FROM OFF-LINE NUMERICAL OPTIMIZATION TO REAL-TIME MEASUREMENT-BASED OPTIMIZATION VIA NCO TRACKING

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Abstract: The problem of optimizing a dynamic system in the presence of uncertainty is typically tackled using measurements. The methods widely used in the literature are based on repetitive optimization of a process model. Recently, tracking of the Necessary Conditions of Optimality (NCO tracking) has been proposed as a computationally less expensive alternative, which is based on the derivation of a *solution model*. So far, the solution model, which contains information on the structure of the input profiles and the set of active constraints, has been derived manually based on physical insight and intuition. In this paper, based on the recent results on the numerical optimization of dynamic systems, we present a systematic and automated approach to come up with a solution model. This concept provides the first steps towards an entirely automated procedure for dynamic optimization under uncertainty via NCO tracking.

Keywords: dynamic real-time optimization, hybrid control, measurements, NCO tracking, numerical methods, solution structure, uncertainty

1. INTRODUCTION

The optimization of dynamic processes has received growing attention in recent years, because it is essential for the process industry to strive for a more efficient and agile manufacturing in the face of saturated markets and global competition. In practical situations, with uncertainties like model-inaccuracies and process disturbances, it is not sufficient to determine numerically an optimal solution by a *nominal optimization* and apply it to the process. Rather, uncertainties have to be taken into account. This can be either accomplished by *robust optimization* (e.g. Zhang *et al.* (2002)), which typically leads to quite conservative solutions, or alternatively by *measurement-based optimization*. Here, process measurements are used to adapt the optimal trajectories to process changes and disturbances. Typically, this is done by a repetitive solution of the dynamic optimization problem over the sampled time horizon *on-line*, i.e. during the process operation. Such techniques are also known as *dynamic real-time optimization*. At each sampling time, the initial conditions for the optimization are updated by means of process measurements. Furthermore, the model parameters might also be updated using measurement information. In most cases, not all required process variables are accessible through measurements. Suitable *estimation* techniques are then required for the computation of unmeasurable quantities (e.g. Lee and Ricker (1994)). Based on these updates, the repetitive optimization can adjust the control variables to the current process state.

A conceptually different way of tackling this problem has been recently proposed by Srinivasan *et al.* (2003*b*). Here, a tracking scheme is derived from the necessary conditions of optimality (NCO), therefore, the approach is referred to as *NCO tracking.* The NCO tracking scheme uses the concept of a *solution model* (Srinivasan and Bonvin, 2004), which is essentially derived by dissecting the optimal input profiles and relating them to the different parts of the NCO. So far, the derivation of the solution model requires experience and physical insight into the process. Current practice is to manually perform numerical optimization studies of the given problem and then interpret the solution profiles by visual inspection.

However, recent results on the numerical optimization of dynamic systems allow not only to compute a nominal optimal solution, but also to extract important structure information such as active path and terminal constraints and the type and sequence of intervals (Schlegel and Marquardt, 2004). The goal of this contribution is therefore to present a scheme for the systematic development of a solution model by combining the aforementioned techniques. This concept provides the first steps towards a fully automated procedure for dynamic optimization under uncertainty.

2. PRELIMINARIES

2.1 Problem formulation

We consider the dynamic optimization problem

$$\min_{\boldsymbol{u}(t),t_f} \ \Phi(\boldsymbol{x}(t_f),\boldsymbol{\theta},t_f) \qquad \text{(P1)}$$

$$\begin{aligned}
\text{s.t.} \quad \dot{\boldsymbol{x}} &= \boldsymbol{f}(\boldsymbol{x},\boldsymbol{u},\boldsymbol{\theta},t)\,, \quad \boldsymbol{x}(t_0)=\boldsymbol{x}_0\,, && (1)\\
\boldsymbol{0} &\geq \boldsymbol{h}(\boldsymbol{x},\boldsymbol{u},\boldsymbol{\theta},t), \quad t\in[t_0,t_f]\,, && (2)\\
\boldsymbol{0} &\geq \boldsymbol{e}(\boldsymbol{x}(t_f),\boldsymbol{\theta})\,. && (3)
\end{aligned}$$

Here, $\boldsymbol{x}(t) \in \mathbb{R}^{n_x}$ denotes the vector of state variables with initial conditions $\boldsymbol{x}_0$. The process model (1) is formulated as the smooth vector function $\boldsymbol{f}$. The time-dependent control variables $\boldsymbol{u}(t) \in \mathbb{R}^{n_u}$ and possibly the final time are the degrees of freedom for the optimization. The objective function Φ is formulated as a terminal cost criterion for simplicity. Further, path constraints $\boldsymbol{h}$ on the states and control variables (2) and endpoint constraints $\boldsymbol{e}$ on the state variables (3) can be employed. For simplicity, assume that each constraint is formulated in terms of simple (lower and upper) bounds on the specific variables. The vector of uncertain parameters $\boldsymbol{\theta}$ includes parametric uncertainty as well as external disturbances.

2.2 Necessary conditions of optimality (NCO)

By employing Pontryagin's Minimum Principle (Bryson and Ho, 1975), (P1) can be reformulated with the *Hamiltonian* function $H(t)$ as

$$\min_{\boldsymbol{u}(t),t_f} \ H(t) = \boldsymbol{\lambda}^T\boldsymbol{f}(\boldsymbol{x},\boldsymbol{u},\boldsymbol{\theta}) + \boldsymbol{\mu}^T\boldsymbol{h}(\boldsymbol{x},\boldsymbol{u},\boldsymbol{\theta}) \quad \text{(P2)}$$

$$\begin{aligned}
\text{s.t.} \quad \dot{\boldsymbol{x}} &= \boldsymbol{f}(\boldsymbol{x},\boldsymbol{u},\boldsymbol{\theta},t)\,, \quad \boldsymbol{x}(t_0)=\boldsymbol{x}_0\,, && (4)\\
\dot{\boldsymbol{\lambda}}^T &= -\frac{\partial H}{\partial \boldsymbol{x}}\,,\ \boldsymbol{\lambda}^T(t_f) = \left(\frac{\partial \Phi}{\partial \boldsymbol{x}} + \boldsymbol{\nu}^T\frac{\partial \boldsymbol{e}}{\partial \boldsymbol{x}}\right)\Bigg|_{t_f}\,, && (5)\\
0 &= \boldsymbol{\mu}^T\boldsymbol{h}(\boldsymbol{x},\boldsymbol{u},\boldsymbol{\theta},t)\,, && (6)\\
0 &= \boldsymbol{\nu}^T\boldsymbol{e}(\boldsymbol{x}(t_f),\boldsymbol{\theta})\,. && (7)
\end{aligned}$$

Here, $\boldsymbol{\lambda}(t) \neq \boldsymbol{0}$ denotes the adjoint variables, $\boldsymbol{\mu}(t) \geq \boldsymbol{0}$ the Lagrange multipliers for the path constraints and $\boldsymbol{\nu} \geq \boldsymbol{0}$ the multipliers for the terminal constraints. The complementarity conditions (6), (7) can be interpreted in a way that a specific Lagrange multiplier is positive if the corresponding constraint is active and zero otherwise.

An optimal solution of problem (P2) fulfills the necessary conditions of optimality:

$$\frac{\partial H(t)}{\partial \boldsymbol{u}} = \boldsymbol{\lambda}^T\frac{\partial \boldsymbol{f}}{\partial \boldsymbol{u}} + \boldsymbol{\mu}^T\frac{\partial \boldsymbol{h}}{\partial \boldsymbol{u}} = \boldsymbol{0}\,, \qquad (8)$$

If a free final time is allowed, an additional transversality condition has to be also satisfied.

$$H(t_f) = \left(\boldsymbol{\lambda}^T\boldsymbol{f} + \boldsymbol{\mu}^T\boldsymbol{h}\right)\Big|_{t_f} = -\left.\frac{\partial \Phi}{\partial t}\right|_{t_f} \qquad (9)$$

The necessary conditions can now be rewritten in the partitioned form of Table 1 by separating:

- The conditions linked to the active constraints from those related to sensitivities (first and second rows in Table 1)
- The conditions linked to path objectives from those related to terminal objectives (first and second columns in Table 1)

Table 1. Separation of the NCO into four distinct parts

	Path objectives	Terminal objectives
Constraints	$\boldsymbol{\mu}^T\boldsymbol{h} = 0$	$\boldsymbol{\nu}^T\boldsymbol{e} = 0$
Sensitivities	$\frac{\partial H}{\partial \boldsymbol{u}} = 0$	$H(t_f) + \left.\frac{\partial \Phi}{\partial t}\right\|_{t_f} = 0$

2.3 Solution structure

An optimal control profile $\boldsymbol{u}(t)$ consists of one or more arcs in such a way, that the control is continuous and differentiable within each arc, but may jump at the switching points. Conclusions about the possible solution structure can be derived from the path objectives of the necessary conditions (6) and (8) (Srinivasan *et al.*, 2003*a*). The solution is either:

(1) $u_i = u_{i,path}$: u_i is determined by an active path constraint (constraint-seeking), or
(2) $u_i = u_{i,sens}$: u_i is not governed by an active path constraint, it is sensitivity-seeking.

Among the constrained-seeking arcs, various cases can be distinguished depending on what type of constaints are active:

(1) $u_i = u_{i,min}$: u_i is at its lower bound,
(2) $u_i = u_{i,max}$: u_i is at its upper bound,
(3) $u_i = u_{i,state}$: u_i is determined by an active state path constraint.

This distinction will be used for an automatic detection of the control structure.

3. NUMERICAL OPTIMIZATION AND STRUCTURE DETECTION

3.1 Numerical solution

There are various solution techniques available for dynamic optimization problems of the form (P1) (Srinivasan *et al.*, 2003*a*). In this work, we use the sequential or single-shooting approach, a direct method which solves the problem by conversion into a nonlinear programming problem (NLP) through discretization of the control variables $\boldsymbol{u}(t)$. Note that our solution approach does not require an explicit derivation of the necessary conditions nor does it use the Hamiltonian two-point boundary value problem formulation (P2).

For the parameterization of the control profiles $u_i(t)$ often piecewise polynomial approximations (e.g. piecewise constant or linear) are applied. The profiles for the state variables $\boldsymbol{x}(t)$ are obtained by forward numerical integration of the model (1) for a given input. With the discretization parameters $\hat{\boldsymbol{u}}$ as degrees of freedom (DOF), problem (P1) can be reformulated as the NLP

$$\min_{\hat{\boldsymbol{u}}, t_f} \Phi = \Phi(\boldsymbol{x}(\hat{\boldsymbol{u}}, \boldsymbol{\theta}, t_f)) \quad \text{(P3)}$$

$$\text{s.t.} \quad 0 \geq \boldsymbol{h}(\boldsymbol{x}, \hat{\boldsymbol{u}}, \boldsymbol{\theta}, t_i), \quad \forall t_i \in \Delta\,, \quad (10)$$

$$0 \geq \boldsymbol{e}(\boldsymbol{x}(t_f), \boldsymbol{\theta})\,, \quad (11)$$

with the path constraints being evaluated at discrete time points contained in Δ. Typically, a sequential quadratic programming (SQP) method (Nocedal and Wright, 1999) is used for the NLP solution.

3.2 Detection of the solution structure

The solution of the NLP provides optimal discretized control profiles for the given problem. However, it is possible to extract further information, namely the control switching structure even without any prior knowledge. Schlegel and Marquardt (2004) have proposed a method which automatically detects the control switching structure and exploits it for an efficient reparameterization of the control profiles.

Due to space limitations, we refer to the aforementioned reference for details about the particular steps in the algorithm. Without going into details, the key is to note that each discrete constraint in (P3) has an associated discrete Lagrange multiplier, $\hat{\mu}_i$ or $\hat{\nu}_i$, respectively. They are related to the Lagrange multipliers $\boldsymbol{\mu}(t)$ and $\boldsymbol{\nu}$ of the continuous problem (P2). The value of each of the discrete multipliers provides information about the status (active or inactive) of the particular constraint at the optimal solution. This information is used for structure detection, reparameterization, and later the derivation of the solution model.

As a result of this procedure, we obtain optimal control profiles parameterized with a minimum number of parameters related to the NCO. The parameterized optimal control is given by

$$\boldsymbol{u}(t) = \mathcal{U}(\boldsymbol{\eta}(t), \boldsymbol{\mathcal{A}}, \boldsymbol{\tau}, t)\,. \quad (12)$$

Each control profile is parameterized by the time-variant arcs $\boldsymbol{\eta}(t) \in \mathbb{R}^L$ and time-invariant parameters $\boldsymbol{\tau} \in \mathbb{R}^L$, where L is the total number of arcs. The boolean set $\boldsymbol{\mathcal{A}}$ of length L describes the type of each particular arc, which can be one out of $\{u_{min}, u_{max}, u_{state}, u_{sens}\}$, as explained in Section 2.3. The switching times of $\boldsymbol{u}$ are collected in the vector $\boldsymbol{\tau} \in \mathbb{R}^L$, with τ_k being the final time of arc k. For fixed final time problems, the last switching time τ_L is fixed. In the numerical solution, the time-variant arcs $\boldsymbol{\eta}(t)$ are further time-parameterized by parameters $\hat{\boldsymbol{\eta}}$. The parameterization is adapted to the type of arc by using coarse piecewise linear approximations on path-constrained and sensitivity seeking arcs and piecewise constant ones on control-bounded arcs.

4. MEASUREMENT-BASED OPTIMIZATION VIA NCO TRACKING

The main idea behind measurement-based optimization via an NCO tracking scheme is that optimality can be achieved by meeting the NCO for the real process. To apply NCO tracking to a dynamic optimization problem, it is important to note that the solution of constrained terminal-time dynamic optimization problems are typically discontinuous and consists of various arcs or intervals. Hence, the NCO has four parts as indicated in Table 1. Thus, enforcing the NCO in dynamic optimization problems corresponds to using control techniques to meet four sets of conditions (a constraint and a sensitivity part both during the operation and at final time) using appropriate measurements.

4.1 Solution Model

The real challenge in NCO tracking lies in the fact that four different objectives are involved in achieving optimality, i.e. meeting constraint and sensitivity conditions both on-line and at final time. Hence, it becomes important to appropriately parameterize the inputs using time functions and scalars and assign them to the different tasks. This assignment, which corresponds to choosing the solution model, is a way of looking at the NCO through the inputs. The generation of a solution model includes two steps:

• *Input dissection:* Based on the effect of uncertainty, this step determines the fixed and free parts of the inputs. For some of the intervals, the inputs are (or are assumed to be) independent of the prevailing uncertainty, e.g., intervals where the inputs are at their bounds, i.e. they can be applied in an open-loop fashion. These input elements can thus be considered fixed in the solution model. In other intervals, the inputs are affected by uncertainty and need to be adjusted for optimality. All the elements affected by uncertainty constitute the free variables of the optimization problem. The choice of the number and sequence of input arcs and the parameterization of the inputs in various arcs form the core issues in input dissection.

• *Linking the input free variables to the NCO:* The next step is to provide an unambiguous link between the free variables of the inputs and the NCO. The active path constraints fix certain time functions and the active terminal constraints certain scalar parameters or time functions. The remaining degrees of freedom are used to meet the path and terminal sensitivities. Note that the pairing is not always unique. An important assumption here is that the set of active constraints is correctly determined and does not vary with uncertainty. Fortunately, this restrictive assumption can often be relaxed.

4.2 Formulation of adaptation laws

Once the solution model is formed, it provides the basis for the adaptation of the various free parts of the inputs using appropriate measurements. However, it is not defined if a controller is implemented on-line or in a run-to-run fashion. On-line implementation requires reliable on-line measurements of the parts of the NCO used in the particular controller. In most of the applications, measurements of the constrained variables are available on-line. If on-line measurements of certain NCO parts are not available, a predictive empirical or fundamental model is used. Also, if alternate measurements are available trajectory following can be implemented.

Otherwise a run-to-run implementation becomes necessary. The corresponding time-functions and parameters are updated in a run-to-run fashion after the full set of batch measurements are collected. Yet, run-to-run adaptation has two main drawbacks: (i) it does not compensate within-run variations since only disturbances that are correlated over several runs can be rejected, and (ii) it requires multiple runs to be optimal. So, it is preferable, if possible, to do most of the adaptation on-line.

However, the required information on the path sensitivities and terminal objectives is typically not available during the run. This necessitates information regarding the future, a task that requires a reliable process model, which was assumed to be unavailable in this study. This implies that full adaptation cannot, in general, be accomplished within a single run. However, the emphasis is to make judicious approximations and formulate strategies to get as much as possible within a single run.

The type of the controllers depend upon the application at hand. However, a PI type controller will usually be sufficient if a good feedforward for the controls is available from the reference solution.

5. FROM THE DETECTED SOLUTION STRUCTURE TO THE SOLUTION MODEL

The NCO tracking approach presented in the previous section requires a robust feasible solution model. For this, problem (P1) is solved for several uncertainty scenarios to compute optimal solutions along with their corresponding structures. If the solution structure – the number, type and sequence of arcs – varies with respect to uncertainty, then a solution model that combines structure detection results from various uncertainty realizations is required. However, the assumption of invariant structure is found to be valid for many examples of batch operation. So, only the issue of deriving the solution model from the nominal numerical solution and its structural information is studied. A solution model is derived from the detected structure using the following steps.

(1) *Decomposition of DOF into constraint-seeking, sensitivity-seeking and bounded DOF:* Expression (12) provides a separate parameterization for all n_u control variables. In the following, each control variable is treated separately. For ease of notation, an index for the control is omitted. η_k refers to the k^{th} arc of a particular control. From the detected solution structure in $\boldsymbol{\mathcal{A}}$,

the time-variant control arcs $\boldsymbol{\eta}(t)$ can be decomposed into constraint-seeking $\boldsymbol{\eta}_{path}(t)$, sensitivity-seeking $\boldsymbol{\eta}_{sens}(t)$ and bounded $[\boldsymbol{\eta}_{min}(t), \boldsymbol{\eta}_{max}(t)]$ arcs. The time-invariant DOF, the switching times $\boldsymbol{\tau}$, are similarly decomposed into the *starting times* of the constraint-seeking arcs ($\boldsymbol{\tau}_{path}$), sensitivity-seeking arcs ($\boldsymbol{\tau}_{sens}$) and bounded arcs ($[\boldsymbol{\tau}_{min}, \boldsymbol{\tau}_{max}]$). Note that the labels of switching times are only referring to the beginning of the arcs and are not necessarily assigning them to the corresponding parts of the NCO.

The next step is to pair the decomposed DOF to the NCO. The time-variant and time-invariant DOF are respectively paired to time-variant and time-invariant functions of the NCO.

(2) *Linking bounded DOF:* Let the arc $\eta_k(t)$ be the i^{th} bounded control arc. It is considered to be fixed in the presence of uncertainty. Then,

$$\eta_{min,i}(t) = \eta_k(t) = u_{min}, t \in [\tau_k, \tau_{k+1}] \text{ or}$$
$$\eta_{max,i}(t) = \eta_k(t) = u_{max}, t \in [\tau_k, \tau_{k+1}]. \quad (13)$$

However, the starting times of these arcs are not fixed, but rather assigned later.

(3) *Linking constraint-seeking DOF:* The time-variant constraint-seeking $\boldsymbol{\eta}_{path}(t)$ are not parameterized. Let the path constraint h_j be active during the arc k which is the i^{th} path constraint-seeking arc $\eta_{path,i}$. Then,

$$\eta_{path,i}(t) = \eta_i(t) = \mathcal{K}_i(h_j(t)), t \in [\tau_k, \tau_{k+1}] \quad (14)$$

where $\mathcal{K}_i$ is an appropriate path controller. The switching times $\boldsymbol{\tau}_{path}$ are assigned to the activation times of the constraints. For the active path constraint h_j, the corresponding switching time $\tau_{path,i}$ for all controls is assigned as

$$\tau_{path,i} = \tau_k = t|_{h_j(t)=0}, \ t \in [0, t_f]. \quad (15)$$

In the single control case, the assignment of the path constraint-seeking DOF is unanimous. But in the multi-input case, the assignment can be non-unique.

(4) *Linking time-invariant bounded DOF:* Depending on the relative degree of an active path constraint h_j, one or more switching times of the bounded arcs that come before are linked to the activation of h_j at the future activation time $\tau_{k+1} = \tau_{path,i}$ in (15). Let τ_k or $\tau_{min/max,i}$ be the starting time of the i^{th} bounded arc. Then,

$$\tau_{min/max,i} = \tau_k = \mathcal{P}_i(h_j(\tau_{k+1})), \quad (16)$$

where $\mathcal{P}_i$ is an appropriate predictive controller that is designed such that in the finite time $(\tau_{k+1} - \tau_k)$ the constraint h_j becomes active at time τ_{k+1}.

The remaining switching times of $\boldsymbol{\tau}_{min/max}$ are linked to some of the active endpoint constraints. A gain matrix that describes the influence of $\boldsymbol{\tau}_{min/max}$ (not determined by the path constraints) on the endpoint constraints is computed. Either a relative gain array analysis or a singular value decomposition is used to choose the combination of the switching times that are linked to the endpoint constraints. For e_j being an active endpoint constraint,

$$\tau_{min/max,i} = \tau_k = \mathcal{E}_i(e_j(t_f)) \quad (17)$$

an appropriate predictive or run-to-run controller $\mathcal{E}_i$ uses the measurements of e_j at the end of batch. For multiple active endpoint constraints that many number of switching times are present in the solution model. This makes the assignment non-unique.

(5) *Linking sensitivity-seeking DOF:* After linking the constraint-seeking DOF, all remaining ones are attributed to the sensitivities, which comprise both, the path and endpoint sensitivities. Furthermore, the remaining active endpoint constraints $\bar{\boldsymbol{e}}$ that are not yet linked are assigned to some of the sensitivity-seeking DOF. Therefore, the arcs are used to simultaneously keep the endpoint constraints active and push the sensitivities to zero. The time-variant sensitivity-seeking arcs $\boldsymbol{\eta}_{sens}$ can be parameterized as in the numerical solution. Alternatively, they can be directly linked to certain time-variant reference trajectories from the nominal solution.

(5.1) *Linking parameterized sensitivity-seeking DOF:* On the i^{th} sensitivity arc, say k in $\boldsymbol{\mathcal{A}}$, the controls $\eta_{sens,i}(t) = \eta_k(t)$ can be further parameterized with the parameters $\hat{\eta}_{sens,i}$ as done in the numerical solution. The sensitivities of the Lagrange function $L = \Phi(t_f) + \hat{\boldsymbol{\nu}}^T \bar{\boldsymbol{e}}(t_f)$ of the parameterized problem (P3) are linked to $\hat{\boldsymbol{\eta}}$ and $\boldsymbol{\tau}_{sens}$ as

$$\hat{\eta}_{sens,i} = \mathcal{T}_{\eta,i}\left(\frac{\partial L}{\partial \hat{\eta}_{sens,i}}\right), \ \forall t \in [\tau_k, \tau_{k+1}] \quad (18)$$

$$\tau_{sens,i} = \tau_k = \mathcal{T}_{\tau,i}\left(\frac{\partial L}{\partial \tau_{sens,i}}\right), \quad (19)$$

where $\mathcal{T}_{\eta,i}$ and $\mathcal{T}_{\tau,i}$ are appropriate controllers for the sensitivities. The sensitivities of Φ and $\bar{\boldsymbol{e}}$ at t_f and the nominal values of the Lagrange multipliers $\hat{\boldsymbol{\nu}}$ of the unassigned active endpoint constraints $\bar{\boldsymbol{e}}$ are required for the sensitivity controllers. Note that the active path constraints are not considered in the Lagrange function. Furthermore, due to the assured feasibility with respect to path constraints in step (3), the sensitivities $\frac{\partial \boldsymbol{h}}{\partial \eta_{sens,i}}, \frac{\partial \boldsymbol{h}}{\partial \tau_{sens,i}}$ can be ignored. The nominal process model with the state measurements/estimates is employed for evaluating the sensitivities on-line during a batch. For details on this sensitivity-based update strategy, the reader is referred to Kadam and Marquardt (2004). If a process model cannot be used on-line, the updates in equations (18) and (19) are done on a run-to-run basis after collecting the measurements at the end of batch.

(5.2) *Linking unparameterized sensitivity-seeking DOF:* Another approach, based on the reference trajectory tracking, is suggested for linking the sensitivity-seeking DOF $\boldsymbol{\eta}_{sens}(t)$. On each sensitivity-seeking arc i, reference trajectories $\boldsymbol{y}_{ref,i}(t)$ for certain measurable variables $\boldsymbol{y} \in \mathbb{R}^{n_y}, n_y \geq n_u$ are linked as

$$\eta_{sens,i}(t) = \eta_k(t) = \mathcal{N}_i(\boldsymbol{y}, \boldsymbol{y}_{ref}), \qquad (20)$$
$$t \in [\tau_k^{ref}, \tau_{k+1}^{ref}]$$
$$\tau_{sens,i} = \tau_k = t|_{y_j(t)=y_{ref,i,j}(\tau_k^{ref})}, \qquad (21)$$

where $\mathcal{N}_i$ is an appropriate controller designed for the reference tracking. The idea is to link $\boldsymbol{\eta}_{sens}$ to n_u directions from the set of reference trajectories $\boldsymbol{y}_{ref}$ which are updated on a run-to-run basis to push the objective function sensitivities to zero. The reference variables are selected such that they are related to the parts of the NCO such as the remaining endpoint constraints $\bar{\boldsymbol{e}}$ and the objective function Φ. τ_k^{ref} and τ_{k+1}^{ref} are the reference start and end times of the sensitivity seeking arcs, which are updated on a run-to-run basis. For brevity, only the pairing equations are given here, we refer to (Kadam *et al.*, 2002) for details on reference trajectory tracking.

6. ILLUSTRATIVE EXAMPLE

6.1 *Bio-reactor with uncertainty*

The example used in this paper is a fed-batch bioreactor with inhibition and a biomass constraint. The objective is to maximize the product concentration at a given final time. The path constraints consist of the bounds on the substrate feed rate u, and an upper bound on the biomass concentration X. Due to space limitations, we refer to Srinivasan *et al.* (2003*a*) for further details about the problem formulation and the model equations. Fig. 1 shows the optimal solution profiles for the feed rate u, the substrate concentration S and the biomass concentration X. We recognize a complex switching structure consisting of $L = 6$ arcs of type $\boldsymbol{\mathcal{A}} = [u_{max}, u_{sens}, u_{min}, u_{path}, u_{sens}, u_{min}]$ with the switching times $\boldsymbol{\tau} = [0.86, 3.84, 5.43, 6.23, 7.93]$ h.

6.2 *Solution model*

The uncertainty considered is the variation of the growth parameter Y_x between the bounds $[0.3, 0.6]$ with the nominal value of 0.4. The structure of the solution does not change with this variation and so the nominal parameter value is used to derive the solution model.

Using the steps given in the previous section, the following solution model is derived from the detected structure.

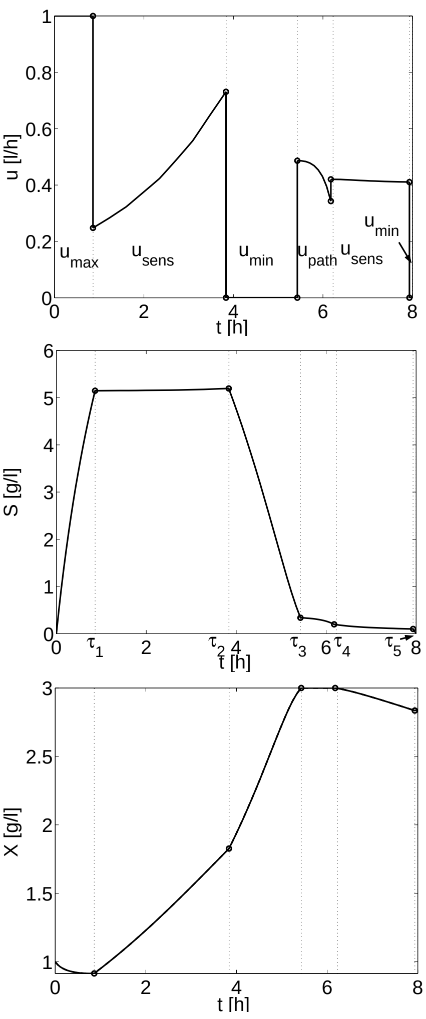

Fig. 1. Optimal nominal solution profiles.

$$u(t) = \begin{cases} u_{max} & 0 \leq t \leq \tau_1 \\ \mathcal{N}_1(S, S_{ref,1}) & \tau_1 \leq t \leq \tau_2 \\ u_{min} & \tau_2 \leq t \leq \tau_3 \\ \mathcal{K}_1(X, X_{max}) & \tau_3 \leq t \leq \tau_4 \\ \mathcal{N}_2(S, S_{ref,2}) & \tau_4 \leq t \leq \tau_5 \\ u_{min} & \tau_5 \leq t \leq t_f \end{cases} \qquad (22)$$

$$\tau_1 = t \text{ s.t. } S(t) = S_{ref,1} \qquad (23)$$
$$\tau_2 = t \text{ s.t. } X_{pred}(t) = 0.95 X_{max} \qquad (24)$$
$$\tau_3 = t \text{ s.t. } X(t) = X_{max} \qquad (25)$$
$$\tau_4 = t \text{ s.t. } S(t) = S_{ref,2} \qquad (26)$$
$$\tau_5 = 0.9 t_f \qquad (27)$$
$$X_{pred} = X - \alpha(1.25 S_{ref,2} - S) \qquad (28)$$

This solution model provides the control action $u(t)$ using the on-line measurements of X and S, without the use of a process model.

Fixed parts: The inputs in intervals 1, 3, and 6 are on the bounds and are considered fixed. The optimal value of the switching time τ_5 is almost constant for different realizations of the uncertain parameter. Therefore, it is also fixed at 7.93 h.

Path constraint: The switching time τ_3 is fixed by the activation of the constraint on X. Note that the third arc to u_{min} is required to bring down S so that X can be kept at X_{max}. This acts as a relative degree 2 system where two switching times are adapted to reach the constraint. An empirical model is developed for predicting X at the end of the u_{min}-arc. It can be observed from the nominal optimal profiles of S and X that, after u is switched to u_{min}, the ratio α between the changes in S and X is almost constant even in the presence of uncertainty. This fact is used for the prediction of X in (28). On the constraint-seeking arc, $\tau_3 \leq t \leq \tau_4$, u is given by the $\mathcal{K}_1$ controller that keeps X at its bound X_{max}. Due to sensitivity issues, a cascade type controller is employed, that calculates a set-point for S which is tracked by manipulating u using a PI controller.

Sensitivity-seeking arcs: A neighboring extremal approach is employed. $S_{ref,1}$ and $S_{ref,2}$ are chosen as constant over time with the values 5.14 and 0.2 g/l, respectively. On the sensitivity-seeking arcs, the optimal values for S corresponding to different realizations of the uncertain parameter value in optimization are almost constant. Therefore, $S_{ref,1}$ and $S_{ref,2}$ need not to be updated necessarily. The switching times τ_1 and τ_4 are assigned as given in equation (23) and (26) as the time when S reaches $S_{ref,1}$ and $S_{ref,2}$, respectively.

6.3 NCO tracking results

The NCO-tracking solution model comprising hybrid PI controllers to update time-variant and invariant parts of the control u is used in simulation. The solution model along with the process model is simulated for different realizations of the uncertain parameter values. Simulation results for two different uncertain parameters values, $Y_x = 0.4$ (nominal) and $Y_x = 0.6$ (perturbed), are reported in Fig. 2 as dashed and dotted lines, respectively. It can be observed that the profiles of X, S and u for nominal value of the uncertain parameter are almost the same as the optimal profiles shown in Fig. 1, which are calculated by rigorously solving the optimization problem. On the constraint seeking arc, X is not exactly at its maximum bound due to the back-off parameter and the use of a simple PI controller for tracking. This can be improved by updating the back-off and using an advanced controller such as a linear time-variant model predictive controller. The switching times are also appropriately updated using only measurements. In particular, the switching time τ_3 following the first sensitivity seeking arc is identical to the optimal one. The empirical model used for predicting X at the end of the u_{min}-arc is sufficiently accurate for updating τ_3. For the perturbed parameter value $Y_x = 0.6$, the same solution model is sufficiently accurate. Fig. 2 shows

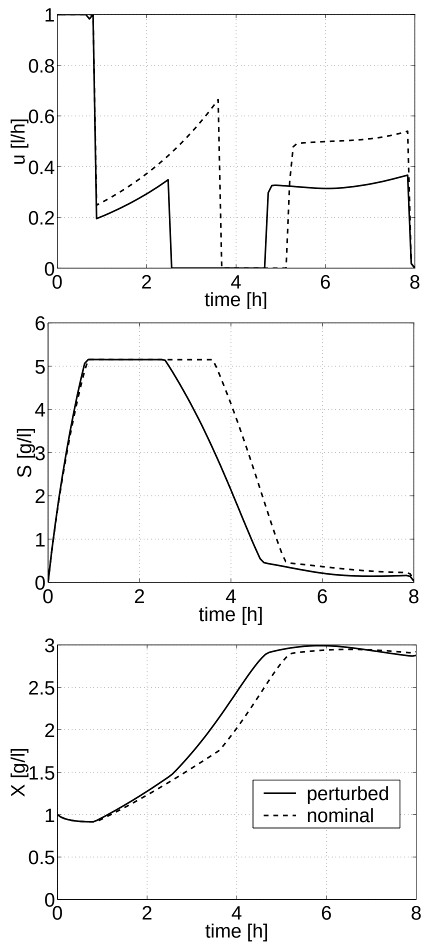

Fig. 2. Solution model profiles for nominal and perturbed parameter

that the batch operation is feasible and close to optimal. τ_3 is lower than nominal, which is accurately calculated. Furthermore, the sensitivity-seeking DOF are close to optimal. The objective function values using the NCO tracking solution model, re-optimized controls and the open-loop implementation of the nominal controls are given in Table 2. Using the solution model, the loss in optimality is very minimal, which can be further reduced by run-to-run updates.

Table 2. Objective function values using different control strategies

Y_x	Solution model	re-optimization
0.4	6.16	6.23
0.6	6.73	6.76

7. CONCLUSIONS

In this paper, we presented a systematic procedure for deriving a solution model for the optimal operation of dynamic processes from a numerical solution. The solution model is used to track the NCO in order to retain a feasible and optimal operation under uncertainty. The example problem used for illustration shows a very complex solution structure which can be automatically detected and systematically converted into a solution model. Investigations of an uncertainty scenario confirmed the robustness of the solution model.

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