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Neighbouring-Extremal Control for Steady-State Optimization Using Noisy Measurements

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Abstract: Optimal operation of chemical plants is usually accomplished by finding the optimal steady state using the nominal set of disturbances and model parameters. The optimization is in most cases model based and therefore subject to uncertainties. This may lead to sub optimal control actions with significant economical losses. One idea to tackle this problem is to use the available measurements to adapt the inputs during operation in a feedback control scheme. This can be achieved by a neighbouring extremal controller that updates the inputs based on the deviation of the measured outputs from their nominal value. In this paper we generalize the neighbouring extremal control design that has been presented in the literature to explicitly handle measurement noise and implementation errors. The benefits of our method are illustrated in a case study where we show that the sensitivity of the controller performance to measurement noise is considerably reduced.

Keywords: optimal operation, neighbouring extremal control, measurement based optimization, robustness, noise

1. INTRODUCTION

We consider the context of steady state process optimization and robust implementation of optimal policies. Our goal is to develop simple polices that guarantee near-optimal operation under all conditions using feedback. Here, 'under all conditions' means for the defined disturbances, plant changes and implementation errors.

One approach is the so called Neighbouring-Extremal (NE) control proposed by Gros et al. (2009), where first-order approximations of the optimal inputs are computed based on the deviations of the measured outputs due to disturbances or parametric uncertainties. This method can be implemented in a simple static output feedback control scheme, which results in near-optimal operation at a negligible online computation costs. Figure 1 illustrates the implementation approach. The main idea with the NE controller is to update the nominal control inputs based on the deviation of the measurements to their nominal value.

However, in practice the economic performance of the NE controller can be severely impaired due to the presence of measurement noise and implementation errors. In this paper we generalize the NE design method to explicitly handle noise and implementation errors. The new design is based on a two-step approach. First, we compute a static estimator which optimally estimates the disturbances using noisy measurements. Then, based on the linearized necessary conditions of optimality the optimal input updates are obtained. Finally, we show that the method can be implemented as a simple static output feedback controller. The strength of the new NE controller for process optimization is illustrated on a continuous chemical reactor.

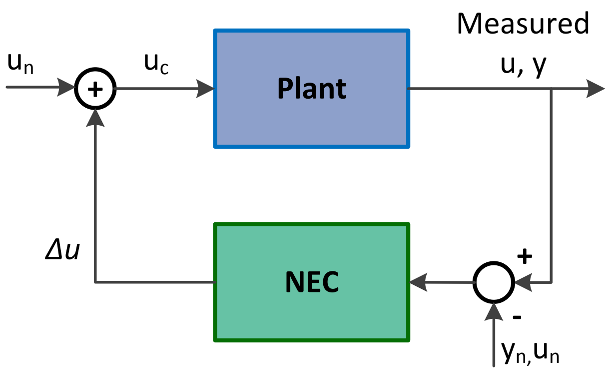

Fig. 1. Schematic of the neigbouring extremal control scheme. The nominal inputs and outputs are represented by u_n and y_n, respectively.

The paper is organized as follows. Section 2 presents the mathematical preliminaries and the problem formulation; Section 3 shows how to extend the NE approach to consider noisy measurements; Section 4 brings a simulation example to illustrate the method; In Section 5 you will find the discussion and conclusions of the paper.

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2. PROBLEM FORMULATION

2.1 Static optimization problem

We consider the following static optimization problem

$$\min_u J(x, u, d) \quad (1)$$

$$\text{s.t. } F(x, u, d) = 0 \quad (2)$$

where $u \in \mathbb{R}^{n_u}$ are the degrees of freedom, $x \in \mathbb{R}^{n_x}$ are the states and $d \in \mathbb{R}^{n_d}$ are the disturbances. Here the objective is $J : \mathbb{R}^{n_x+n_u+n_d} \mapsto \mathbb{R}$, and $F : \mathbb{R}^{n_x+n_u+n_d} \mapsto \mathbb{R}^{n_x}$ denotes the model equations. The output equations at steady-state read

$$y = R(x, u, d) \quad (3)$$

with the mapping $R : \mathbb{R}^{n_x+n_u+n_d} \mapsto \mathbb{R}^{n_y}$.

2.2 Optimality conditions

Let us define the Lagrangian function $L(x, u, d, \lambda) = J(x, u, d)+\lambda^T F(x, u, d)$ where λ are the multipliers. Under a suitable second-order condition and constraint qualification such as LICQ, the necessary conditions of optimality of problem (1)-(2) are

$$L_u = J_u + \lambda^T F_u = 0 \quad (4)$$

$$L_x = J_x + \lambda^T F_x = 0 \quad (5)$$

$$L_\lambda = F^T = 0 \quad (6)$$

where the notation $(\cdot)_X = \frac{\partial(\cdot)}{\partial X}$.

We can combine (4)-(5) to have:

$$L_u = J_u - J_x F_x^{-1} F_u = \frac{dJ}{du} = 0 \quad (7)$$

where this total derivative is the (reduced) gradient of the cost function with respect to u and will be denoted by the n_u dimensional vector $g \equiv \frac{dJ}{du}$. Here we assume that F_x is invertible.

2.3 First-order variation of the NCO

We consider small variations in the disturbance $\Delta d = d - d_{nom}$ around the nominal value d_{nom}. The linearized optimality conditions can be written as (François et al., 2014):

$$\Delta L_u \approx L_{ux}\Delta x + L_{uu}\Delta u + F_u^T \Delta\lambda + L_{ud}\Delta d = 0 \quad (8)$$

$$\Delta L_x \approx L_{xx}\Delta x + L_{xu}\Delta u + F_x^T \Delta\lambda + L_{xd}\Delta d = 0 \quad (9)$$

$$\Delta L_\lambda \approx F_x^T \Delta x + F_u^T \Delta u + F_d^T \Delta d = 0 \quad (10)$$

where the notation Δ indicates the deviation of the variable with respect to the nominal value.

We may use equations (8) and (9) to express the Δx and $\Delta\lambda$ in terms of Δu and Δd

$$\Delta x = -F_x^{-1} F_u \Delta u - F_x^{-1} F_d \Delta d \quad (11)$$

$$\Delta\lambda = -F_x^{-T} L_{xx}\Delta x - F_x^{-T} L_{xu}\Delta u - F_x^{-T} L_{xd}\Delta d \quad (12)$$

Here the notation $(\cdot)^{-T} = (\cdot)^{-1^T}$. Combining (11) and (12) with (8) we get

$$\Delta L_u = J_{uu}\Delta u + J_{ud}\Delta d \quad (13)$$

where

$$J_{uu} \equiv L_{uu} - L_{ux}F_x^{-1}F_u - F_u^T F_x^{-T} L_{xu} + F_u^T F_x^{-T} L_{xx} F_x^{-1} F_u \quad (14)$$

$$J_{ud} \equiv L_{ud} - L_{ux}F_x^{-1}F_d - F_u^T F_x^{-T} L_{xd} + F_u^T F_x^{-T} L_{xx} F_x^{-1} F_d \quad (15)$$

where $J_{uu} = \frac{d^2 J}{du^2}$ is the $n_u \times n_u$ reduced Hessian matrix and $J_{ud} = \frac{d^2 J}{du\, dd}$ is a $n_u \times n_d$ matrix.

The term ΔL_u is the first order approximation of the reduced gradient for the perturbed system, and we want to enforce it to zero. Therefore, the variation Δu that is necessary to optimally offset the effect of Δd is

$$\Delta u_{opt} = -J_{uu}^{-1} J_{ud} \Delta d \quad (16)$$

If the variations Δd are known, it is straightforward to compute the input corrections to keep the gradient equal to zero despite the disturbances. However, Δd is generally unknown and the challenge is to infer it from the noisy measurements.

2.4 Linear model

The linearized output equations is given by

$$\Delta y = R_x\Delta x + R_u\Delta u + R_d\Delta d \quad (17)$$

Upon linearising the model equation (2) and solving for the state deviations we get

$$\Delta x = -F_x^{-1} F_u \Delta u - F_x^{-1} F_d \Delta d \quad (18)$$

This results in

$$\Delta y = G\Delta u + G_d\Delta d \quad (19)$$

where

$$G = R_u - R_x F_x^{-1} F_u \quad (20)$$

$$G_d = R_d - R_x F_x^{-1} F_d \quad (21)$$

2.5 Measurement noise and input disturbance

We assume that our measurements are corrupted with noise ($y_m = y + \eta_y$) and that the computed inputs (by the optimization/controller) u_m differ from the actual plant inputs u due to input disturbances η_u. In deviation variables we have

$$\Delta y_m = \Delta y + \eta_y \quad (22)$$

$$\Delta u_m = \Delta u - \eta_u \quad (23)$$

where η_y and η_u are zero-mean Gaussian measurement noise. For simplicity, we will use the following notation

$$\eta = \begin{bmatrix} \eta_y \\ -\eta_u \end{bmatrix} \quad (24)$$

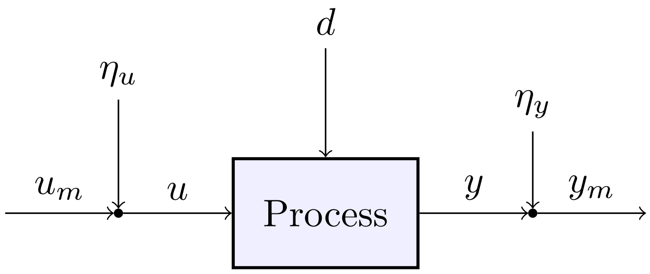


Fig. 2. Plant setup with disturbances and noise

3. DEALING WITH MEASUREMENT NOISE

3.1 Optimal static estimator open-loop

We would like to find an estimator in the form

$$\Delta\hat{d} = \underbrace{[H_1\ H_2]}_{H} \begin{bmatrix} \Delta y_m \\ \Delta u_m \end{bmatrix} \tag{25}$$

that optimally approximate the disturbance Δd in the case of noisy measurements. By optimal it is meant here that we want to minimize the prediction error

$$e = \Delta d - \Delta\hat{d} \tag{26}$$

Let us consider the augmented linear model

$$w = \begin{bmatrix} \Delta y \\ \Delta u \end{bmatrix} = \underbrace{\begin{bmatrix} G \\ I \end{bmatrix}}_{G_u^w} \Delta u + \underbrace{\begin{bmatrix} G_d \\ 0 \end{bmatrix}}_{G_d^w} \Delta d \tag{27}$$

It can be shown that the prediction error is given by

$$e(H) = [-HG_u^w \quad (I - HG_d^w) \quad -H_1 \quad -H_1 G] \begin{bmatrix} \Delta u \\ \Delta d \\ \eta_y \\ \eta_u \end{bmatrix} \tag{28}$$

Next, the magnitudes of the disturbances, measurement errors and inputs are quantified by the scaling diagonal matrices W_d, W_{du}, W_n and W_u respectively so that we can write

$$\Delta u = W_u u' \tag{29}$$

$$\Delta d = W_d d' \tag{30}$$

$$\eta_y = W_n \eta_y' \tag{31}$$

$$\eta_u = W_{du} \eta_u' \tag{32}$$

where the elements u', d', η_y' and η_u' are assumed to be normally distributed with zero mean and unit standard deviation. The diagonal scaling matrices contain the standard deviations of the elements in Δu, Δd, η_y and η_u. The prediction error can be expressed by

$$e(H) = \overbrace{[-HG_u^w W_u \quad (I - HG_d^w) W_d \quad -H_1 W_n \quad -H_1 G W_{du}]}^{M(H)} \begin{bmatrix} u' \\ d' \\ \eta_y' \\ \eta_u' \end{bmatrix} \tag{33}$$

It can be shown that the expected value of the 2-norm of the prediction error is

$$E(\|e\|_2) = \|M(H)\|_F^2 \tag{34}$$

See Ghadrdan et al. (2013) for a similar proof. The matrix M can be rewritten as

$$M = Y - HX \tag{35}$$

where

$$Y = [0 \quad W_d \quad 0] \tag{36}$$

$$X = [G_u^w W_u \quad G_d^w W_d \quad \tilde{W}_n \quad G_u^w W_{du}] \tag{37}$$

and

$$\tilde{W}_n = \begin{bmatrix} W_n \\ 0 \end{bmatrix} \tag{38}$$

Minimizing the estimation error variance ($\|e\|_2$) is equivalent to minimizing $\|M(H)\|_F^2$. The optimization problem can be written as

$$\min_H \|Y - HX\|_F \tag{39}$$

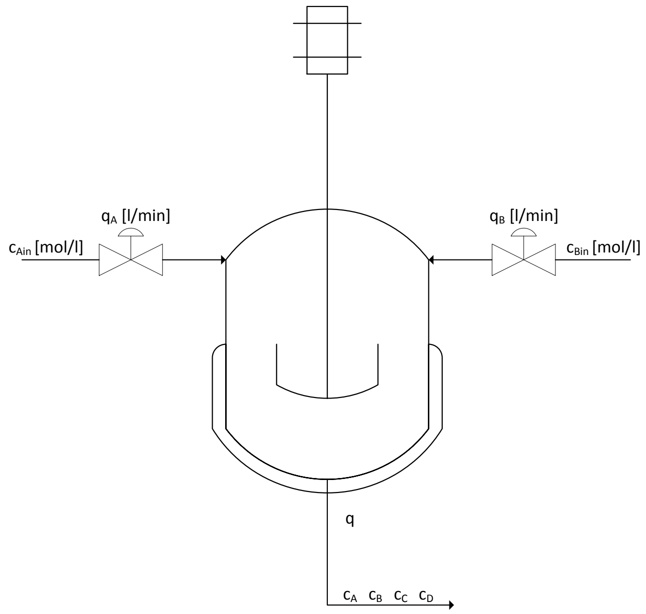


Fig. 3. Schematic diagram of a CSTR

which we recognize as a least-squares problems with explicit solution

$$H = YX^{\dagger} \tag{40}$$

Note that this is not the same as simply finding the least squares solution for d from measurement equation (19), as it has been proposed by Gros et al. (2009).

3.2 Neighbouring-extremal considering measurement noise and input disturbances

The next step is to combine the optimal disturbance estimator (25) with the optimal input update (16) to obtain the iterative control rule

$$\Delta u_{k+1} = K_u \Delta u_{m.k} + K_y \Delta y_{m,k} \tag{41}$$

where

$$K_y = -J_{uu}^{-1} J_{ud} H_1 \tag{42}$$

$$K_u = -J_{uu}^{-1} J_{ud} H_2$$

Figure 1 depicts a simplified block diagram of the proposed implementation approach. Note that the neighbouring extremal controller updates the control input based on the deviation of the measurements to their nominal value. In the next section we will illustrate the application of the method for the optimization of a chemical reactor.

4. SIMULATION EXAMPLE

Consider the steady state optimization of an isothermal continuously stirred reactor (CSTR) in which the reactions $A + B \rightarrow C$ and $2B \rightarrow D$ are taking place, see Fig. 3. The example is borrowed from (Gros et al., 2009). The operational goal is to determine the feed rates q_A and q_B of the components A and B into the reactor to maximize the production of the component C at steady state. This optimization problem can be formulated as

$$\max_u J(u) = \frac{c_C^2 (q_A + q_B)^2}{q_A\, c_{Ain}} - 0.5(q_A^2 + q_B^2) \tag{43}$$

Table 1. Nominal model parameters and operating conditions

Parameter	*Value*	*Unit*
k_1	0.65	l/(mol h)
k_2	0.014	l/(mol h)
c_{Ain}	2	mol/l
c_{Bin}	1.5	mol/l
V	500	l

subject to

$$\begin{aligned} 0 &= -k_1 c_A c_B + \frac{q_A}{V} c_{Ain} - \frac{q_A + q_B}{V} c_A \\ 0 &= -k_1 c_A c_B - 2k_2 c_B^2 + \frac{q_B}{V} c_{Bin} - \frac{q_A + q_B}{V} c_B \\ 0 &= k_1 c_A c_B - \frac{q_A + q_B}{V} c_C \end{aligned} \tag{44}$$

Where $u = [q_A, q_B]^T$, c_X describes the molar concentration of component X, V is the volume of liquid in the reactor, k_1 and k_2 are the rate constants of the chemical reactions, c_{Ain} and c_{Bin} are the concentrations of the feed streams. The nominal model parameters are given in table 1. The main disturbances are the rate constants k_1 and k_2. Solving the optimization problem under nominal conditions gives

$$u_n = \begin{bmatrix} q_A \\ q_B \end{bmatrix} = \begin{bmatrix} 0.56 \\ 0.77 \end{bmatrix}, \quad y_n = \begin{bmatrix} c_A \\ c_B \\ c_C \end{bmatrix} = \begin{bmatrix} 0.058 \\ 0.05 \\ 0.78 \end{bmatrix} \tag{45}$$

which are referred to as nominal optimal conditions.

4.1 Design of the new neighbouring extremal control

The task now is to design neighbouring extremal controllers to update the nominal inputs to keep the process operating near optimal conditions despite the uncertainties. The main disturbance d are the rate constants ($d = [k_1, k_2]^T$). Our measurement vector is defined as $y = [c_A, c_B, c_C]^T$. The second order derivatives at the nominal point are

$$J_{uu} = \begin{bmatrix} 18.17 & -12.12 \\ -12.12 & 9.71 \end{bmatrix}, \quad J_{ud} = \begin{bmatrix} -0.17 & -28.6 \\ -0.06 & 22.9 \end{bmatrix} \tag{46}$$

The only information missing for the computation of the controller (42) is the matrix $H = [H_1, H_2]$. For this we need to compute the matrices G and G_d of the linearized model (27). Using symbolic differentiation and inserting the nominal optimal inputs we get

$$G = \begin{bmatrix} 0.54 & -0.36 \\ -0.45 & 0.36 \\ 0.34 & -0.28 \end{bmatrix}, \quad G_d = \begin{bmatrix} -0.06 & 0.71 \\ -0.03 & -0.73 \\ 0.06 & -0.71 \end{bmatrix} \tag{47}$$

Next, we assume the parameters k_1 and k_2 may lie in the range $\pm 50\%$ with 95% probability. This gives the scaling matrices $W_d = \text{diag}(0.1625, 0.0035)$ and $W_u = \text{diag}(0.0017, 0.0025)$. We also assume an expected measurement noise of 10% standard deviation, resulting in $W_n = \text{diag}(0.0003, 0.0003, 0.0039)$ and $W_{du} = \text{diag}(0.0028, 0.0038)$. Gathering all these pieces we are now able to solve (40) to obtain

$$H = \begin{bmatrix} -11.69 & -11.95 & 0.29 & 0.84 & 0.24 \\ 0.07 & -0.71 & -0.25 & -0.27 & 0.21 \end{bmatrix} \tag{48}$$

which results in the following controller gains

$$K_y = \begin{bmatrix} -1.34 & -0.66 & 0.26 \\ -1.76 & -0.49 & 0.46 \end{bmatrix}, \qquad K_u = \begin{bmatrix} -0.35 & 0.17 \\ -0.57 & 0.32 \end{bmatrix} \tag{49}$$

4.2 Neighbouring extremal controller design ignoring noise

For comparison we will follow the neighbouring extremal approach of Gros et al. (2009) where the estimation of the disturbance Δd comes from the direct invention of the linearized model (19). This results in the following gains

$$K_y^{Gros} = \begin{bmatrix} -0.87 & -0.42 & 0.86 \\ -1.21 & -0.07 & 1.21 \end{bmatrix}, \quad K_u^{Gros} = \begin{bmatrix} -0.015 & 0.08 \\ 0.22 & -0.06 \end{bmatrix} \tag{50}$$

4.3 Results

In this section we will compare the controllers for several disturbances realizations and for different measurement noise levels. For completeness, we also included the results for a trivial open-loop policy, in which the control inputs are kept constant at their nominal values.

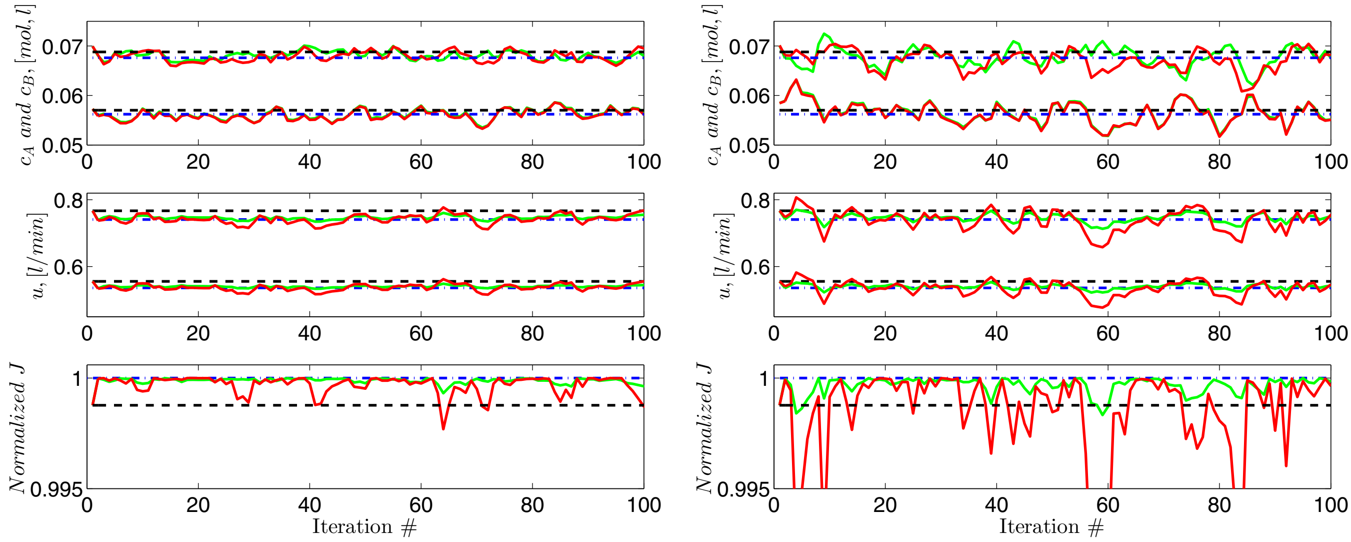
Table 2 summarizes the different disturbance cases that were tested. We compared the controllers using four levels of measurement noise: 0%, 5%, 10% and 20% standard deviation Gaussian noise. We ran every case 1000 times and computed the average performance. Figure 5 shows the results for cases 1 to 4. Both strategies are significantly better than the open-loop policy in the noise-free case (top left plot in Fig. 5).

Not surprisingly, the neighbouring extremal controller (50), which was designed neglecting the noise, results in better performance in the noise-free experiment. Nonetheless, the economic benefits of (50) decrease significantly as the noise level increases. The proposed approach remain consistently better than open-loop policy in all cases.

Figure 4 exemplifies the performance obtained for different noise levels. In all cases we show c_A and c_B measurements, the control inputs and the objective function to be maximized. Measurement of c_C was omitted from the plot to ease the visualization. The red solid line is the NE controller (50) designed assuming perfect measurements; the green solid line is the proposed method; the dashed **black** line represent the open-loop solutions using nominal inputs; the blue lines represent the optimal solution. The objective function was normalized with respect to the optimal value.

5. DISCUSSION AND CONCLUSION

It is worth pointing out that the NE control updates can be beneficial up to some noise level, in which there would be no gain compared to the open-loop strategy. This threshold, however, depends on the size of the disturbance Δ d, but it can be analytically computed as shown in Gros et al. (2009). The intuition is that we need to be able to detect the effect of the process disturbance in the noisy measurements y_m. For a fixed level of noise, the relative efficiency (with respect to the open-loop policy) of the NE approaches improves with an increase in the magnitude of Δd.



(a) Case 4 with 10% standard deviation Gaussian noise

(b) Case 4 with 20% standard deviation Gaussian noise

Fig. 4. Comparison of the different approaches for two different measurement noise levels. The red lines are given by the NE controller (50) that was designed without taking noise in consideration. The green lines are the result of the proposed NE controller (49). Note that the new method is considerably less sensitive to noise.

Table 2. Disturbance cases

Case	*Disturbance*	*Optimal inputs*
case 1	$k_1 = k_{1,nom} + 20\%$ $k_2 = k_{2,nom} + 20\%$	$q_A = 0.57$ $q_B = 0.78$
case 2	$k_1 = k_{1,nom} - 20\%$ $k_2 = k_{2,nom} - 20\%$	$q_A = 0.54$ $q_B = 0.75$
case 3	$k_1 = k_{1,nom} + 20\%$ $k_2 = k_{2,nom} - 20\%$	$q_A = 0.57$ $q_B = 0.79$
case 4	$k_1 = k_{1,nom} - 20\%$ $k_2 = k_{2,nom} + 20\%$	$q_A = 0.53$ $q_B = 0.74$

Both NE control methods are based on linearization of the problem around some operation point. For this reason we restricted our simulations to a local neighbourhood of the nominal case. Due to the inherent nonlinearity of real processes, little can be said about the performance NE controllers for excessively large parameter variations. Nonetheless, in our proposed method we are able to define the range of expected disturbances and find the best option for the given range.

Our design approach is based on two steps: first we find the optimal static estimator and then we combine it with the optimal sensitivities to obtain the NE gains K_u and K_y. An interesting question that arises is whether we can compute the optimal gains in one step, that is, can we directly find gains K_u and K_y that minimizes the average loss? It is not perfectly clear that the solution to this problem is equivalent to the solution obtained with the two step approach. More in depth analysis of these questions will be presented in a future paper.

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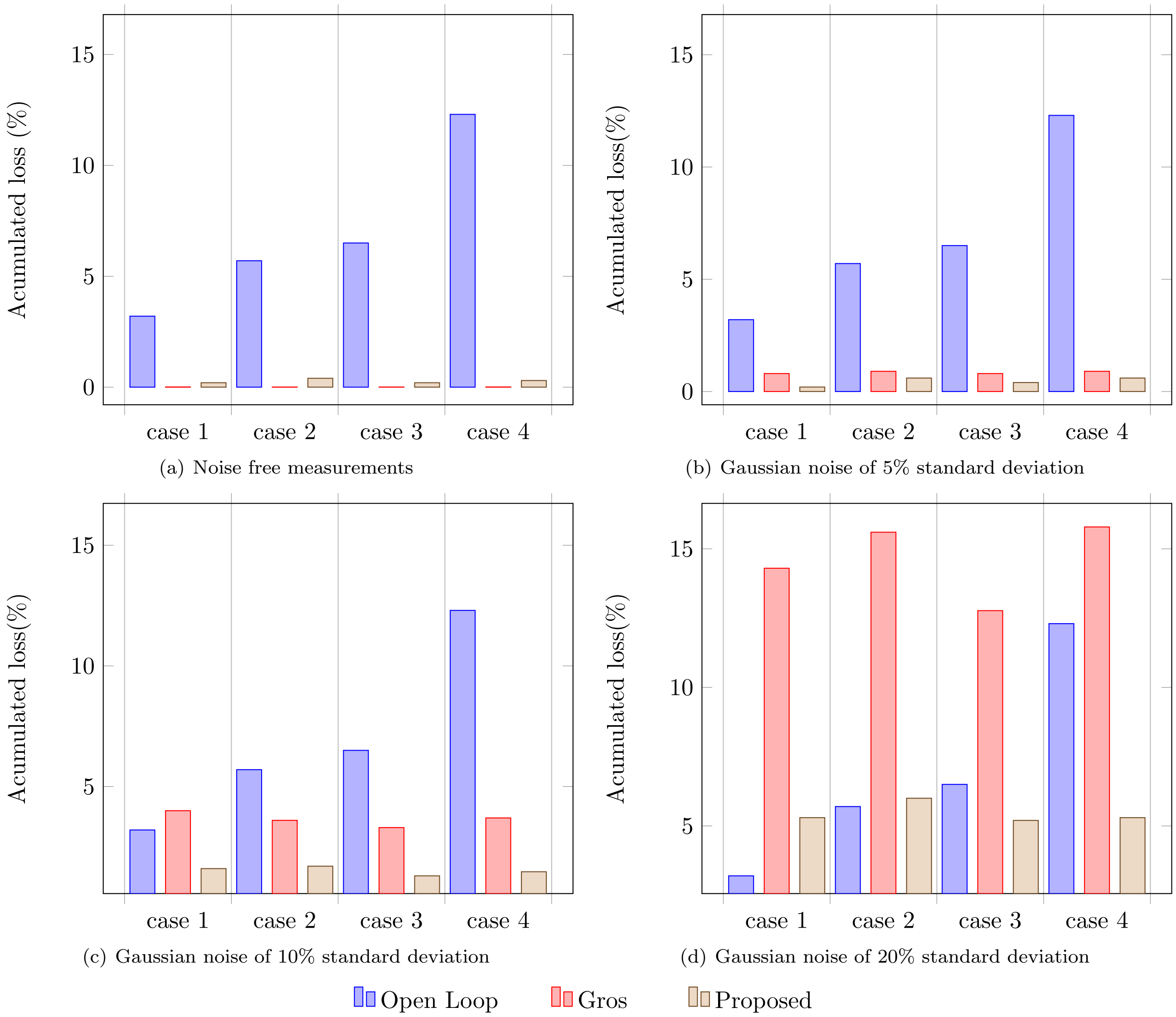

Fig. 5. Comparison of control strategies with different disturbances affecting the system. The results represent an average over 1000 runs considering different levels of measurement noise.