions closely resembling the optimal active constraint regions. For the worst-case loss (Fig. 7(b)), the resulting economic loss is still small when compared to the values attained dynamically in Fig. 6.

8.5. Discussion of example 2

This example illustrates the application of the proposed method to nonlinear systems. If a nonlinear model is available, it must be first locally approximated as a QP problem with linear measurements, see Eqs. (3), (4) and (9). With this, the method is applied in the same way as described for example 1, and the results illustrate the obtained steady-state performance. It is no longer possible to attain perfect disturbance rejection as there is model mismatch, but the performance can still be deemed acceptable, with small losses in the neighborhood of the design point. The use of a gradient estimate based on the exact local method led to a lower maximum loss in the domain of interest when compared to the extended nullspace method, which favors the effect of the modeled disturbances over the possible measurement errors.

The values chosen for W_d and W_{n^y} reflect the expected behavior of the real system when compared to that of the approximate model used for design. This was possible because the nonlinear model was available for evaluation. In practice, these are tuning parameters that weight the importance of disturbance rejection versus the presence of measurement error, and they can therefore be chosen based on process knowledge.

9. Conclusion

The optimal local gradient estimate for use in steady-state real-time optimization is simply $\hat{J}_u = H^J(y_m - y^*) + J_u^*$ with H^J as in Eq. (13) (Theorem 1). This gradient estimate is optimal also in the constrained case when used with the KKT optimality conditions (2) (Theorem 2). The gradient estimate $\hat{J}_u$ may be used in a multitude of control applications (Figs. 1 to 4) where it is desired to include the optimality conditions (2) directly into the feedback control layer. In summary, the proposed gradient estimate is simple to implement and may form the basis for solving industrial RTO problems in an efficient manner.

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CRediT authorship contribution statement

Lucas Ferreira Bernardino: Writing – original draft, Visualization, Software, Methodology, Investigation, Formal analysis, Conceptualization. **Sigurd Skogestad:** Writing – review & editing, Supervision, Project administration.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

Appendix A. Proof: Optimal gradient estimate for the constrained case

We begin by describing the loss function for the constrained optimization problem, resulting in a simple form. Then, we show that the ideal variables for a given set of active constraints are the projection of the unconstrained gradient estimate onto the nullspace of the gradient of the active constraints, in the sense that they minimize the expected loss.

A.1. Loss for constrained optimization problem

From Eq. (3), we have:

$$
\begin{aligned}
L = J(u,d) - J^{opt}(d) &= J_u^{*T}(u - u^{opt}) \\
&+ \frac{1}{2}(u-u^*)^T J_{uu}(u-u^*) + (d-d^*)^T J_{ud}^T (u-u^{opt}) \\
&- \frac{1}{2}(u^{opt}-u^*)^T J_{uu}(u^{opt}-u^*)
\end{aligned}
$$

$$
\begin{aligned}
L = &\left(J_u^* + J_{ud}(d-d^*)\right)^T (u-u^{opt}) + \frac{1}{2}(u-u^*)^T J_{uu}(u-u^*) \\
&- \frac{1}{2}(u^{opt}-u^*)^T J_{uu}(u^{opt}-u^*)
\end{aligned}
\tag{39}
$$

The optimality conditions state that:

$$
\begin{aligned}
&\mathcal{L}_u(u^{opt}, d, \lambda^{opt}) = J_u(u^{opt}, d) + g_u^{*T}\lambda^{opt} = 0 \\
&\implies J_u^* + J_{uu}(u^{opt}-u^*) + J_{ud}(d-d^*) + g_u^{*T}\lambda^{opt} = 0 \\
&\implies J_u^* + J_{ud}(d-d^*) = -(J_{uu}(u^{opt}-u^*) + g_u^{*T}\lambda^{opt})
\end{aligned}
\tag{40}
$$

We can therefore rewrite Eq. (39) as:

$$
\begin{aligned}
L = &-\left(J_{uu}(u^{opt}-u^*) + g_u^{*T}\lambda^{opt}\right)^T (u-u^{opt}) \\
&+ \frac{1}{2}(u-u^*)^T J_{uu}(u-u^*) - \frac{1}{2}(u^{opt}-u^*)^T J_{uu}(u^{opt}-u^*) \\
= &-\lambda^{opt^T} g_u^*(u-u^{opt}) + \frac{1}{2}(u-u^*)^T J_{uu}(u-u^*) \\
&- \frac{1}{2}(u^{opt}-u^*)^T J_{uu}(u^{opt}-u^*) - (u^{opt}-u^*)^T J_{uu}(u-u^{opt}) \\
= &-\lambda^{opt^T} g_u^*(u-u^{opt}) + \frac{1}{2}(u-u^*)^T J_{uu}(u-u^*) \\
&- \frac{1}{2}(u^{opt}-u^*)^T J_{uu}(u^{opt}-u^*) - (u^{opt}-u^*)^T J_{uu}(u-u^*) \\
&+ (u^{opt}-u^*)^T J_{uu}(u^{opt}-u^*) \\
= &-\lambda^{opt^T} g_u^*(u-u^{opt}) + \frac{1}{2}(u-u^*)^T J_{uu}(u-u^*) \\
&- (u^{opt}-u^*)^T J_{uu}(u-u^*) + \frac{1}{2}(u^{opt}-u^*)^T J_{uu}(u^{opt}-u^*)
\end{aligned}
$$

From this, we conclude that:

$$
L = \frac{1}{2}(u-u^{opt})^T J_{uu}(u-u^{opt}) - \lambda^{opt^T} g_u^*(u-u^{opt}) \tag{41}
$$

This expression is very similar to Eq. (7), the difference being the linear term $\lambda^{opt^T} g_u^*(u-u^{opt})$, which is related to constraint control. Because the optimal Lagrange multipliers for the inactive constraints are zero, we have that $\lambda^{opt^T} g_u^*(u-u^{opt}) = \lambda_{\mathcal{A}}^{opt^T} g_{u,\mathcal{A}}(u-u^{opt})$, with $g_{u,\mathcal{A}}$ defined as the gradient of the active constraints with respect to the inputs. If the optimal active constraint set $\mathcal{A}$ is perfectly controlled, we have:

$$
\begin{aligned}
&\begin{cases}
g_{\mathcal{A}}(u^{opt}, d) = g_{\mathcal{A}}^* + g_{u,\mathcal{A}}(u^{opt}-u^*) + g_{d,\mathcal{A}}(d-d^*) = 0 \\
g_{\mathcal{A}}(u, d) = g_{\mathcal{A}}^* + g_{u,\mathcal{A}}(u-u^*) + g_{d,\mathcal{A}}(d-d^*) = 0
\end{cases} \\
&\implies g_{u,\mathcal{A}}(u-u^{opt}) = 0
\end{aligned}
\tag{42}
$$

This means that only the quadratic term on Eq. (41) is relevant when the correct constraints are controlled, with the additional restriction on the allowed directions of $(u-u^{opt})$, which are in the nullspace of $g_{u,\mathcal{A}}$. Define $N_{\mathcal{A}}$ as a basis for the nullspace of $g_{u,\mathcal{A}}$. This means that the loss from Eq. (41) is further simplified when the correct constraints are controlled to give:

$$
L = \frac{1}{2}(u-u^{opt})^T J_{uu}(u-u^{opt}) = \frac{1}{2} w^T {N_{\mathcal{A}}}^T J_{uu} N_{\mathcal{A}} w \tag{43}
$$

Here, w is an appropriately sized vector that represents the unconstrained degrees of freedom.

A.2. Connection with the unconstrained problem

We now show that the ideal controlled variables for this problem are directly linked to the ones from the unconstrained problem. First, note that the matrix $J_{ww} = {N_{\mathcal{A}}}^T J_{uu} N_{\mathcal{A}}$ is invertible by definition, and therefore we can write:

$$
L = \frac{1}{2} w^T J_{ww} J_{ww}^{-1} J_{ww} w \tag{44}
$$

From this, we can see that the loss variable z_w for this problem can be represented by:

$$
z_w = J_{ww}^{-1/2} {N_{\mathcal{A}}}^T J_{uu} N_{\mathcal{A}} w = J_{ww}^{-1/2} {N_{\mathcal{A}}}^T J_{uu}(u-u^{opt}) \tag{45}
$$

Similarly to Eq. (8), we can write z_w in terms of the unconstrained CVs c as:

$$
\begin{aligned}
z_w &= J_{ww}^{-1/2} {N_{\mathcal{A}}}^T J_{uu}(HG^y)^{-1}(c-c^{opt}) \\
&= J_{ww}^{-1/2} {N_{\mathcal{A}}}^T J_{uu}^{1/2} M_n (c-c^{opt})
\end{aligned}
$$

We can similarly write z_w in terms of the unconstrained gradient:

$$
\begin{aligned}
&J_u = J_u(u^{opt}, d) + J_{uu}(u-u^{opt}) \\
&\implies z_w = J_{ww}^{-1/2} {N_{\mathcal{A}}}^T (J_u - J_u(u^{opt}, d))
\end{aligned}
$$

Note that, because of the optimality conditions, we have that:

$$
J_u(u^{opt}, d) + g_u^{*T}\lambda^{opt} = 0 \implies {N_{\mathcal{A}}}^T J_u(u^{opt}, d) = 0
$$

and with the choice of $M_n = J_{uu}^{-1/2}$, we compare both expressions for z_w and we see that:

$$
\begin{aligned}
&{N_{\mathcal{A}}}^T J_u = {N_{\mathcal{A}}}^T (c - c^{opt}) \\
&= {N_{\mathcal{A}}}^T \left(H(y_m - y^*) - Hn^y - H(y^{opt}(d) - y^*)\right)
\end{aligned}
\tag{46}
$$

This formulation is similar to that of Eq. (18), with the exception that now $u^{opt}(d)$ and $y^{opt}(d)$ represent a constrained optimal point, and therefore are a different function of the disturbances, $(y^{opt}(d) - y^*) = F_{\mathcal{A}}(d-d^*)$. We can determine $F_{\mathcal{A}}$ from the constrained optimization problem as follows:

$$
\begin{bmatrix} J_{uu} & g_{u,\mathcal{A}}^T \\ g_{u,\mathcal{A}} & 0 \end{bmatrix}
\begin{bmatrix} \Delta u^{opt} \\ \Delta \lambda_{\mathcal{A}}^{opt} \end{bmatrix}
= \begin{bmatrix} -J_{ud} \\ -g_{d,\mathcal{A}} \end{bmatrix} \Delta d \tag{47}
$$

First we eliminate Δu^{opt} by premultiplying both sides by $\left[g_{u,\mathcal{A}} J_{uu}^{-1} \quad -I\right]$, leading to the solution $\Delta \lambda_{\mathcal{A}}^{opt} = W_{\mathcal{A}} \Delta d$, where

$$
W_{\mathcal{A}} = \left(g_{u,\mathcal{A}} J_{uu}^{-1} g_{u,\mathcal{A}}^T\right)^{-1} \left(g_{d,\mathcal{A}} - g_{u,\mathcal{A}} J_{uu}^{-1} J_{ud}\right)
$$

The solution for the new optimal inputs follows as $\Delta u^{opt} = -J_{uu}^{-1}\left((g_{u,\mathcal{A}})^T W_{\mathcal{A}} + J_{ud}\right)\Delta d$, and the optimal sensitivity matrix $F_{\mathcal{A}}$ can be obtained as:

$$
F_{\mathcal{A}} = F - G^y J_{uu}^{-1} g_{u,\mathcal{A}}^T W_{\mathcal{A}} \tag{48}
$$

with F being the unconstrained optimal sensitivity matrix. The second term of $F_{\mathcal{A}}$ is related to constraint control, and we can see that, with $M_n = J_{uu}^{-1/2}$:

$$
\begin{aligned}
{N_{\mathcal{A}}}^T H F_{\mathcal{A}} &= {N_{\mathcal{A}}}^T H F - {N_{\mathcal{A}}}^T \overbrace{H G^y J_{uu}^{-1}}^{=I} g_{u,\mathcal{A}}^T W_{\mathcal{A}} \\
&= {N_{\mathcal{A}}}^T H F - \overbrace{{N_{\mathcal{A}}}^T g_{u,\mathcal{A}}^T}^{=0} W_{\mathcal{A}} = {N_{\mathcal{A}}}^T H F
\end{aligned}
$$

This means that the last two terms in Eq. (46) are minimized by the unconstrained self-optimizing control solution for $H = H^J$ (13), and therefore the reduced gradient estimate

$$N_A{}^T \hat{J}_u = N_A{}^T H^J (y_m - y^*) \tag{49}$$

is the unconstrained CV that should be kept at zero to minimize the expected norm of z_w.

Appendix B. Effect of nominal setpoint

Here, we evaluate the effect of having a non-optimal reference point. From Eq. (16) and choosing $M_n = J_{uu}^{-1/2}$, we have:

$$c(u, d) - c(u^{opt}(d), d) = J_u(u, d) - J_u(u^{opt}(d), d)$$

The same expression is valid for the nominal point, according to:

$$c(u^*, d^*) - c(u^{opt}(d^*), d^*) = J_u(u^*, d^*) - J_u(u^{opt}(d^*), d^*)$$

Here, we assume that $u^* \neq u^{opt}(d^*)$, that is, the nominal point is not optimal. For the unconstrained problem, $J_u(u^{opt}(d), d) = J_u(u^{opt}(d^*), d^*) = 0$, and we subtract the two equations to give:

$$J_u(u, d) = J_u(u^*, d^*) + c(u, d) - c(u^*, d^*) - \left(c(u^{opt}(d), d) - c(u^{opt}(d^*), d^*)\right)$$

or

$$J_u(u, d) = J_u(u^*, d^*) + H(y^m - y^*) - H \underbrace{(y_m - y)}_{n^y} - HF(d - d^*) \tag{50}$$

Choosing the exact local method solution for H from (13), we minimize the last two terms from the previous equation, and the optimal gradient estimate to be controlled is given by:

$$\hat{J}_u(u, d) = H^J (y^m - y^*) + J_u(u^*, d^*)$$

as stated in Eq. (20). As previously shown, this gradient estimate is also valid for the constrained region, with the corresponding reduced gradient estimate being the optimal variable to be controlled.

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