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Null-space method for optimal operation of transient processes

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Abstract: We consider batch process optimization and robust implementation of optimal control policies. The dynamic optimization of such processes is in most cases model based, and therefore subject to uncertainties. This may lead to sub-optimal control trajectories with significant economical losses. In this paper we extended the concept of self-optimizing control for the optimal operation of transient processes. The main idea is to find a function of the measurements whose trajectory is optimally invariant to disturbances, and then track the trajectory using standard feedback controllers. Doing so results in near-optimal economic operation in spite of varying disturbances without the need for re-optimization. We show that the invariant trajectories can be computed as linear combinations of the measurement vector, where the combination matrix is easily obtained from optimal sensitivities. We illustrate the application of the proposed method in a semi-batch reactor case study.

1. INTRODUCTION

Optimal economic operation of chemical processes may be in general formulated as a dynamic optimization problem. This includes problems that are transient in nature, where the dynamic behaviour must be considered, such as batch operations, grade changes and start-up and shut-down of continuous plants. The optimal solutions should not be implemented in an open-loop manner in most cases because of uncertain and unknown disturbances, which may lead to large economic losses or even infeasibility.

Two paradigms exist for implementation of near optimal control: an on-line approach, where the optimization problem is solved in real-time at every sample time when new information is available. An example of this approach is the economic model predictive control (EMPC)(Ellis et al., 2014).

An example of the offline optimization paradigm is self-optimizing control, which combines an off-line analysis with an on-line implementation using feedback control to track the optimal properties of the solution. For processes whose economics are defined by the steady-state behaviour the concept of self-optimizing control was introduced by Skogestad (2000).

Self-optimizing control focuses on selecting a set of controlled variables c that, when kept at constant setpoints, indirectly result in near-optimal economic operation in spite of disturbances without the need for re-optimization. Diverse systematic methods are available to find the right variables to control for steady-state problems. Skogestad and Postlethwaite (2005) proposed the Maximum Gain Rule to select individual measurements. Alstad and Skogestad (2007) presented the Null Space method to select optimal linear combinations of measurements to be controlled. The Null Space method is very simple and yet gives zero economical loss if enough measurements are available and measurement noise is negligible.

In this paper we extended the steady state Null Space method to optimal control of batch processes. The main idea is to find a function of the measurements $c_r(t)$ whose trajectory is optimally invariant to disturbances and then track the trajectory using standard feedback controllers. By doing so, the input trajectories are optimally updated in case disturbances occur.

In this paper, we show that the invariant trajectories can be computed as linear combinations of the measurement vector. The optimal combination matrix can be easily computed off-line using optimal sensitivity information, which is easy to calculate. Our proposed control structure is shown in Fig. 1 where $c_r(t)$ is the optimally invariant reference trajectory that we track. As illustrated in a fedbatch case study, the proposed method is very simple and intuitive and yet is able to give near-optimal results.

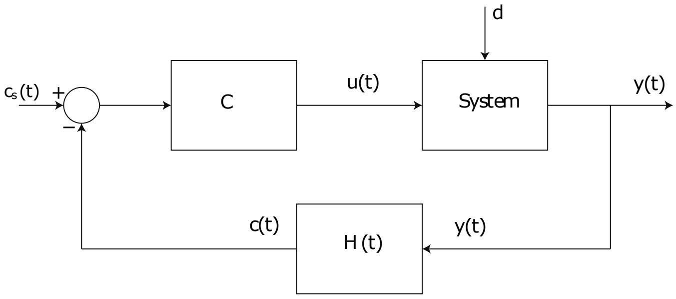

Fig. 1. Proposed implementation based on simple feedback

There are alternative approaches for self-optimizing control of batch processes currently available in the literature (see for instance (Grema et al., 2015; Jaschke et al., 2011; Wuhua Hu, 2012)). However, the method presented in this paper stands out for its simplicity and ease of implementation.

The paper is divided as follows: Section 2 outlines the proposed method; Section 3 gives the results for the semi-batch reactor case study; Sections 4 and 5 show a discussion and the conclusion for the paper, respectively.

2. NULL-SCAPE METHOD FOR TRANSIENT PROCESSES

Consider the following dynamic optimization problem:

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

subject to:

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

$$y = g(x) \tag{3}$$

$$p(x, u) \leq 0 \tag{4}$$

where t_f is the final time, $x \in \mathcal{R}^{n_x}$ are the state variables and $u \in \mathcal{R}^{n_u}$ are the control inputs. In addition, we define $y \in \mathcal{R}^{n_y}$ as the vector of known variables (measurements), which may include states, disturbances and control inputs. The optimization problem depends explicitly on the uncertain parameters by $d \in \mathcal{R}^{n_d}$. State and input constraints are summarized by $p(x, u)$. In this paper we make the assumption that the active constraint set does not change with the disturbances and time.

Assume the nominal optimal input sequence $u_0(t)$ and nominal optimal measurements $y_0(t)$ for a given disturbance d_0 is known a priori. The goal is to obtain all the neighbouring solutions for deviations $\Delta d = d - d_0$ in the problem parameters without the need for re-optimization. It can be shown that if the cost function J is twice continuously differentiable in a neighbourhood of the nominal solution and the linear independence constraint qualifications and the sufficient second-order conditions hold, then the optimal sensitivity matrix F is well defined:

$$F(t) = \frac{\partial y_{opt}(t, d)}{\partial d} \tag{5}$$

and, a first order, local approximation of the optimal solution in terms of outputs y in the neighbourhood can be obtained from

$$y_{opt}(t, d) \approx y_0(t, d_0) + F(t)\Delta d \tag{6}$$

To find the invariant measurement combination, $c(y(t), d)$ whose optimal value is independent of Δd, i.e., we want $c_{opt}(y(t), d) = c_0(y(t), d_0)$ for any Δd sufficiently small. A simple choice is a linear combination of the measurements:

$$c(t) \equiv H(t)y(t) \tag{7}$$

where $H(t)$ is a $n_u \times n_y$ matrix, and $c(t)$ is a $n_u \times 1$ vector. This way we can write

$$c_{opt}(t, d) = H(t)[y_0(t, d_0) + F(t)\Delta d] \tag{8}$$

and we define the nominal combination of measurements:

$$c_0(t, d_0) = H(t)y_0(t, d_0) \tag{9}$$

By subtracting (9) from (8) we obtain:

$$c_{opt}(t, d) - c_0(t, d_0) = H(t)F(t)\Delta d \tag{10}$$

To have optimality with the given control policy, we must require that $c_{opt}(t) = c_0(t)$ or

$$c_{opt}(t, d) - c_0(t, d_0) = 0 \tag{11}$$

or

$$H(t)(y_{opt}(t) - y_0(t)) = 0 \tag{12}$$

or

$$H(t)F(t)\Delta d = 0 \tag{13}$$

Since this must hold for any value of Δd, we must select $H(t)$ such that for any t we have $H(t)F(t) = 0$. This is always true if $H(t)$ lies in the left null space of $F(t)$. The main result is summarized in the following theorem.

Theorem 1 (Nullspace method for dynamic systems) Consider a disturbance vector Δd consisting of perturbations in the initial value of certain system parameters, and let $F(t)$ denote the optimal sensitivity matrix of the measured outputs y with respect to these disturbances, that is, $\frac{\partial y_{opt}}{\partial d}(d) = F(t)\Delta d$. Then for a small disturbance (within a range where $F(t)$ is independent of the magnitude of Δd) the controlled system, with the control policy $c(t) = c_0(t)$, behaves optimally if we select $H(t)$ such that it lies in the nullspace of $F^T(t)$, that is

$$H(t)F(t) = 0, \quad \forall t \tag{14}$$

A non-trivial optimal solution $H(t)$ of rank n_u can always be found if we have sufficient number of independent measurements $y(t)$. This requires that $n_y \geq n_u + n_d$.

In this approach there is an indirect assumption of 'perfect control' since we assume that we can adjust $u(t)$ such that $c(t)$ is kept at its setpoint $c_0(t)$ for all t. This may seem limiting but this is often not the case. First, we know that there does exists a feasible $u(t)$, because this is how we obtain $c_0(t)$ and $\frac{\partial y_{opt}}{\partial d}(d) = F(t)\Delta d$. Second, there may be fundamental limitations, such as time delay, which limits perfect control, but this will not be important for the economics if the time scale required for optimal dynamic operation is much longer than the achievable closed-loop time constant for control.

Using this approach we obtain a trajectory $c_{opt}(t, d)$ that is optimally invariant due to disturbance. We can transform the problem of implementing $u(t)$ in a 'open-loop' manner to a reference tracking problem with optimal setpoints $c_r(t, d) = c_{opt}(t, d)$ (see Fig. 1). By tracking c_r, a simple controller automatically generates inputs u that are optimal for any disturbance d sufficiently small and thus, the online optimization is avoided.

The whole procedure has offline and online steps which are summarized as follows:

Offline:

- Solve the dynamic optimization problem with d_0;
- Select appropriate measurements y;
- Compute the optimal sensitivities $F(t)$ and the combination $H(t)$;
- Compute the reference trajectories $c_r(t) = H(t)y_0(t)$.

Online:

- Track the reference c_r by a feedback controller.

The first step of the offline analysis is often the most time-consuming step of the procedure because a large nonlinear optimization problem needs to be solved in order to obtain u_0 and $y_0(t)$. In the second step, the measurements should be selected to ensure good controllability, which is achieved by having high input-output gains.

An important assumption in our approach is the time-scale separation between the (slower) dynamic evolution of the overall trajectory and the (faster) optimal input update given by the feedback control. That is, the local convergence to the setpoint ($c(t) = c_s(t)$) is much faster than the evolution of $c_s(t)$ and may be considered instantaneous from the slower scale point of view.

Remark 1. The proposed approach is closely related to the neighbouring-extremal (NE) control introduced in the seventies (see Bryson and HO (1975) for details). In NE control, and optimum state feedback law is applied to compute fast corrections of the control trajectory for small deviations. However, the controller is obtained from a boundary value problem whose solution is not straightforward. Furthermore, differently from our approach, in NE control all the states are required to be measured or estimated.

Remark 2. The optimal sensitivity has been used recently to compute online fast optimal control updates in the context of nonlinear model predictive control (as for example in Zavala and Biegler (2009)) and real time dynamic optimization as in Würth et al. (2009). However, in both cases the proposed methods required measurement or estimation of the disturbance/model uncertainty Δd. Here we only require enough independent measurements y and the solution is given by an simple output feedback controller.

3. SIMULATION EXAMPLE: FED-BATCH REACTOR

Consider the fed batch reactor optimization problem studied in Srinivasan et al. (2003), Jaschke et al. (2011) and Gros et al. (2009) where we have two chemical reactions:

$$A + B \longrightarrow C \text{ and } B \longrightarrow D \tag{15}$$

where C is the product and D is the undesired side product. A is already presented in the reactor while B is fed during the batch. The goal is to maximize the difference between the amount of C and D at the end of the batch.The dynamics are given by:

$$\begin{aligned} \dot{c}_A &= -k_1 c_A c_B - c_A u/V \\ \dot{c}_B &= -k_1 c_A c_B - 2k_2 c_B - (c_B - c_{B_{in}})u/V \\ \dot{V} &= u, \end{aligned} \tag{16}$$

where c_A and c_B are the concentrations [mol/l] of A and B respectively, V [l] is the volume and u [l/min] is the inlet feed rate and $c_{B_{in}}$ is the inlet concentration [mol/l]. The initial conditions $c_A(0) = c_{A0}$, $c_B(0) = c_{B0}$ and $V(0) = V_0$. Additionally, the initial product concentration is zero.

Concentrations $c_C(t)$ and $c_D(t)$ are obtained from mass balance and are written as:

$$c_C(t) = \frac{1}{V}(c_{A0}V_0 - c_A(t)V(t)) \tag{17}$$

and

$$c_D(t) = \frac{1}{2V}[(c_A(t) + c_{B_{in}} - c_B(t))V(t) - (c_{A0} + c_{B_{in}} - c_{B0})V_0] \tag{18}$$

The optimization problem is thus formulated as:

$$\min_u J(t_f) = -(c_C(t_f) - c_D(t_f)) \tag{19}$$

subject to the dynamic model (16) and $u \leq u_{max}$ and $u \geq u_{min}$. The final time is fixed. All the problem parameters for the nominal conditions are summarized in Table 1.

3.1 Nominal optimal solution

The input and output trajectories for the nominal conditions are given in Fig. 2 and Fig. 3 respectively.

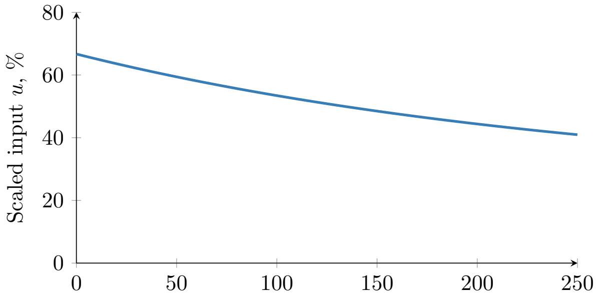

Fig. 2. Scaled input for the nominal case (optimal solution for $d = d_0$)

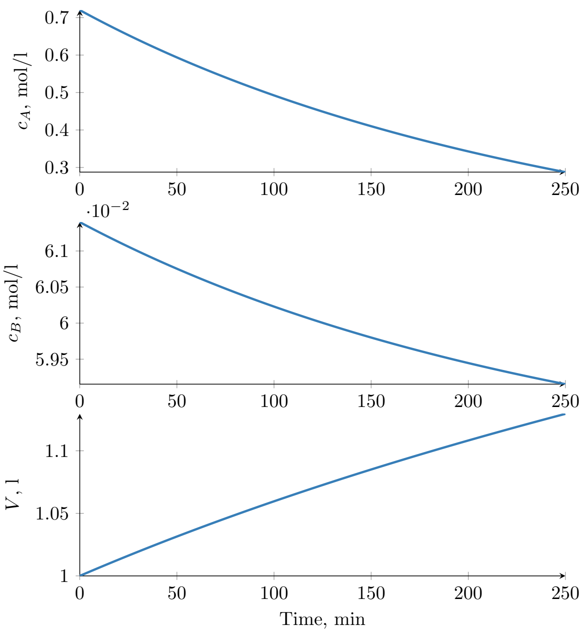

Fig. 3. State variables for the nominal case (optimal solution for $d = d_0$)

3.2 Disturbances and measurements

We consider here 20% disturbance on the kinetic parameters k_1 and k_2 ($d = [k_1, \ k_2]^T$). Because we consider

Table 1. Nominal parameters values

Symbol	Value	Unit
k_1	0.053	l/(mol×min)
k_2	0.128	l/(mol×min)
$c_{B_{in}}$	5	mol/l
t_f	250	min
u_{min}	0	l/min
u_{max}	0.001	l/min
c_{A0}	0.72	mol/l
c_{B0}	0.0614	mol/l
c_{C0}	0	mol/l
c_{D0}	0	mol/l
V_0	1	l

two disturbances ($n_d = 2$) and we have one manipulated variable ($n_u = 1$), we will make use of thee measurements to satisfy the condition $n_y \geq n_u + n_d = 3$. We consider measurements of concentrations c_A and c_B in addition to the volume V. Thus, our measurement vector becomes

$$y = [c_A \ c_B \ V]^T \tag{20}$$

3.3 Computing invariant trajectories

Once the important disturbances d and the measurement vector y have been defined the next step is to compute the optimal sensitivity $F(t)$. A simple practical method to obtain F is to use finite differences, where we recompute the optimal solution for a perturbed problem and approximate the sensitivities using the deviation from the nominal solution, that is

$$F(t) \approx \frac{y_{opt}^{d^*}(t) - y_0(t)}{d^* - d_0} \tag{21}$$

where d^* is the perturbed parameter vector and $y_{opt}^{d^*}$ is the optimized for the perturbed problem. Note that the deviation $\|d^* - d_0\|$ should be small to bound the approximation error. Nonetheless, this approach may be computationally demanding for large dimension problems with large number of disturbances. For such cases, we may use more efficient methods for calculations of the sensitivities as those provided by (Pirnay et al., 2012). In that approach, the basic strategy is based on the application of the Implicit Function Theorem to the KKT conditions of the NLP, where it can be shown that sensitivities can be obtained simply by solving a linearization of the KKT conditions. The main implementation idea is to take advantage of the exact second derivatives used in the intermediate steps of the NLP algorithm to computed exact parametric sensitivities with very little added computation (Pirnay et al., 2012).

Finally, the final step is to compute the optimal invariant trajectory $c_0(t) = H(t)y_0(t)$ such that $F(t)H(t) = 0$. The optimal combination matrix $H(t) = [h_1(t) \quad h_2(t) \quad h_3(t)]$ for our problem is depicted in the bottom of Fig. 4. Note that the weights are fairly constant, a fact that may simplify the implementation tasks, such as the control tuning. Figure 4 also shows the invariant $c_0(t)$. The final step is the online implementation, where we design a feedback controller to track the reference $c_0(t)$. The controller used here is a simple PI.

3.4 Closed-loop evaluation

In this simulation study we consider four disturbance cases, which are summarized in Table 2. Figures 5 and 6 show the performance of the proposed method in comparison with the reoptimized solution and the open-loop nominal solution for the disturbance case 2 (see Table 2). Note in Fig. 5 that the optimal solution (red line) consists of a short boundary arc $u(t) = u_{min}$ of about $\Delta t = 2.5$ min followed by a sensitivity seeking arc. Interestingly, although the proposed controller starts with nominal values, it rapidly catches up with the optimal input trajectory. As a consequence, the state trajectories in the proposed method (shown in 6) are nearly identical to the optimal ones.

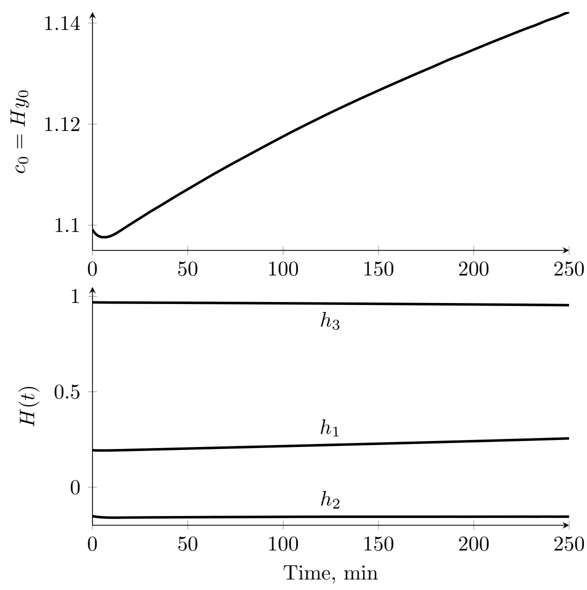

Fig. 4. Nominal inputs

Table 2. Disturbances

Case	k_1	k_2
Nominal	0.0530	0.1280
Case 1	0.0424	0.1024
Case 2	0.0424	0.1536
Case 3	0.0636	0.1024
Case 4	0.0636	0.1536

In Gros et al. (2009) Neighbouring-Extremal (NE) controller for singular optimal control problems is proposed. The main idea of that NE consists in linearizing the necessary conditions of optimality around an optimal trajectory of the corresponding undisturbed problem leading to a state-feedback control law. The NE feedback law computes directly the updates δu to the nominal control input u_n so that $u = \delta u + u_n$. We compare the proposed controller with the one presented in Gros et al. (2009) for different disturbance scenarios. Table 3 summarizes the comparisons. As it can be seen, the self-optimizing controller and

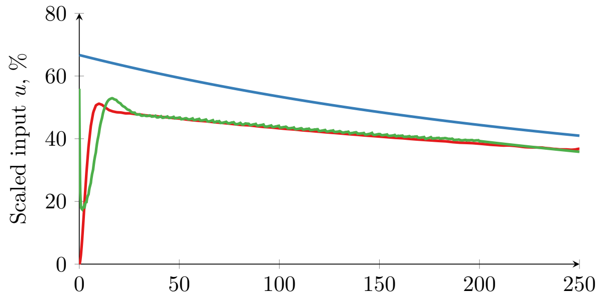

Fig. 5. Case 2: Control input. Blue line: open-loop nominal input; red line: optimal solution; green line: proposed approach. Note that the input trajectory in our approach stays near the optimal solution without the need for re-optimization.

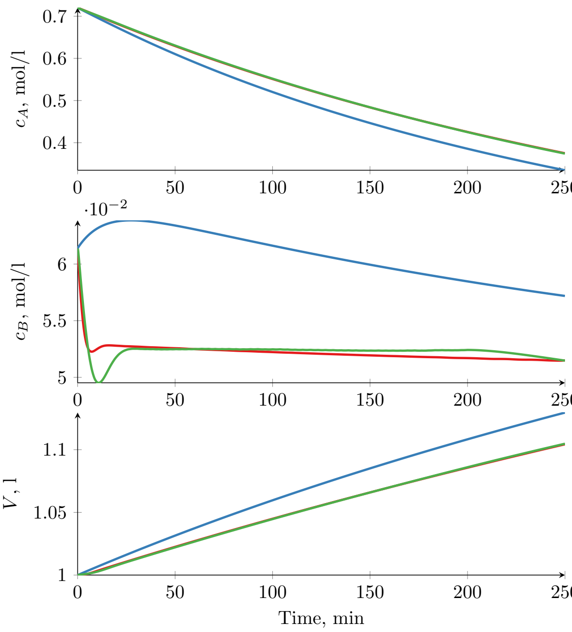

Fig. 6. Case 2: Measurements. Blue lines: open-loop nominal input; red lines: optimal solution; green lines: proposed approach.

$NE(\theta)$ give very good results for all cases. Both methods are based on linearized conditions of optimality and should theoretically yield the same economic performance. However, the implementation philosophies of both cases are fundamentally different. In the NE approach the feedback law is derived directly from the linearized optimization problem and we have no control over important closed-loop dynamic properties, such as stability margins. In the proposed approach, the optimization and the control objectives are decoupled, that is, the design of feedback controller is an independent decision that can be made after the optimal invariant trajectories are obtained.

Table 3. Results for different disturbances on k_1 and k_2. J_{opt} is the optimal cost with the perturbed system, J_{soc} is the cost with the proposed approach, J_{OL} is the cost of the open-loop strategy, J_{NE}^{θ} is the cost of the NE controller proposed in Gros et al. (2009) considering the parametric uncertainty and J_{NE} is the NE controller proposed in Gros et al. (2009) ignoring the uncertainty.

Case	$-J_{opt}$	$-J_{soc}$	$-J_{OL}$	$-J_{NE}^{\theta}$	$-J_{NE}$
Case 1	0.2435	0.2434	0.2431	0.2435	0.2433
Case 2	0.1957	0.1957	0.1904	0.1956	0.1857
Case 3	0.3476	0.3474	0.3437	0.3475	0.3398
Case 4	0.2952	0.2952	0.2950	0.2952	0.2950

4. DISCUSSION

A drawback of this approach is that it cannot explicitly handle constraints. Therefore, for a realistic implementation the proposed method should be combined with a periodic solution of the dynamic optimization where a new reference solution is obtained, and new invariant trajectories $c(t)$ are computed. The idea is to recompute the optimal sensitivities $F(t)$ online after solving the current NLP and then apply the approach shown in Fig 1 in between two successive optimizations. Similar idea has been published in (Würth et al., 2009) where the authors proposed to use sensitivity based neighbouring-extremal updates combined with real-time optimization. In this way, the frequency of optimizations can be greatly reduced.

For simplicity, in this paper we have assumed a fixed final time in the dynamic optimization problem formulation. However, it is often necessary to consider a variable final time to handle uncertainties. In fact, many practical applications can be formulated as minimum time problems. The main complication here is the fact that nominal and disturbed trajectories may be misaligned in time. Thus, in order to apply our method in such cases we would need to synchronize the different trajectories using a new time variable (a 'warped-time' variable) that is comparable in all cases. An example of a typical candidate could be the distance between the current measured state and an end-point state active constraint.

5. CONCLUSION

In this paper we extend the concept of self-optimizing control to the dynamic optimization of batch processes. The main idea is to find a function of the measurements whose trajectory is optimally invariant to disturbances and then track the trajectory using standard feedback controllers. The invariant trajectory is computed as a time-varying linear combination of the measurements and the optimal combination is obtained from optimal sensitivities that are easily computed. The proposed method was tested in a semi-batch reactor case study, where near-optimal performance was achieved for various disturbances.

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