Preprints of the 8th IFAC Symposium on Nonlinear Control Systems
University of Bologna, Italy, September 1-3, 2010

Selective Input Adaptation in Parametric Optimal Control Problems with Path Constraints ⋆

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Abstract: This paper is concerned with input adaptation in dynamic processes in order to guarantee feasible and optimal operation despite the presence of uncertainty. For optimal control problems having mixed control-state constraints, two sets of directions can be distinguished in the input function space: the so-called sensitivity-seeking directions, along which a small input variation does not affect the active constraints, and the complementary constraint-seeking directions, along which an input variation does affect the respective constraints. Two selective input adaptation scenarios can be defined, namely, adaptation along each set of input directions. This paper proves the important result that the cost variation due to the adaptation along the sensitivity-seeking directions is typically smaller than that due to the adaptation along the constraint-seeking directions.

Keywords: Parametric optimal control, mixed control-state constraints, sensitivity-seeking directions, constraint-seeking directions, linear integral equations, selective input adaptation.

1. INTRODUCTION

Transient processes constitute an important class of engineering processes. Many processes in resource industries and alternative energy-generation systems are either inherently transient or operated in an unsteady-state manner. Batch and semi-batch processes in chemical engineering are examples of processes characterized by the absence of a steady state.

We will consider the problem of optimal control of transient processes for which the uncertainties in the process model are represented in the form of parametric variations. If the optimal input profiles that are computed off-line, are applied to the process in an open-loop manner, plant-model mismatch and process disturbances can result in suboptimal process operation or, worse, infeasible operation. One way to avoid re-solving the optimal control problem is to *adapt* the nominal optimal inputs in accordance with the magnitude of the parametric variations. In this approach, one needs a *sensitivity analysis* of the parametric optimal control problems, i.e., a study of the effect of parametric variations on the optimal inputs. See Ito and Kunisch [1992, 2008] and Maurer and Augustin [2001] for extensive references to sensitivity analysis of parametric optimal control problems.

The use of sensitivity analysis to adapt all parts of the input profiles is difficult in practice, and may not be necessary from a performance viewpoint. Hence, partial or selective input adaptation strategies that result in acceptable performance loss compared to optimal operation of the perturbed process have a great potential for practical applications. The main focus of this work will be to define certain *components* of the input variations, which will help implement *selective* input adaptation schemes

For optimal control problems having control-state path constraints, the possibility of splitting the input space, at each time instant, into so-called pointwise *sensitivity- and constraint-seeking* directions has been discussed in Deshpande et al. [2009]. A small input variation along the former set of directions at a given time does not change the values of the active path constraints at that time. However, note that, since the system is dynamic, it is necessary to consider the current and all past input variations for computing the change in path constraints and capture the dynamic essence of the problem.

The latter approach is developed in this paper. In this case, a sensitivity-seeking direction turns out to be the solution of a certain set of linear integral equations. Thus, in this case, the sensitivity- and constraint-seeking directions are *directions* in the input function space $\mathcal{C}[t_0, t_\mathrm{f}]^{n_\mathbf{u}}$ as opposed to directions in the Euclidean space $\mathbb{R}^{n_\mathbf{u}}$ at each time instant as in Deshpande et al. [2009], where t_0 and t_f are the initial and final times, respectively, and $n_\mathbf{u}$ represents the number of input variables. The main result of this paper is that, for small parametric variations, the cost variation due to the adaptation along the sensitivity-seeking directions is typically *smaller* than that due to the adaptation along the constraint-seeking directions.

⋆ This work was supported by the Swiss National Science Foundation (SNSF) under Grant #200020-113292.

The practical significance of the result is that, for small parametric variations, meeting the active constraints will have a greater impact on optimality than forcing the sensitivity condition to zero.

The outline of the paper is as follows. The general mathematical formulation of the parametric optimal control problem involving path constraints is given in Section 2. A summary of the necessary conditions of optimality (NCO) and the terminology of *switching times* and related notation are also introduced in this section. In Section 3, the sensitivity- and constraint-seeking directions are defined, and the concept of selective input adaptation along either one of these directions is introduced. Section 4 presents a quantitative analysis of the cost variation brought about by selective input adaptation on response to parametric variations. In Section 5, a numerical approach is proposed to compute the sensitivity- and constraint-seeking directions. A numerical case study is presented in Section 6. Finally, Section 7 summarizes the results and identifies future research directions.

2. PRELIMINARIES

This section comprises the general mathematical formulation of the parametric optimal control problem involving path constraints and a summary of the NCOs. The terminology of switching times is also introduced.

2.1 Problem Formulation and Assumptions

The following parametric optimal control problem in the parameters $\boldsymbol{\theta}$, subject to the mixed control-state inequality constraints $\boldsymbol{\Omega} \leq \mathbf{0}$, with given initial time t_0 and terminal time t_{f}, is considered $(\mathrm{OC}(\boldsymbol{\theta}))$: [1]

$$\dot{\mathbf{x}}(t) = \mathbf{f}(t, \mathbf{x}(t), \mathbf{u}(t), \boldsymbol{\theta}); \quad \mathbf{x}(t_0) = \mathbf{h}(\boldsymbol{\theta}), \tag{1}$$

$$\Omega_i(t, \mathbf{x}(t), \mathbf{u}(t), \boldsymbol{\theta}) \leq 0, \quad i \in \mathcal{I}_{n_{\boldsymbol{\Omega}}}, \tag{2}$$

$$\min_{\mathbf{u}(t)} \; J(\mathbf{u}) = \psi(t_{\mathrm{f}}, \mathbf{x}(t_{\mathrm{f}}), \boldsymbol{\theta}) + \int_{t_0}^{t_{\mathrm{f}}} \phi(t, \mathbf{x}(t), \mathbf{u}(t), \boldsymbol{\theta})\, dt, \tag{3}$$

where $t \in [t_0, t_{\mathrm{f}}]$, $\mathbf{u}(t) \in \mathbb{R}^{n_{\mathbf{u}}}$ and $\mathbf{x}(t) \in \mathbb{R}^{n_{\mathbf{x}}}$. Moreover, the functions $\mathbf{f}$, Ω_i, ψ and ϕ are assumed to be continuously differentiable with respect to all their arguments.

Let the nominal values of the system parameters be $\boldsymbol{\theta}_0$, and let $(\mathbf{u}^*(t), \mathbf{x}^*(t))$ be an optimal pair for the problem $\mathrm{OC}(\boldsymbol{\theta}_0)$. We assume the following constraint qualification to hold [Maurer and Augustin, 2001]: [2]

$$\mathrm{rank}\{\boldsymbol{\Omega}^a_{\mathbf{u}}(t, \mathbf{x}^*(t), \mathbf{u}^*(t), \boldsymbol{\theta}_0)\} = n_{\boldsymbol{\Omega}^a}(t), \forall\, t \in [t_0, t_{\mathrm{f}}],$$

where $n_{\boldsymbol{\Omega}^a}(t)$ denotes the number of active path constraints at time t. Introducing the Hamiltonian function $\mathcal{H}$,

$$\mathcal{H}(t, \mathbf{x}, \mathbf{u}, \boldsymbol{\lambda}, \boldsymbol{\mu}, \boldsymbol{\theta}) := \phi(t, \mathbf{x}, \mathbf{u}, \boldsymbol{\theta}) + \boldsymbol{\lambda}^T \mathbf{f}(t, \mathbf{x}, \mathbf{u}, \boldsymbol{\theta}) + \boldsymbol{\mu}^T \boldsymbol{\Omega}(t, \mathbf{x}, \mathbf{u}, \boldsymbol{\theta}),$$

and assuming that the problem $\mathrm{OC}(\boldsymbol{\theta}_0)$ is not abnormal, the first-order necessary conditions of optimality must hold almost everywhere (a.e.) in $[t_0, t_{\mathrm{f}}]$ [Hartl et al., 1995]:

$$\mathbf{0} = \mathcal{H}_{\mathbf{u}}(t, \mathbf{x}^*(t), \mathbf{u}^*(t), \boldsymbol{\lambda}^*(t), \boldsymbol{\mu}^*(t), \boldsymbol{\theta}_0), \tag{4}$$

$$\dot{\boldsymbol{\lambda}}^*(t) = -\mathcal{H}_{\mathbf{x}}(t, \mathbf{x}^*(t), \mathbf{u}^*(t), \boldsymbol{\lambda}^*(t), \boldsymbol{\mu}^*(t), \boldsymbol{\theta}_0), \tag{5}$$

$$\boldsymbol{\lambda}^*(t_{\mathrm{f}}) = \psi_{\mathbf{x}}(t_{\mathrm{f}}, \mathbf{x}^*(t_{\mathrm{f}}), \boldsymbol{\theta}_0)$$

$$0 = \mu_i^*(t)\Omega_i(t, \mathbf{x}^*(t), \mathbf{u}^*(t), \boldsymbol{\theta}_0), \quad \forall\, i \in \mathcal{I}_{n_{\boldsymbol{\Omega}}}, \tag{6}$$

$$0 \leq \mu_i^*(t), \quad \forall\, i \in \mathcal{I}_{n_{\boldsymbol{\Omega}}},$$

for some $\boldsymbol{\lambda}^*(t) \in \mathbb{R}^{n_{\mathbf{x}}}$, $\boldsymbol{\mu}^*(t) \in \mathbb{R}^{n_{\boldsymbol{\Omega}}}$, $t \in [t_0, t_{\mathrm{f}}]$, along with (1) and (2).

Two additional assumptions are introduced:

- Strict complementarity slackness holds, i.e. the multiplier functions $\mu_i^*(t)$, $\forall\, t \in [t_0, t_{\mathrm{f}}]$, corresponding to the active mixed control-state constraints are strictly nonzero. The vector of these multiplier functions at time t is denoted by $\boldsymbol{\mu}^a(t)$.
- The Hamiltonian function is *regular*, which implies that the optimal inputs $\mathbf{u}^*(t)$ are continuous in $[t_0, t_{\mathrm{f}}]$ [Maurer and Augustin, 2001].

2.2 Switching Times

For problems having mixed control-state constraints, a constraint can be active over several time intervals. Let the structure of the nominal optimal inputs be such that the constraint Ω_i is active on N_i disjoint intervals $[a_{ik}, b_{ik}] \subset [t_0, t_{\mathrm{f}}], k \in \mathcal{I}_{N_i}$. Therefore,

$$\Omega_i(t, \mathbf{x}^*(t), \mathbf{u}^*(t), \boldsymbol{\theta}_0) = 0, \quad i \in \mathcal{I}_{n_{\boldsymbol{\Omega}}},$$

for $t \in \{[a_{i1}, b_{i1}], \ldots, [a_{iN_i}, b_{iN_i}]\}$.

The time instants a_{ik} and b_{ik} are called the *switching times* for the constraint Ω_i, and the vector of active constraints at time t is denoted by $\boldsymbol{\Omega}^a(t, \mathbf{x}^*(t), \mathbf{u}^*(t), \boldsymbol{\theta}_0)$. Henceforth, the set of all switching times in the nominal solution, including the initial and final times, is represented by

$$\mathcal{T} = \{t_0^*, \ldots, t_N^*\},$$

with $t_0 = t_0^* < \cdots < t_N^* = t_{\mathrm{f}}$. It is important to note that the set of active constraints in any subinterval $[t_{k-1}^*, t_k^*]$ is constant, while the sets of active constraints in different subintervals $[t_{p-1}^*, t_p^*]$ and $[t_{k-1}^*, t_k^*]$ are different.

3. SENSITIVITY- AND CONSTRAINT-SEEKING DIRECTIONS

In this section, the sensitivity- and constraint-seeking directions in input space are characterized by considering small variations of the inputs around their nominal optimal values $\mathbf{u}^*(t)$.

Consider a small variation around the nominal optimal inputs $\mathbf{u}^*(t)$ in the directions $\boldsymbol{\xi}^{\mathbf{u}} \in \hat{\mathcal{C}}[t_0, t_{\mathrm{f}}]^{n_{\mathbf{u}}}$,

$$\tilde{\mathbf{u}}(t; \eta) = \mathbf{u}^*(t) + \eta\, \boldsymbol{\xi}^{\mathbf{u}}(t), \quad \forall\, t \in [t_0, t_{\mathrm{f}}], \tag{7}$$

with $|\eta| \ll 1$, and where $\hat{\mathcal{C}}[t_0, t_{\mathrm{f}}]^{n_{\mathbf{u}}}$ stands for the linear space of piecewise-continuous functions on $[t_0, t_{\mathrm{f}}]$.

Let $\tilde{\mathbf{x}}(t)$ denote the resulting perturbed states so that the pair $(\tilde{\mathbf{x}}(t), \tilde{\mathbf{u}}(t))$ satisfies (1) for the parameter values $\boldsymbol{\theta}_0$. From the continuous differentiability of $\mathbf{f}$ with respect to the inputs and states at $(\mathbf{x}^*(t), \mathbf{u}^*(t))$, Taylor expansion of $\mathbf{f}$ around $(\mathbf{x}^*(t), \mathbf{u}^*(t))$ gives: [3]

[1] The following notation is used throughout the paper: $\mathcal{I}_n := \{1, \ldots, n\}$.

[2] The notation $\mathbf{g}_{\mathbf{z}}$ is used for the Jacobian matrix of the vector function $\mathbf{g}$ with respect to the vector $\mathbf{z}$.

[3] The compact notation $y^*[t] := y(t, \mathbf{x}^*(t), \mathbf{u}^*(t), \boldsymbol{\theta}_0)$ is used throughout the paper.

$$\dot{\tilde{\mathbf{x}}}(t) - \dot{\mathbf{x}}^*(t) = \mathbf{f}(t, \tilde{\mathbf{x}}(t), \tilde{\mathbf{u}}(t), \boldsymbol{\theta}_0) - \mathbf{f}^*[t]$$
$$= \mathbf{f}^*_{\mathbf{x}}[t]\,\{\tilde{\mathbf{x}}(t) - \mathbf{x}^*(t)\} + \eta\, \mathbf{f}^*_{\mathbf{u}}[t]\boldsymbol{\xi}^{\mathbf{u}}(t) + O(\eta^2).$$

A first-order approximation of $\tilde{\mathbf{x}}(t;\eta)$ is obtained as

$$\tilde{\mathbf{x}}(t;\eta) = \mathbf{x}^*(t) + \eta\, \boldsymbol{\xi}^{\mathbf{x}}(t) + O(\eta^2), \tag{8}$$

where $\boldsymbol{\xi}^{\mathbf{x}}(t)$ is the solution of

$$\dot{\boldsymbol{\xi}}^{\mathbf{x}}(t) = \mathbf{f}^*_{\mathbf{x}}[t]\boldsymbol{\xi}^{\mathbf{x}}(t) + \mathbf{f}^*_{\mathbf{u}}[t]\boldsymbol{\xi}^{\mathbf{u}}(t), \quad \forall\, t \in [t_0, t_\mathrm{f}],$$
$$\boldsymbol{\xi}^{\mathbf{x}}(t_0) = \mathbf{0}. \tag{9}$$

The unique solution of the above linear system can be written in the following form [Rugh, 1993],

$$\boldsymbol{\xi}^{\mathbf{x}}(t) = \sum_{i=1}^{k-1} \int_{t^*_{i-1}}^{t^*_i} \boldsymbol{\Phi}^{\mathbf{f}^*_{\mathbf{x}}}(t,s)\mathbf{f}^*_{\mathbf{u}}[s]\boldsymbol{\xi}^{\mathbf{u}}(s)\, ds + \int_{t^*_{k-1}}^{t} \boldsymbol{\Phi}^{\mathbf{f}^*_{\mathbf{x}}}(t,s)\mathbf{f}^*_{\mathbf{u}}[s]\boldsymbol{\xi}^{\mathbf{u}}(s)\, ds, \tag{10}$$

for each $t \in (t^*_{k-1}, t^*_k]$, $k \in \mathcal{I}_N$, where $\boldsymbol{\Phi}^{\mathbf{A}}(t,s)$ stands for the state-transition matrix of the homogeneous linear system

$$\dot{\mathbf{z}}(t) = \mathbf{A}(t)\mathbf{z}(t),\ \forall\, t \geq t_0; \quad \mathbf{z}(t_0) = \mathbf{z}_0. \tag{11}$$

The variation of the active constraints $\boldsymbol{\Omega}^a$ at time $\underline{t} \in [t_0, t_\mathrm{f}]$ caused by the input variation (7) is given by the Gâteaux derivative [Cesari, 1983] of $\boldsymbol{\Omega}^a$ in the direction $\boldsymbol{\xi}^{\mathbf{u}}(t)$ at $\mathbf{u}^*(t)$:

$$\delta\boldsymbol{\Omega}^a(\mathbf{u}^*;\boldsymbol{\xi}^{\mathbf{u}}) := \frac{\partial}{\partial\eta}\boldsymbol{\Omega}^a(\underline{t}, \tilde{\mathbf{x}}(\underline{t};\eta), \tilde{\mathbf{u}}(\underline{t};\eta), \boldsymbol{\theta}_0)\Big|_{\eta=0}$$
$$= \boldsymbol{\Omega}^{a*}_{\mathbf{x}}[\underline{t}]\boldsymbol{\xi}^{\mathbf{x}}(\underline{t}) + \boldsymbol{\Omega}^{a*}_{\mathbf{u}}[\underline{t}]\boldsymbol{\xi}^{\mathbf{u}}(\underline{t}).$$

Using (10), this variation can be rewritten as

$$\delta\boldsymbol{\Omega}^a(\mathbf{u}^*;\boldsymbol{\xi}^{\mathbf{u}}) = \boldsymbol{\Omega}^{a*}_{\mathbf{x}}[\underline{t}] \sum_{i=1}^{k-1} \int_{t^*_{i-1}}^{t^*_i} \boldsymbol{\Phi}^{\mathbf{f}^*_{\mathbf{x}}}(\underline{t},s)\mathbf{f}^*_{\mathbf{u}}[s]\boldsymbol{\xi}^{\mathbf{u}}(s)\, ds$$
$$+ \boldsymbol{\Omega}^{a*}_{\mathbf{x}}[\underline{t}] \int_{t^*_{k-1}}^{\underline{t}} \boldsymbol{\Phi}^{\mathbf{f}^*_{\mathbf{x}}}(\underline{t},s)\mathbf{f}^*_{\mathbf{u}}[s]\boldsymbol{\xi}^{\mathbf{u}}(s)\, ds + \boldsymbol{\Omega}^{a*}_{\mathbf{u}}[\underline{t}]\boldsymbol{\xi}^{\mathbf{u}}(\underline{t}). \tag{12}$$

If the value of $\boldsymbol{\Omega}^a$ is unaffected by a small variation in the direction $\boldsymbol{\xi}^{\mathbf{u}}(t)$ around $\mathbf{u}^*(t)$, for all $t \in [t_0, t_\mathrm{f}]$, then $\boldsymbol{\xi}^{\mathbf{u}}(t)$ is called a *sensitivity-seeking (SS) direction* at $\mathbf{u}^*(t)$. This concept is formalized in the following definition.

Definition 1. (Sensitivity-Seeking Directions). A function $\boldsymbol{\xi}^{\mathbf{u}} \in \hat{\mathcal{C}}[t_0, t_\mathrm{f}]^{n_{\mathbf{u}}}$ is called a *sensitivity-seeking direction* for the optimal control problem $\mathrm{OC}(\boldsymbol{\theta}_0)$ at $\mathbf{u}^*(t)$ if

$$\mathbf{0} = \mathcal{D}_{\boldsymbol{\Omega}^a,t}\boldsymbol{\xi}^{\mathbf{u}} := \boldsymbol{\Omega}^{a*}_{\mathbf{x}}[t] \sum_{i=1}^{k-1} \int_{t^*_{i-1}}^{t^*_i} \boldsymbol{\Phi}^{\mathbf{f}^*_{\mathbf{x}}}(t,s)\mathbf{f}^*_{\mathbf{u}}[s]\boldsymbol{\xi}_{\mathbf{u}}(s)\, ds$$
$$+ \boldsymbol{\Omega}^{a*}_{\mathbf{x}}[t] \int_{t^*_{k-1}}^{t} \boldsymbol{\Phi}^{\mathbf{f}^*_{\mathbf{x}}}(t,s)\mathbf{f}^*_{\mathbf{u}}[s]\boldsymbol{\xi}_{\mathbf{u}}(s)\, ds + \boldsymbol{\Omega}^{a*}_{\mathbf{u}}[t]\boldsymbol{\xi}^{\mathbf{u}}(t), \tag{13}$$

for $t \in (t^*_{k-1}, t^*_k]$, $k \in \mathcal{I}_N$.

Thus, a SS direction is a solution of the linear integral equation (13) for all $t \in [t_0, t_\mathrm{f}]$. Clearly, any linear combination of SS directions is itself a SS direction. Therefore, the set of SS directions for $\mathrm{OC}(\boldsymbol{\theta}_0)$ at $\mathbf{u}^*(t)$, denoted by

$$\mathcal{V}^s := \{\boldsymbol{\xi} \in \hat{\mathcal{C}}[t_0, t_\mathrm{f}]^{n_{\mathbf{u}}} :\ \mathcal{D}_{\boldsymbol{\Omega}^a,t}\boldsymbol{\xi} = \mathbf{0},\ t \in [t_0, t_\mathrm{f}]\},$$

yields a linear subspace of $\hat{\mathcal{C}}[t_0, t_\mathrm{f}]^{n_{\mathbf{u}}}$. It will be referred to as the *sensitivity-seeking subspace* for $\mathrm{OC}(\boldsymbol{\theta}_0)$ at $\mathbf{u}^*(t)$.

Next, a constraint-seeking (CS) direction is defined as one that is *orthogonal* to the sensitivity-seeking subspace.

Definition 2. (Constraint-Seeking Directions). A function $\boldsymbol{\xi}^{\mathbf{u}} \in \hat{\mathcal{C}}[t_0, t_\mathrm{f}]^{n_{\mathbf{u}}}$ is called a *constraint-seeking direction* for the optimal control problem $\mathrm{OC}(\boldsymbol{\theta}_0)$ at $\mathbf{u}^*(t)$ if $\boldsymbol{\xi}^{\mathbf{u}}(t)$ is orthogonal to $\mathcal{V}^s$,

$$0 = \langle \boldsymbol{\xi}^{\mathbf{u}}, \boldsymbol{\varphi} \rangle, \quad \forall\, \boldsymbol{\varphi} \in \mathcal{V}^s,$$

where $\langle\cdot,\cdot\rangle$ stands for any inner product on $\hat{\mathcal{C}}[t_0, t_\mathrm{f}]^{n_{\mathbf{u}}}$.

Let $\mathcal{V}^c$ denote the set of all CS directions for $\mathrm{OC}(\boldsymbol{\theta}_0)$ at $\mathbf{u}^*(t)$ by $\mathcal{V}^c$. By the sesquilinearity property of an inner product, $\mathcal{V}^c$ is itself a linear subspace in $\hat{\mathcal{C}}[t_0, t_\mathrm{f}]^{n_{\mathbf{u}}}$ and will be referred to as the *constraint-seeking subspace* for $\mathrm{OC}(\boldsymbol{\theta}_0)$ at $\mathbf{u}^*(t)$.

Lemma 3. No non-zero $\mathbf{v}_c \in \mathcal{V}^c$ satisfies (13), that is,

$$\mathcal{V}^s \cap \mathcal{V}^c = \{\mathbf{0}\}.$$

Proof: Let $\boldsymbol{\xi} \in \mathcal{V}^s \cap \mathcal{V}^c$. By construction, we have $\langle\boldsymbol{\xi},\boldsymbol{\xi}\rangle = 0$, which by the elementary properties of an inner product implies $\boldsymbol{\xi} = \mathbf{0}$. □

At this point, the concept of *selective input adaptation* can be introduced.

Definition 4. (Selective Input Adaptation). The process of adapting the nominal optimal inputs $\mathbf{u}^*(t)$ according to (7) in any nonzero direction $\boldsymbol{\xi}^{\mathbf{u}} \in \mathcal{V}^s$ is called *selective input adaptation in a sensitivity-seeking direction*. Likewise, the process of adapting $\mathbf{u}^*(t)$ in any nonzero direction $\boldsymbol{\xi}^{\mathbf{u}} \in \mathcal{V}^c$ is called *selective input adaptation in a constraint-seeking direction*.

4. SELECTIVE INPUT ADAPTATION UNDER PARAMETRIC UNCERTAINTY

Parametric perturbations from $\boldsymbol{\theta}_0$ to $\tilde{\boldsymbol{\theta}}(\eta) := \boldsymbol{\theta}_0 + \eta\,\boldsymbol{\xi}^{\boldsymbol{\theta}}$, with $|\eta| \ll 1$, are considered in this section. Suppose that one wishes to avoid repeating the whole solution procedure to compute the optimal inputs $\tilde{\mathbf{u}}^*(t)$ for the perturbed system. Either one of two options are possible:

(1) *No Input Adaptation:* The nominal optimal inputs $\mathbf{u}^*$ are applied 'as is' to the perturbed system. Let the pair of perturbed states and resulting cost be denoted by $(\hat{\mathbf{x}}(t), \hat{J})$. Thus, $(\hat{\mathbf{x}}(t), \mathbf{u}^*(t))$ satisfies (1) for $\tilde{\boldsymbol{\theta}}$. Because of the continuous differentiability of $\mathbf{f}$ with respect to $\mathbf{x}$ and $\boldsymbol{\theta}$, $\hat{\mathbf{x}}(t)$ has a first-order approximation around $\mathbf{x}^*(t)$ as

$$\hat{\mathbf{x}}(t;\eta) = \mathbf{x}^*(t) + \eta\boldsymbol{\xi}^{\hat{\mathbf{x}}}(t) + O(\eta^2),$$

where

$$\dot{\boldsymbol{\xi}}^{\hat{\mathbf{x}}}(t) = \mathbf{f}_{\mathbf{x}}[t]\boldsymbol{\xi}^{\hat{\mathbf{x}}}(t) + \mathbf{f}_{\boldsymbol{\theta}}[t]\boldsymbol{\xi}^{\boldsymbol{\theta}}, \tag{14}$$
$$\boldsymbol{\xi}^{\hat{\mathbf{x}}}(t_0) = \mathbf{h}_{\boldsymbol{\theta}}(\boldsymbol{\theta}_0)\boldsymbol{\xi}^{\boldsymbol{\theta}}.$$

(2) *Selective Input Adaptation:* The nominal optimal inputs are adapted along a general direction $\boldsymbol{\xi}^{\mathbf{u}} \in \hat{\mathcal{C}}[t_0, t_\mathrm{f}]$ and the resulting inputs (7) are then applied to the perturbed system. Let the pair of perturbed states and resulting cost be denoted by $(\tilde{\mathbf{x}}(t), \tilde{J})$, respectively. Thus, $(\tilde{\mathbf{x}}(t), \tilde{\mathbf{u}}(t))$ satisfies (1) for $\tilde{\boldsymbol{\theta}}$. Because of the continuous differentiability of $\mathbf{f}$ with respect to $\mathbf{x}$, $\mathbf{u}$ and $\boldsymbol{\theta}$, $\tilde{\mathbf{x}}(t)$ also has a first-order approximation around $\mathbf{x}^*(t)$ as

$$\tilde{\mathbf{x}}(t;\eta) = \mathbf{x}^*(t) + \eta\boldsymbol{\xi}^{\tilde{\mathbf{x}}}(t) + O(\eta^2),$$

where

$$\dot{\boldsymbol{\xi}}^{\tilde{\mathbf{x}}}(t) = \mathbf{f}_{\mathbf{x}}[t]\boldsymbol{\xi}^{\tilde{\mathbf{x}}}(t) + \mathbf{f}_{\mathbf{u}}[t]\boldsymbol{\xi}^{\mathbf{u}}(t) + \mathbf{f}_{\boldsymbol{\theta}}[t]\boldsymbol{\xi}^{\boldsymbol{\theta}}, \qquad (15)$$
$$\boldsymbol{\xi}^{\tilde{\mathbf{x}}}(t_0) = \mathbf{h}_{\boldsymbol{\theta}}(\boldsymbol{\theta}_0)\boldsymbol{\xi}^{\boldsymbol{\theta}}.$$

Subscript s or c will be added to various notations when the direction of input adaptation $\boldsymbol{\xi}^{\mathbf{u}}(t)$ under consideration is a SS or a CS direction, respectively.

Evidently, both of the above options will result in suboptimal process operation, although Option 2 can be expected to perform better under judicious choice of the input adaptation directions. The cost difference between selective adaptation and no adaptation is given by $\delta J(\boldsymbol{\xi}^{\mathbf{u}}) := \tilde{J} - \hat{J}$. The objective here is to compare the cost variations $\delta J(\boldsymbol{\xi}_s^{\mathbf{u}})$ and $\delta J(\boldsymbol{\xi}_c^{\mathbf{u}})$.

Following common practice in optimal control theory [Bryson and Ho, 1975], the cost functionals are augmented as

$$J^a := \psi(t_\mathrm{f}, \mathbf{x}(t_\mathrm{f}), \boldsymbol{\theta}) + \sum_{k=1}^{N} \int_{t_{k-1}^*}^{t_k^*} \phi(t, \mathbf{x}(t), \mathbf{u}(t), \boldsymbol{\theta})\, dt + \sum_{k=1}^{N} \int_{t_{k-1}^*}^{t_k^*} \boldsymbol{\pi}(t)^T \left(\mathbf{f}(t, \mathbf{x}(t), \mathbf{u}(t), \boldsymbol{\theta}) - \dot{\mathbf{x}}(t)\right) dt,$$

for some multiplier functions $\boldsymbol{\pi} \in \mathcal{C}^1[t_0, t_\mathrm{f}]^{n_\mathrm{x}}$ —the linear space of continuously differentiable functions on $[t_0, t_\mathrm{f}]$. It should be clear that $J^a = J$ for *any* such multiplier function provided that the pair $(\mathbf{x}(t), \mathbf{u}(t))$ satisfies (1) for $\boldsymbol{\theta}$. In this case, minimizing J with respect to $\mathbf{u}$ is equivalent to minimizing J^a with respect to $\mathbf{u}$. Using integration by parts, then Taylor expansions of various terms in the expression of $\delta J(\boldsymbol{\xi}^{\mathbf{u}})$ around $(\hat{\mathbf{x}}(t), \mathbf{u}^*(t))$, and finally suitable rearrangement, gives: [4]

$$\begin{aligned}\delta J(\boldsymbol{\xi}^{\mathbf{u}}) = \eta \Bigg\{ & \left[\hat{\psi}_{\mathbf{x}}[t_\mathrm{f}]^T - \boldsymbol{\pi}(t_\mathrm{f})^T\right] \left[\boldsymbol{\xi}^{\tilde{\mathbf{x}}}(t) - \boldsymbol{\xi}^{\hat{\mathbf{x}}}(t)\right] \\ & + \sum_{k=1}^{N} \int_{t_{k-1}^*}^{t_k^*} \left[\hat{\phi}_{\mathbf{x}}[t]^T + \boldsymbol{\pi}(t)^T \hat{\mathbf{f}}_{\mathbf{x}}[t] + \dot{\boldsymbol{\pi}}(t)^T\right] \left[\boldsymbol{\xi}^{\tilde{\mathbf{x}}}(t) - \boldsymbol{\xi}^{\hat{\mathbf{x}}}(t)\right] dt \\ & + \sum_{k=1}^{N} \int_{t_{k-1}^*}^{t_k^*} \left[\hat{\phi}_{\mathbf{u}}[t]^T + \boldsymbol{\pi}(t)^T \hat{\mathbf{f}}_{\mathbf{u}}[t]\right] \boldsymbol{\xi}^{\mathbf{u}}(t)\, dt \Bigg\} + O(\eta^2). \end{aligned} \qquad (16)$$

Choosing the multiplier functions $\boldsymbol{\pi}$ to be the (unique) solution $\hat{\boldsymbol{\pi}}$ of the linear system:

$$\dot{\hat{\boldsymbol{\pi}}}(t) = -\hat{\mathbf{f}}_{\mathbf{x}}[t]^T \hat{\boldsymbol{\pi}}(t) - \hat{\phi}_{\mathbf{x}}[t]; \qquad \hat{\boldsymbol{\pi}}(t_\mathrm{f}) = \hat{\psi}_{\mathbf{x}}[t_\mathrm{f}], \qquad (17)$$

and Taylor expanding the terms $\hat{\phi}_{\mathbf{u}}[t]$, $\hat{\mathbf{f}}_{\mathbf{x}}[t]$ and $\hat{\mathbf{f}}_{\mathbf{u}}[t]$ around $(\mathbf{x}^*(t), \mathbf{u}^*(t), \boldsymbol{\theta}_0)$, the cost difference reduces to:

$$\delta J(\boldsymbol{\xi}^{\mathbf{u}}) = \eta \sum_{k=1}^{N} \int_{t_{k-1}^*}^{t_k^*} \left[\phi_{\mathbf{u}}^*[t]^T + \hat{\boldsymbol{\pi}}(t)^T \mathbf{f}_{\mathbf{u}}^*[t]\right] \boldsymbol{\xi}^{\mathbf{u}}(t)\, dt + O(\eta^2). \qquad (18)$$

Since the optimality condition (4) holds along the nominal optimal trajectory $\mathbf{u}^*(t)$, (18) can be rewritten as

$$\delta J(\boldsymbol{\xi}^{\mathbf{u}}) = \eta \sum_{k=1}^{N} \int_{t_{k-1}^*}^{t_k^*} \left[\hat{\boldsymbol{\beta}}(t)^T \mathbf{f}_{\mathbf{u}}^*[t] - \boldsymbol{\mu}^a(t)^T \boldsymbol{\Omega}_{\mathbf{u}}^{a*}[t]\right] \boldsymbol{\xi}^{\mathbf{u}}(t)\, dt + O(\eta^2), \qquad (19)$$

[4] The compact notations $\hat{y}[t] := y(t, \hat{\mathbf{x}}(t), \mathbf{u}^*(t), \tilde{\boldsymbol{\theta}})$, and $\tilde{y}[t] := y(t, \tilde{\mathbf{x}}(t), \tilde{\mathbf{u}}(t), \tilde{\boldsymbol{\theta}})$ are used in the remainder of the paper.

where $\hat{\boldsymbol{\beta}}(t) := \hat{\boldsymbol{\pi}}(t) - \boldsymbol{\lambda}^*(t)$.

It can be shown that $\hat{\boldsymbol{\beta}}(t) = \boldsymbol{\beta}^*(t) + O(\eta)$, where $\boldsymbol{\beta}^*(t)$ is the unique solution of

$$\dot{\boldsymbol{\beta}}^*(t) = -\mathbf{f}_{\mathbf{x}}^*[t]^T \boldsymbol{\beta}^*(t) + \boldsymbol{\Omega}_{\mathbf{u}}^{a*}[t]^T \boldsymbol{\mu}^a(t); \quad \boldsymbol{\beta}^*(t_\mathrm{f}) = \mathbf{0}.$$

Substituting the expression of $\boldsymbol{\beta}^*(t)$ in (19), gives

$$\begin{aligned}\delta J(\boldsymbol{\xi}^{\mathbf{u}}) = {} & O(\eta^2) - \eta \sum_{k=1}^{N} \int_{t_{k-1}^*}^{t_k^*} \boldsymbol{\mu}^a(t)^T \boldsymbol{\Omega}_{\mathbf{u}}^{a*}[t] \boldsymbol{\xi}^{\mathbf{u}}(t)\, dt \\ & - \eta \sum_{k=1}^{N} \int_{t_{k-1}^*}^{t_k^*} \Bigg\{ \int_{t}^{t_k^*} \boldsymbol{\mu}^a(s)^T \boldsymbol{\Omega}_{\mathbf{x}}^{a*}[s] \boldsymbol{\Phi}^{\mathbf{f}_{\mathbf{x}}^*}(s,t) \mathbf{f}_{\mathbf{u}}^*[t]\, ds \\ & + \sum_{i=k+1}^{N} \int_{t_{i-1}^*}^{t_i^*} \boldsymbol{\mu}^a(s)^T \boldsymbol{\Omega}_{\mathbf{x}}^{a*}[s] \boldsymbol{\Phi}^{\mathbf{f}_{\mathbf{x}}^*}(s,t) \mathbf{f}_{\mathbf{u}}^*[t]\, ds \Bigg\} \boldsymbol{\xi}^{\mathbf{u}}(t)\, dt. \end{aligned}$$

By changing the order of integration in all double integral terms in the last expression, then a suitable rearrangement of the double sum term, and finally using (13), we get

$$\boxed{\delta J(\boldsymbol{\xi}^{\mathbf{u}}) = -\eta \sum_{k=1}^{N} \int_{t_{k-1}^*}^{t_k^*} \boldsymbol{\mu}^a(t)^T \left(\mathcal{D}_{\boldsymbol{\Omega}^a, t} \boldsymbol{\xi}^{\mathbf{u}}\right) dt + O(\eta^2).} \qquad (20)$$

The main result of the paper can now be stated:

Theorem 5. (Order of Selective Input Adaptation). Let $\mathbf{u}^*$ be an optimal solution for the optimal control problem $\mathrm{OC}(\boldsymbol{\theta}_0)$, and consider parametric variations of the form $\tilde{\boldsymbol{\theta}}(\eta) = \boldsymbol{\theta}_0 + \eta\, \boldsymbol{\xi}^{\boldsymbol{\theta}}$, with $|\eta| \ll 1$. The variation in cost upon selective input adaptation is $O(\eta^2)$ in any (nonzero) SS direction $\boldsymbol{\xi}_s^{\mathbf{u}} \in \mathcal{V}^s$, whereas it is $O(\eta)$ in any (nonzero) CS direction $\boldsymbol{\xi}_c^{\mathbf{u}} \in \mathcal{V}^c$.

Proof: By Definition 1, $\boldsymbol{\xi}_s^{\mathbf{u}}$ satisfies (13). Therefore, from (20), $\delta J(\boldsymbol{\xi}_s^{\mathbf{u}}) = O(\eta^2)$. On the other hand, no nonzero direction in $\mathcal{V}^c$ satisfies (13) from Lemma 3. Since strict complementarity slackness holds for the path constraints at $\mathbf{u}^*$ by assumption, it follows that the first-order term in (20) is nonzero in general, that is, $\delta J(\boldsymbol{\xi}_c^{\mathbf{u}}) = O(\eta)$. □

5. NUMERICAL PROCEDURE TO COMPUTE SENSITIVITY- AND CONSTRAINT-SEEKING DIRECTIONS

This section proposes a numerical procedure to compute SS and CS directions.

Let $\boldsymbol{\xi}^{\mathbf{u}}(t)$ denote a given direction in the input function space. We would like to compute the SS and CS components $\boldsymbol{\xi}_s^{\mathbf{u}} \in \mathcal{V}_s$ and $\boldsymbol{\xi}_c^{\mathbf{u}} \in \mathcal{V}_c$ of $\boldsymbol{\xi}^{\mathbf{u}}(t)$, respectively.

To avoid the difficulty of computing projections on the infinite-dimensional function spaces $\mathcal{V}_c$ and $\mathcal{V}_s$, we propose to approximate the optimal control problem by a nonlinear programming problem (NLP) as follows:

(1) Approximate the input profiles $\mathbf{u}(t)$ using a control vector parameterization (e.g., piecewise constant or affine) in terms of n parameters, the vector of which will be denoted by $\boldsymbol{\omega}$. Thus, we have the following expression relating $\boldsymbol{\omega}$ to $\mathbf{u}(t)$:

$$\mathbf{u}(t) = \mathcal{U}(t, \boldsymbol{\omega}), \quad \forall\, t \in [t_0, t_\mathrm{f}]. \qquad (21)$$

(2) Transform the optimal control problem into an NLP in terms of the decision variables $\boldsymbol{\omega}$. Note that the path constraints in the original optimal control problem will have to be transformed into a set of m discrete –typically nonlinear– constraints in the variables $\boldsymbol{\omega}$. m may be chosen equal to n.

(3) Solve the resulting NLP numerically to obtain the optimal values $\boldsymbol{\omega}^*$, and denote by $\mathbf{G}^a$ the set of active constraints of the NLP at $\boldsymbol{\omega}^*$.

(4) From the singular value decomposition of $\mathbf{G}^a_{\boldsymbol{\omega}}$ at $\boldsymbol{\omega}^*$, find the orthogonal matrices $\mathbf{V}_c$ and $\mathbf{V}_s$ that define the CS and SS directions, respectively, *of the NLP problem*; see Chachuat et al. [2008] for details.

(5) Parameterize the given direction $\boldsymbol{\xi}^{\mathbf{u}}(t)$ in terms of the vector $\boldsymbol{\xi}^{\boldsymbol{\omega}} \in \mathbb{R}^n$, such that:

$$\boldsymbol{\xi}^{\mathbf{u}}(t) = \mathcal{U}(t, \boldsymbol{\xi}^{\boldsymbol{\omega}}), \quad \forall t \in [t_0, t_f].$$

(6) Compute the orthogonal projections of the vector $\boldsymbol{\xi}^{\boldsymbol{\omega}}$ on the column space of $\mathbf{V}_c$ and $\mathbf{V}_s$, respectively:

$$\begin{aligned} \boldsymbol{\xi}^{\boldsymbol{\omega}}_c &= \mathbf{V}_c {\mathbf{V}_c}^T \boldsymbol{\xi}^{\boldsymbol{\omega}}, \\ \boldsymbol{\xi}^{\boldsymbol{\omega}}_s &= \mathbf{V}_s {\mathbf{V}_s}^T \boldsymbol{\xi}^{\boldsymbol{\omega}}. \end{aligned} \tag{22}$$

(7) $\boldsymbol{\xi}^{\boldsymbol{\omega}}_c$ and $\boldsymbol{\xi}^{\boldsymbol{\omega}}_s$ provide the approximations of the desired profiles $\boldsymbol{\xi}^{\mathbf{u}}_c(t)$ and $\boldsymbol{\xi}^{\mathbf{u}}_s(t)$, respectively, under the same parameterization as used in Step 1, i.e.,

$$\begin{aligned} \boldsymbol{\xi}^{\mathbf{u}}_c(t) &= \mathcal{U}(t, \boldsymbol{\xi}^{\boldsymbol{\omega}}_c), \quad \forall t \in [t_0, t_f], \\ \boldsymbol{\xi}^{\mathbf{u}}_s(t) &= \mathcal{U}(t, \boldsymbol{\xi}^{\boldsymbol{\omega}}_s), \quad \forall t \in [t_0, t_f]. \end{aligned}$$

Steps 5 to 7 are depicted in Figure 1.

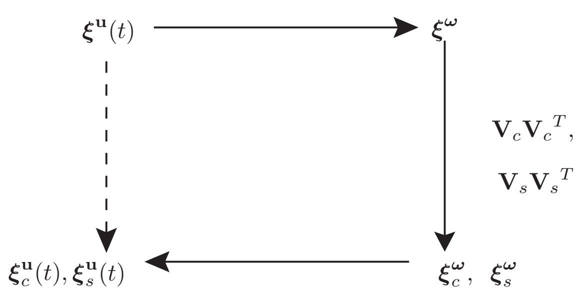

Fig. 1. *Approximate* computation of SS and CS directions. Exact computations (dotted arrow). Approximate computations (solid arrows).

In practice, one can expect the approach to yield better approximations of the desired directions $\boldsymbol{\xi}^{\mathbf{u}}_c(t)$ and $\boldsymbol{\xi}^{\mathbf{u}}_s(t)$ as the number n of parameters in the control parameterization increases.

In case of small parametric variations around $\boldsymbol{\theta}_0$, a possible choice of the input adaptation direction is $\boldsymbol{\xi}^{\mathbf{u}^*}(t)$, where

$$\boldsymbol{\xi}^{\mathbf{u}^*}(t) = \mathcal{U}(t, \boldsymbol{\xi}^{\boldsymbol{\omega}^*}), \quad \forall t \in [t_0, t_f], \tag{23}$$

$\boldsymbol{\xi}^{\boldsymbol{\omega}^*}$ being the (first-order) sensitivity of the NLP optimal solution $\boldsymbol{\omega}^*$ with respect to the uncertain parameters at $\boldsymbol{\theta}_0$. Such sensitivity information can be computed, under mild conditions, via linearization of the first-order optimality conditions (KKT conditions); see Fiacco [1983] for details. Steps 5 to 7 above will then yield the specific input adaptation directions $\boldsymbol{\xi}^{\mathbf{u}^*}_c \in \mathcal{V}_c$ and $\boldsymbol{\xi}^{\mathbf{u}^*}_s \in \mathcal{V}_s$, respectively.

6. ILLUSTRATIVE EXAMPLE

Consider the following parametric optimal control problem with one input variable and one path constraint:

$$\begin{aligned} \min_{u(t)} \quad & \int_0^1 \left(x_1^2(t) + x_2^2(t) + 0.005u^2(t)\right) dt, \\ \text{s.t.} \quad & \dot{x}_1(t) = x_2(t); \quad x_1(0) = 0, \\ & \dot{x}_2(t) = -x_2(t) + \theta\, u(t); \quad x_2(0) = -0.2, \\ & x_2(t) - u(t) + 0.5 - 8(t - 0.5)^2 \le 0, \quad 0 \le t \le 1, \end{aligned} \tag{24}$$

where θ stands for the uncertain system parameter, with nominal value $\theta_0 = 1$.

The nominal solution $u^*(t) = \mathcal{U}(t, \boldsymbol{\omega}^*)$ for Problem (24) is shown in Figure 2. This solution was obtained upon applying a piecewise-constant control vector parameterization on $n = 200$ equidistant stages and discretizing the path constraint at the end of each stage. It can be inferred from this plot that $u^*(t)$ consists of 3 arcs: an interior arc, followed by a boundary arc, and finally another interior arc.

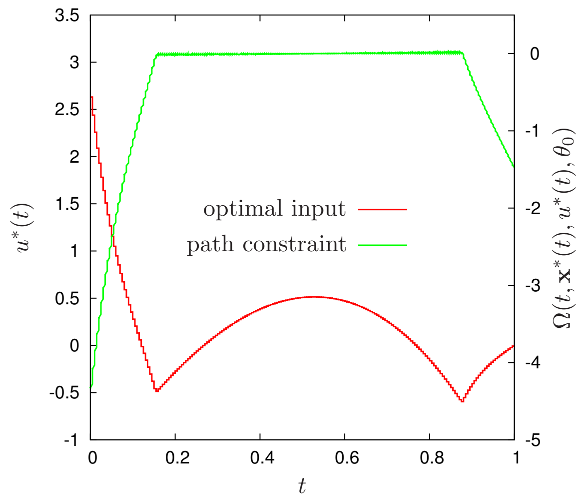

Fig. 2. Optimal nominal solution.

It is found that 144 constraints are active at the solution $\boldsymbol{\omega}^*$ of the NLP problem. The projection matrices $\mathbf{V}_c{\mathbf{V}_c}^T$ and $\mathbf{V}_s{\mathbf{V}_s}^T$ are computed in Step 4 of the numerical procedure described in Section 5.

With the choice of the input adaptation direction as in (23), Steps 5 to 7 yield the corresponding CS and SS directions. The adaptation direction $\boldsymbol{\xi}^{u^*}(t)$ as well as its projections on the CS and SS subspaces, $\boldsymbol{\xi}^{u^*}_c(t)$ and $\boldsymbol{\xi}^{u^*}_s(t)$, respectively, are shown in Figure 3.

The two scenarios of -4% and -8% variation in the parameter value are considered, i.e. for $\xi^\theta = 1$, $\eta = -0.04$ and $\eta = -0.08$, respectively. For these scenarios, the costs J_c and J_s resulting from selective input adaptation along the CS and SS directions are calculated. The cost J_f due to full first-order input adaptation, i.e. $u_f(t, \eta) = u^*(t) + \eta \xi^{u^*}(t)$, is also computed. In Table 1, the results are compared with the costs associated with no input adaptation ($\hat{J}$) and with the perturbed optimal cost ($\tilde{J}^*$).

In either scenario, adaptation along the CS direction results in larger cost improvement compared to adaptation

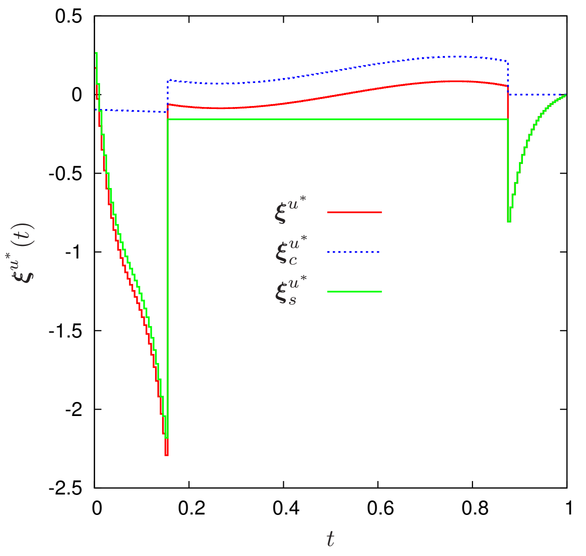

Fig. 3. First-order input variation and corresponding CS and SS directions.

Table 1. Costs of the perturbed system resulting from various input adaptations, and corresponding fractional cost recovery. $\hat{J}$: cost with no adaptation; J_s: cost with adaptation along the SS directions; J_c: cost with adaptation along the CS directions; J_f: cost with full first-order adaptation; $\tilde{J}^*$: perturbed optimal cost.

	$\eta = -0.04$	$\eta = -0.08$
$\hat{J}$	6.6078×10^{-3}	6.6447×10^{-3}
J_s	6.5819×10^{-3}	6.5395×10^{-3}
J_c	6.4988×10^{-3}	6.4659×10^{-3}
J_f	6.4587×10^{-3}	6.3087×10^{-3}
$\tilde{J}^*$	6.4537×10^{-3}	6.2895×10^{-3}
$\frac{\hat{J}-J_s}{\hat{J}-\tilde{J}^*}$	16.8%	29.6%
$\frac{\hat{J}-J_c}{\hat{J}-\tilde{J}^*}$	70.7%	50.3%
$\frac{\hat{J}-J_f}{\hat{J}-\tilde{J}^*}$	96.7%	94.6%

along the SS direction. However, the relative improvement of an adaptation along the CS direction with respect to the full first-order adaptation decreases as the uncertainty gets bigger.

7. CONCLUSIONS

Due to the complexity of solving optimal control problems, methods that do not require recomputing the exact solution appear to be very much desirable.

For problems involving mixed control-state constraints, the directions in the input function space along which small variation in the nominal optimal inputs *do not* cause any change in the active constraints for all $t \in [t_0, t_f]$ are defined as the SS directions. They are shown to be solutions of certain linear integral equations. The directions orthogonal to the set of SS directions are defined as the CS directions.

For the case of the parametric variation $\boldsymbol{\theta}_0 + \eta\boldsymbol{\xi}^{\boldsymbol{\theta}}$, it is shown that the cost improvement due to selective input adaptation along SS directions –over no adaptation– is $O(\eta^2)$, whereas it is $O(\eta)$ with selective input adaptation along CS directions. Hence, the main implication of the theory developed in this paper for optimal control problems with path constraints is that, for small parametric variations, adapting the inputs along the CS directions has the largest impact on cost, while the consequences of not adapting the inputs along the SS directions will remain small in comparison.

These results might prove applicable in the field of a recently developed methodology for constrained optimal control problems called NCO tracking [Srinivasan and Bonvin, 2007], in which parts of the input profiles can be adapted selectively. Hence, prioritization of selective-adaptation strategies is crucial for developing practical NCO-tracking controllers.

Extensions of these results to problems involving discontinuous $\mathbf{u}^*(t)$, problems having non-regular Hamiltonians and singular arcs as well as problems having a combination of terminal and path constraints will be addressed in future work.

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