On the Role of Constraints in Optimization under Uncertainty

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Abstract

This thesis addresses the problem of industrial real-time process optimization that suffers from the presence of uncertainty. Since a process model is typically used to compute the optimal operating conditions, both plant-model mismatch and process disturbances can result in suboptimal or, worse, infeasible operation. Hence, for practical applications, methodologies that help avoid re-optimization during process operation, at the cost of an acceptable optimality loss, become important. The design and analysis of such approximate solution strategies in real-time optimization (RTO) demand a careful analysis of the components of the necessary conditions of optimality. This thesis analyzes the role of constraints in process optimality in the presence of uncertainty.

This analysis is made in two steps. Firstly, a general analysis is developed to quantify the effect of input adaptation on process performance for static RTO problems. In the second part, the general features of input adaptation for dynamic RTO problems are analyzed with focus on the constraints. Accordingly, the thesis is organized in two parts:

1. For static RTO, a joint analysis of the *model* optimal inputs, the *plant* optimal inputs and a class of adapted inputs, and
2. For dynamic RTO, an analytical study of the effect of local adaptation of the *model* optimal inputs.

The first part (Chapters 2 and 3) addresses the problem of adapting the inputs to optimize the *plant*. The investigation takes a constructive viewpoint, but it is limited to static RTO problems modeled as parametric nonlinear programming (pNLP) problems. In this approach, the inputs are not limited to being local adaptation of the model optimal inputs but, instead, they can change significantly to optimize the plant. Hence, one needs to consider the fact that the set of active constraints for the model and the plant can be different. It is proven that, for a wide class of systems, the detection of a change in the active set contributes only negligibly to optimality, as long as the adapted solution remains feasible. More precisely, if η denotes the magnitude of the parametric variations and if the linear independence constraint qualification (LICQ) and strong second-order sufficient condition (SSOSC) hold for the underlying pNLP, the optimality loss due to any feasible input that conserves only the strict nominal active set is of magnitude $O(\eta^2)$, irrespective of whether or not there is a change in the set of active constraints. The implication of this result for a static RTO algorithm is to prioritize the satisfaction of only a core set of constraints, as long as it is possible to meet the feasibility requirements.

The second part (Chapters 4 and 5) of the thesis deals with a way of adapting the *model* optimal inputs in dynamic RTO problems. This adaptation is made along two sets of directions such that one type of adaptation does not affect the nominally active constraints, while the other does. These directions are termed the sensitivity-seeking (SS) and the constraint-seeking (CS) directions, respectively. The SS and CS directions are defined as elements of a fairly general function space of input variations. A mathematical criterion is derived to define SS directions for a general class of optimal control problems involving both path and terminal constraints. According to this criterion, the SS directions turn out to be solutions of linear integral equations that are completely defined by the model optimal solution. The CS directions are then chosen orthogonal to the subspace of SS directions, where orthogonality is defined with respect to a chosen inner product on the space of input variations. It follows that the corresponding subspaces are infinite-dimensional subspaces of the function space of input variations. It is proven that, when uncertainty is modeled in terms of small parametric variations, the aforementioned classification of input adaptation leads to clearly distinguishable cost variations. More precisely, if η denotes the magnitude of the parametric variations, adaptation of the model optimal inputs along SS directions causes a cost variation of magnitude $O(\eta^2)$. On the other hand, the cost variation due to input adaptation along CS directions is of magnitude $O(\eta)$.

Furthermore, a numerical procedure is proposed for computing the SS and CS components of a given input variation. These components are projections of the input variation on the infinite-dimensional subspaces of SS and CS directions. The numerical procedure consists of the following three steps: approximation of the optimal control problem by a pNLP problem, projection of the given direction on the finite-dimensional SS and CS subspaces of the pNLP and, finally, reconstruction of the SS and CS components of the original problem from those of the pNLP.

Keywords:

Static Real-Time Optimization, Dynamic Real-Time Optimization, Parametric Uncertainty, Nonlinear Programming, Optimal Control.

Résumé

Cette thèse aborde le problème de l'optimisation en temps réel des procédés industriels en présence d'incertitude. Pour déterminer les conditions opératoires optimales, un modèle du procédé est généralement utilisé. En conséquence, les erreurs de modélisation, l'incertitude paramétrique et les perturbations vont typiquement conduire à la sous-optimalité voire à l'infaisabilité si l'on utilise telles quelles les conditions opératoires optimales ainsi obtenues. Il est donc grandement nécessaire, pour les applications pratiques, de disposer de méthodes qui garantissent une perte d'optimalité acceptable, sans pour autant nécessiter de réoptimisation en ligne, basée sur le modèle. Pour concevoir et analyser de telles stratégies d'optimisation en temps réel (OTR), il convient d'effectuer une analyse approfondie des composantes des conditions nécessaires d'optimalité. Cette thèse analyse le rôle des contraintes pour l'optimalité des procédés, en présence d'incertitude.

Cette analyse est faite en deux étapes. Premièrement, une analyse générale est réalisée, pour mesurer l'effet de l'adaptation des entrées pour les problèmes d'OTR statiques. Dans la deuxième partie, les caractéristiques générales de l'adaptation des entrées pour des problèmes d'OTR dynamiques sont analysées, avec l'emphase sur les contraintes. En conséquence, la thèse est organisée en deux parties :

1. Pour l'OTR statique, une analyse commune des entrées optimales du modèle, des entrées optimales du procédé réel et d'une classe d'entrées adaptées, et
2. Pour l'OTR dynamique, une étude analytique de l'effet de l'adaptation locale des entrées optimales du modèle.

La première partie (Chapitres 2 and 3) traite du problème de l'adaptation des entrées pour optimiser le procédé. La recherche prend un point de vue constructif, mais elle est limitée aux problèmes d'OTR statiques, formulés comme des problèmes de programmation non linéaire paramétrique (PNLp). L'adaptation des entrées n'est pas limitée au voisinage des entrées optimales du modèle mais, a contrario, les entrées peuvent changer de manière significative. Par conséquent, on ne peut écarter que les ensembles de contraintes actives à l'optimum du modèle et à l'optimum du procédé puissent être différents. Dans cette thèse, il est montré que pour une large classe de systèmes, la détection d'un changement de l'ensemble des contraintes actives ne

contribue que de façon négligeable à l'optimalité, tant que la solution adaptée demeure faisable. Plus précisément, si η désigne l'ampleur des variations paramétriques, sous couvert de la *linear independence constraint qualification* (LICQ) et la *strong second-order sufficient conditions* (SSOSC) pour la PNLp, pour toutes les entrées appliquées au procédé qui préservent inchangé l'ensemble des contraintes strictement actives obtenues avec le modèle nominal, la perte d'optimalité est de l'ordre de $O(\eta^2)$, indépendamment de, si oui ou non, les ensembles de contraintes actives du modèle et du procédé diffèrent. L'implication de ce résultat pour un algorithme d'OTR statique est de donner la priorité à la satisfaction d'un ensemble de base de contraintes, tant qu'il est possible de répondre aux exigences de faisabilité.

La deuxième partie (Chapitres 4 et 5) de la thèse étudie l'adaptation des entrées optimales du modèle pour les problèmes d'OTR dynamiques. Il est proposé de réaliser cette adaptation selon deux ensembles de directions selon que l'adaptation modifie ou pas les contraintes nominalement actives. Ces directions sont respectivement appelées *sensitivity-seeking directions* (i.e. directions qui cherchent les sensibilités) et *constraint-seeking directions* (i.e. directions qui cherchent les contraintes), et sont notées SS et CS, respectivement. Les directions SS et CS sont définies comme les éléments d'un espace fonctionnel correspondant à une large classe de variations d'entrée. Un critère mathématique est dérivé pour définir les directions SS pour une classe générale de problèmes de commande optimale, impliquant des contraintes de chemin et des contraintes terminales. Selon ce critère, les directions SS se révèlent être les solutions d'équations intégrales linéaires qui sont complètement définies par la solution optimale du modèle. Les directions CS sont alors choisies orthogonales à l'espace des directions SS, où l'orthogonalité est définie au moyen d'un produit scalaire choisi dans l'espace des variations d'entrée. Il s'ensuit que les sous-espaces correspondants sont des sous-espaces de dimensions infinies de l'espace fonctionnel des variations d'entrée.

Il est prouvé que, lorsque l'incertitude est modélisée en termes de petites variations paramétriques, séparer les adaptations des entrées selon les ensembles de directions susmentionnés, conduit à des variations du coût clairement identifiables. Plus précisément, si η désigne l'ampleur des variations paramétriques, l'adaptation des entrées optimales du modèle dans des directions SS entraîne une variation des coûts de l'ordre de $O(\eta^2)$, tandis que selon de directions CS elle est de l'ordre de $O(\eta)$.

Par ailleurs, une procédure numérique est proposée pour calculer les composantes SS et CS d'une variation d'entrée donné. Ces composantes sont des projections de la variation de l'entrée sur les sous-espaces de dimensions infinies des directions SS et CS. La procédure numérique est constituée des trois étapes suivantes: l'approximation du problème de contrôle optimal par un problème de PNLp, la projection de la direction donnée sur les sous-espaces SS et CS de dimensions finies du problème de PNLp et, enfin, la reconstruction des composantes SS et CS du problème original à partir du problème de PNLp.

Mots-clés:

Optimisation Statique en Temps Réel, Optimisation Dynamique en Temps Réel, Incertitude Paramétrique, Programmation Non Linéaire, Contrôle Optimal.

Contents

Nomenclature

Roman symbols used in Static Real-Time Optimization (SRTO)

δJ	Optimality loss ((2.10))
$\mathbf{G}$	Vector of constraints
$\mathbf{u}$	Vector of inputs
$\hat{\mathbf{u}}$	Vector of adapted inputs ((3.7))
$\mathbf{u}^*$	Vector of nominal optimal inputs
$\tilde{\mathbf{u}}$	Vector of optimal inputs for the perturbed system
J	Cost function

Greek symbols used in SRTO

η	Magnitude of parametric perturbations in (2.8)
$\boldsymbol{\lambda}^*$	Vector of nominal Lagrange multipliers
$\tilde{\boldsymbol{\lambda}}$	Vector of Lagrange multipliers for the perturbed system
$\boldsymbol{\theta}$	Vector of uncertain parameters
$\boldsymbol{\theta}_0$	Vector of nominal parameters
$\tilde{\boldsymbol{\theta}}$	Vector of perturbed parameters ((2.8))
$\boldsymbol{\xi}^{\boldsymbol{\theta}}$	Direction of parametric perturbations in (2.8)

Calligraphic symbols used in SRTO

$\mathcal{A}^*$	$\mathcal{I}^* \cup \mathcal{J}^*$
$\tilde{\mathcal{A}}$	$\tilde{\mathcal{I}} \cup \tilde{\mathcal{J}}$

$\mathcal{I}^*$	Set of indices of strictly active constraints at $(\mathbf{u}^*, \boldsymbol{\theta}_0)$
$\tilde{\mathcal{I}}$	Set of indices of strictly active constraints at $(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}})$
$\mathcal{J}^*$	Set of indices of marginally active constraints at $(\mathbf{u}^*, \boldsymbol{\theta}_0)$
$\tilde{\mathcal{J}}$	Set of indices of marginally active constraints at $(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}})$
$\mathcal{K}^*$	Set of indices of inactive constraints at $(\mathbf{u}^*, \boldsymbol{\theta}_0)$
$\tilde{\mathcal{K}}$	Set of indices of inactive constraints at $(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}})$
$\mathcal{N}^s$	Null space of Jacobian of strongly active constraints (defined in (2.11))

Roman symbols used in Dynamic Real-Time Optimization (DRTO)

δJ	Difference between $\tilde{J}$ and $\hat{J}$
$\hat{J}$	Cost resulting from application of nominal inputs to perturbed system
$\tilde{J}$	Cost resulting from application of adapted inputs of type (5.1) to perturbed system
$\mathbf{T}$	Vector of terminal constraints
t_k^*	k^{th} switching time in $\mathcal{T}$
$\mathbf{u}^*$	Nominal optimal inputs
$\tilde{\mathbf{u}}$	Adapted inputs of type (5.1)
$\hat{\mathbf{x}}$	States resulting from application of nominal inputs to perturbed system
$\mathbf{x}^*$	Nominal optimal states
$\tilde{\mathbf{x}}$	States associated with the inputs $\tilde{\mathbf{u}}$
J	Cost functional
$\text{OC}(\boldsymbol{\theta})$	Parametric optimal control problem (4.1) – (4.4)

Greek symbols used in DRTO

$\delta\boldsymbol{\psi}(\mathbf{u}^*, \boldsymbol{\xi}^{\mathbf{u}})$	Gâteaux derivative of function $\boldsymbol{\psi}(\mathbf{u})$ in the direction $\boldsymbol{\xi}^{\mathbf{u}}$ at $\mathbf{u}^*$
$\boldsymbol{\lambda}^*$	Nominal adjoint states
$\boldsymbol{\mu}^a$	Vector of nominal multiplier functions of active path constraints
$\boldsymbol{\mu}^*$	Vector of nominal multiplier functions of path constraints
$\boldsymbol{\Omega}$	Vector of mixed path constraints
$\boldsymbol{\Omega}^a$	Vector of active path constraints
ϕ	Integrand of the integral term in cost

$\boldsymbol{\Phi}^{\mathbf{A}}$	State-transition matrix of system (5.6)
$\boldsymbol{\rho}^{a}$	Vector of nominal multipliers of active terminal constraints
$\boldsymbol{\rho}^{*}$	Vector of nominal multipliers of terminal constraints
$\boldsymbol{\theta}$	Vector of uncertain parameters
$\boldsymbol{\theta}_0$	Vector of nominal parameters
$\tilde{\boldsymbol{\theta}}$	Vector of perturbed parameters
φ	Component of cost due to terminal state
$\boldsymbol{\xi}^{\mathbf{u}}$	Input variation functions
$\boldsymbol{\xi}^{\boldsymbol{\theta}}$	Direction of parametric perturbations

Calligraphic symbols used in DRTO

$\mathcal{C}^1[p,q]^k$	Linear space of continuously differentiable vector functions of size k on $[p,q]$
$\hat{\mathcal{C}}[p,q]^k$	Linear space of piecewise-continuous vector functions of size k on $[p,q]$
$\mathcal{H}$	Hamiltonian of OC($\boldsymbol{\theta}$)
$\mathcal{T}$	Set of all nominal switching times, including initial and final times
$\mathcal{U}(t,\boldsymbol{\omega})$	Vector of piecewise-constant functions of type (5.13) characterized by vector of variables $\boldsymbol{\omega}$
$\mathcal{V}^c$	Set of CS directions for OC($\boldsymbol{\theta}_0$)
$\mathcal{V}^s$	Set of SS directions for OC($\boldsymbol{\theta}_0$)

Chapter 1

Introduction

1.1 Motivation

When it comes to choosing one from a multitude of options, it is possible to systematically choose the best option only if we know the result of the choice of each option. If repeated choice is not possible or if the number of options is enormous, as frequently happens in real-life, we need to have some knowledge of cause-effect type between available options and possible results.

In engineering processes, this knowledge is the *model* of a process that relates inputs of the process to its outputs. Mathematical process models are widely used in engineering. Since engineering processes are man-made, there is naturally always a choice from a multitude of inputs. As can be expected, choice of best inputs is always a problem in engineering and it is solved by applying optimization techniques to the available process model.

Consider, for example, the problem of

- choice of the speed of a rocket that is intended to put a satellite in a desired orbit in minimum time, with the constraint that the rocket engine cannot generate speeds above a certain limit and that body temperature of the rocket should remain below a safety limit, or
- choice of the rate at which a raw material is to be fed to a chemical reactor so that the amount of the chemical produced in a given time is the largest, with the constraint that the physical equipment attached to the reactor cannot handle feed rates larger than a certain limiting value and the reactor temperature cannot cross above a safety limit.

Thus, while choosing best inputs, we have to choose the ones that satisfy properties of both feasibility (satisfaction of the constraints) and optimality.

It is already evident that there is always a *tension* between constraints and optimality in an optimization problem. Consider, for example, the hypothetical case:

- if the rocket engine could produce speeds higher than what is possible, the time needed to reach the desired orbit could possibly be reduced further, or
- if the equipment of the reactor could handle larger feed rates than is possible, the amount of the chemical produced in a given time period could possibly be higher.

Such *confidence* stems from the fact that our knowledge of the rocket dynamics or the chemical reaction, in other words our process *model*, tells us that increasing the rocket speed reduces the time to reach the desired orbit or that increasing the feed rate of the raw materials increases the amount of the chemical produced. But how *complete* or *perfect* is our knowledge? Consider, for example, the scenario that

- unforeseen strong local winds are generated that cross the path of the rocket through atmosphere and the same rocket speeds result in higher friction that raises the rocket body temperature beyond its safety limit, or
- catalytic degradation about which we are unaware slows down the chemical reaction and, for the same feed rates of raw materials, the amount of chemical produced is of lower than expected.

In practice, it is perfectly natural to be unable to foresee complex natural phenomena like occasional local winds or to be unaware of changes in processes designed some time ago, for example the catalyst degradation. Thus, unforeseen events or lack of knowledge are the causes of uncertainty in process operation.

An important question follows: despite having a fairly good knowledge of the process, will the uncertainty during process operation always result in less than best operation or even disastrous operation? Well, if we could compensate for the effect of uncertainty on the process operation, then things should be fine. After all, what we lack is the knowledge of the uncertainty, not the knowledge of the process!

The main difficulty seems to be the fact that, in most cases, we will be aware of the uncertainty only *during* process operation and, as noted earlier, possibility of repeat operation is not always available. But, this difficulty is compensated by the fact that we can collect various types of measurement data by observing the process operation. Consider, for example, that it is possible to

- measure the altitude gained by the rocket at each instant, or
- measure the reactor temperature at each instant.

Then, using our knowledge of the rocket dynamics or chemical reaction, we can

- compare the altitude measurements with those predicted by the *model* of rocket dynamics, or
- compare the reactor temperature measurements with those predicted by the *model* of chemical reaction,

and thus, we can have some (indirect) *knowledge* about the effect of uncertainty.

What remains is to feed this knowledge back to the optimization routine *in a suitable form* and get back the optimal inputs for the real-time operation of the *plant* in contrast with those for the *model*.[1] The big difficulty with this scheme is to perform these computations during process operation, i.e., in real-time.

It turns out that to surmount these two challenges, it is necessary to answer the following questions:
Given the *tension* between feasibility and optimality, how different is the impact of uncertainty on feasibility and optimality of the plant? From the relative impact of uncertainty on the two, can we deduce the *importance* of feasibility for plant optimality? Can this knowledge be combined with that of the model-based optimal solution and the data available from process operation to obtain the desired plant optimum instead of performing a re-optimization?

The present thesis is an analytical study of some aspects of these questions.

1.2 State of the Art

If a mathematical model of a process is available, methods of mathematical optimization enable the computation of process inputs or decision variables that optimize the performance of the process. However, real-time performance of the optimum calculated using a model naturally depends on how truly does the model represent reality. Unfortunately, highly accurate process models are rarely available in practice. This is especially true for highly complex industrial processes that have become commonplace as well as for highly complex physical phenomena such as atmospheric,

[1] In contrast to the cases where optimization is used as a tool to design a feedback mechanism for controlling a process, here, we seem to witness the case of a feedback mechanism needed to bring about optimal operation.

biological or nuclear processes. Many practical factors also go against the development of very complex models, e.g. lack of knowledge of underlying phenomena, tradeoff between efforts needed to develop complex models versus the relative benefits brought in by them, efforts needed for detection of errors and for maintenance, tradeoff between computational efforts needed to solve the problems formed using complex models versus the benefits brought in by the computed solutions, ease of regularly updating the models, if needed, and so on.

The lack of accurate knowledge of process operation gives rise to uncertainty about the process operation. As already noted, plant-model mismatch is the most obvious source of uncertainty. Another source of uncertainty in process operation is the influence of events that are extraneous to the process itself, and so not included in the model, but are part of the environment in the process operates. The effect of unforeseen changes in operating environment on process operation is another source of uncertainty. The last two types of uncertainty are generally clubbed under the term *disturbances*. See [10, 32, 109] for excellent discussions on various sources of uncertainty in dynamic chemical processes.

It is very common to represent process uncertainty in a mathematical model using parameters. In this approach, it is assumed that the available model is valid for some set of *nominal* values of parameters. Then, the uncertainty in operation is thought to be generated due to deviation of the parameters from their nominal values. This is referred to as process uncertainty represented in terms of *parametric perturbations* or parametric uncertainty for short. In particular, we will deal exclusively with the approach of parametric uncertainty throughout the thesis.

Since, the nominal and perturbed values of parameters correspond, respectively, to process model and plant, the latter two will be referred to as nominal and perturbed model, respectively. Naturally, all entities associated with the model will be referred by the epithet *nominal* while those for the plant by *perturbed*. For example, model and plant optimum will, be referred to as nominal and perturbed optimum, respectively.

Optimization of a large class of processes that are operated at steady-state necessitates the choice of a *finite number* of decision variables or inputs. Such problems are termed as *steady-state* or *static* optimization problems. Optimization of transient processes consists of the choice of complete *profiles* of decision variables or inputs.

The latter are termed as *dynamic* optimization problems. Methods of optimal control theory address the problem of dynamic optimization [13, 89].

Since parametric uncertainty is a very common way of accounting for plant-model mismatch or process disturbances, most optimization problems under uncertainty, of both static and dynamic type, can be cast in the framework of parametric optimization problems. For example, nonlinear programming problems (NLP) are, probably, the largest class of static optimization problems studied and used in practice; see [27, 96] for examples of optimization problems of chemical processes modeled as nonlinear programs. Naturally, most static optimization problems subject to uncertainty can be modeled as parametric nonlinear programming problems [14]. On the other hand, parametric optimal control problems form a natural framework for dynamic optimization problems subject to uncertainty [74]. To be a bit more concrete, let us consider example of a static optimization problem, in which a set of inputs $\mathbf{u}$ is to be found to minimize a given cost $J(\mathbf{u})$ subject to given operational constraints $G_i(\mathbf{u}) \leq 0$, $i = 1, \ldots, n_{\mathbf{G}}$. That is

$$\begin{aligned} \min_{\mathbf{u}\in\mathbb{R}^{n_{\mathbf{u}}}} \quad & J(\mathbf{u}) \\ \text{s.t.} \quad & G_i(\mathbf{u}) \leq 0, \quad i = 1, \ldots, n_{\mathbf{G}}. \end{aligned} \tag{1.1}$$

The formulation above is valid only if the knowledge of the functions J and G_i is perfect. On the other hand, if, as a result of uncertainty, functions J and G_i for the plant are known only up to certain parameters $\theta_1, \ldots, \theta_{n_{\boldsymbol{\theta}}}$, then the optimization problem for the plant becomes:

$$\begin{aligned} \min_{\mathbf{u}\in\mathbb{R}^{n_{\mathbf{u}}}} \quad & J(\mathbf{u}, \boldsymbol{\theta}) \\ \text{s.t.} \quad & G_i(\mathbf{u}, \boldsymbol{\theta}) \leq 0, \quad i = 1, \ldots, n_{\mathbf{G}}, \\ \boldsymbol{\theta} := & \begin{bmatrix} \theta_1 \\ \vdots \\ \theta_{n_{\boldsymbol{\theta}}} \end{bmatrix}. \end{aligned} \tag{1.2}$$

Clearly, (1.1) is a special case of (1.2) (for $\boldsymbol{\theta} = \mathbf{0}$). Let $\mathbf{u}^*$ be a optimal solution of the former while $\tilde{\mathbf{u}}$ be that of the latter. In general, $\tilde{\mathbf{u}}$ will be different from $\mathbf{u}^*$.

Naturally, if we apply the model-based optimal solution ($\mathbf{u}^*$ above) to plant in real-time operation, both plant-model mismatch and process disturbances can result in suboptimal process operation or, worse, infeasible operation [33, 109, 113]. Ideally, one would need to compute the perturbed values of the parameters that correspond to plant and to repeat the computation for optimization with perturbed parameters to obtain the optimal inputs for plant. As the deviation between model and plant can become evident only during the process operation, the re-optimization needs to be done in real-time. Since static optimization problems involving hundreds of decision variables and constraints are common in practice, real-time re-optimization to compute plant optimum can turn out to be a challenging task. Given the complexity of solving realistic optimal control problems [8, 87, 108], re-solving the dynamic optimization problem in real-time is also a challenge in most practical cases. Note that computing the perturbed parameter values, or their estimates, itself is rarely possible for complex industrial processes [1].

Another point of view regarding real-time optimization is to use the model-based solution computed offline and appropriate process measurements to compute online (approximations of) the plant optimal solution, while avoiding online re-optimization, if possible.

This situation gives rise to the *problem of optimization in the presence of uncertainty*, viz., the real-time computation of optimal inputs for the plant, preferably without repeating the optimization, but possibly using the knowledge of the model optimum and any data that can be measured from the actual process operation.

1.2.1 A Survey of Methods for Optimization in the Presence of Uncertainty

There exist numerous methods for optimization in the presence of uncertainty. In Figure 1.1, we have shown a broad classification of such methods.

The idea behind the classification is as follows:

- *Level 1* of the classification is based on whether or not the concerned optimization methods make use of *measurements* on-line.
- *Level 2* of the classification is based on whether or not the concerned optimization methods use a process *model* on-line.

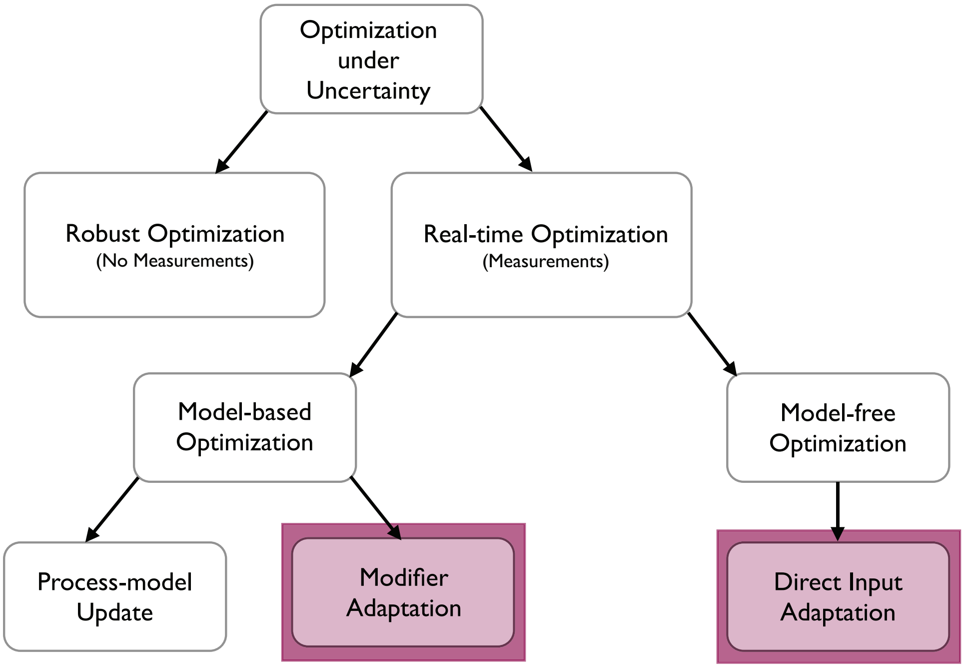

Figure 1.1 A broad classification of existing approaches for optimization under uncertainty. The approaches in the shaded boxes are mainly the sources of the research questions dealt with in the thesis.

- *The last level* of the classification is based on the process *adaptation strategy* employed by the concerned optimization methods.

These aspects will become clear in the following broad overview of methods for optimization under uncertainty. An attempt has been made in the overview to outline key ideas underlying each method. For a more detailed and refined discussion about these methods, as well as their comparison, we refer the reader to the excellent surveys in [17] for static optimization problems and in [103] for dynamic optimization problems as well as to the individual references that will be cited.

In the next Section, we will abstract certain key features of some of the most promising methods and see what analytical results exist that underlie the methods.

Robust and real-time optimization methods constitute the first level of classification in Figure 1.1.

Robust optimization methods do not make use of measurement data. To handle the effects of uncertainty, these methods introduce conservatism in process operation so that the operational feasibility is guaranteed for the complete range of perturbed parameters. See, for example, [81, 114] for static robust optimization and [79, 80, 117] for dynamic robust optimization. A comprehensive reference, especially for analytical results, on both static and dynamic robust optimization is [7].

Real-time optimization (RTO) methods include some of the most commonly used methods in practice for optimization in the presence of uncertainty [34]. The most significant feature of real-time optimization methods is to use measurement data from real-time process operation to adapt process operation on-line so as to compensate for process change and disturbances. Henceforth, we will concentrate on different types of RTO methods.

Second level of classification in Figure 1.1 consists of two broad categories of RTO methods: **model-based** and **model-free**. The distinction between the two is that the former need to use a process model during online operation while the latter do not.

Model-based RTO methods can further be divided in two classes, viz., **process-model update** and **modifier adaptation**, depending on the on-line process adaptation strategy used. On the other hand, the process adaptation strategy in most model-free RTO methods can be classified as **direct input adaptation**. Thus, the last level of classification in Figure 1.1 is based on the process adaptation strategy used by corresponding RTO methods. Next, we discuss a number of RTO methods that belong to the three classes in this level.

1.2.1.1 Process-Model Update Methods

Process-model update methods for static RTO (SRTO) take a two-step approach that consists of repeated identification of process parameters using output measurements followed by optimization of the process model that uses the identified parameters. Hence, they are also called as **model-parameter adaptation** methods. See [18, 73] for examples of model-parameter adaptation methods in SRTO problems.

Discussion of model-parameter adaptation methods for within run optimization of dynamic RTO (DRTO) problems can be seen in [1, 26, 40, 55, 85, 95]. Some examples of such methods addressing run-to-run optimization of DRTO problems are included in [19, 30, 35, 100, 102].

In DRTO problems, there is an additional possibility of using process measurements to update current states, rather than model parameters, followed by re-optimization of the process model. Model predictive control (MPC) [2, 76, 77, 82, 98] is the most well-known example of methods utilizing the said approach. Using the measurement of the current state, MPC recomputes, at each sampling instant, the input that optimizes a performance criterion over the future prediction horizon. Only the first part of the computed input is applied to the process. Because the measured current state of the process is used to recompute the input, the measurements provide the feedback that helps reject disturbances and reduce the sensitivity to process-model mismatch.

1.2.1.2 Modifier Adaptation Methods

Modifier Adaptation methods add modifier terms to cost or constraints of an SRTO problem. These methods use process measurements to adapt certain modifier terms in the optimization problem formulation instead of updating model parameters as in model-parameter adaptation methods. Hence, these methods are sometimes also termed as *fixed-model* methods [70]. The adaptation of the modifier terms is done in such way that after repeated online optimization the necessary conditions of optimality (NCO) for the adapted problem and the plant match. Important examples of modifier adaptation methods are as follows:

- The **bias update** method [32] and the **constraint-adaptation** method [16] add modifier term *only* to the process constraints. The modifier term is simply the *constraint bias*, i.e., the difference between the measured and predicted constraint values.
- The **iterative set-point control** method in [107] proposes to add to cost a gradient correction term, i.e., the difference between measured and predicted cost gradients, as a cost modifier that needs to be adapted iteratively using process measurements.

  There exists a whole group of methods under the umbrella of **ISOPE** (Integrated System Optimization and Parameter Estimation) [12, 91, 92] that can be considered as hybrids between model-parameter adaptation methods and modifier adaptation methods that use a cost-gradient modifier term.

- The method in [39] uses a constraint bias term and a constraint-gradient correction term as modifiers of constraints that need to be adapted iteratively. The constraint-gradient correction is the difference between measured and predicted constraint gradients. It is shown that, if the method converges, then the NCO at the converged points match those of the plant optimum.
- The method in [72] proposes the use of constraint biases, cost-gradient correction terms and constraint-gradient correction terms as modifier terms for the respective entities. This ensures that, if the method converges, then the NCO at the converged points match those of the plant optimum.

In contrast to the SRTO case, not many modifier adaptation methods are available for DRTO problems. Some examples of modifier adaptation methods for run-to-run dynamic optimization can be seen in [22, 71].

1.2.1.3 Direct Input Adaptation Methods

Direct Input Adaptation methods avoid repeated on-line optimization by *adapting* the known model optimal inputs during process operation in such a way that the process operation tends towards the unknown plant optimum. Thus, in contrast to methods based on process-model update and modifier adaptation, these methods do not need to use a process model during online operation. Since these methods use only the nominal model (in offline computations), they are also sometimes termed as *fixed-model* methods [70].

- Methods based on **sensitivity analysis** make use of the analytical results on the change in optimal solutions of parametric optimization problems due to change in parameters.

  Recall from Section 1.2 that we are considering problems in which plant-model mismatch or process disturbances are modeled using parametric perturbations, so that the optimization problems in the presence of uncertainty that are under consideration are *parametric optimization* problems. Hence, knowledge of how optimal solutions change with parametric perturbations can be used for directly adapting the known model optimum ($\mathbf{u}^*$ corresponding to (1.1)) to obtain the desired, but unknown, plant optimum ($\tilde{\mathbf{u}}$ corresponding to (1.2)), thereby avoiding the re-optimization completely.

As a simple example, assume that the magnitude of parametric variations is *small* and the properties of the underlying parametric optimization problem (1.2) ensure that the plant optimum is *differentiable* with respect to parameters. In this case, one can write a first-order expansion of plant optimal solution with respect to model optimal input as follows:

$$\tilde{\mathbf{u}} = \mathbf{u}^* + \eta\, \boldsymbol{\xi}^{\mathbf{u}^*} + O(\eta^2), \tag{1.3}$$

where $\eta = ||\boldsymbol{\theta}||$ and $\boldsymbol{\xi}^{\mathbf{u}^*}$ is called the first-order *sensitivity* of the optimal solution with respect to parameters. For sufficiently *small* perturbations, i.e., $\eta \ll 1$, the $O(\eta^2)$ term will, in practice, be negligible compared to $\eta\, \boldsymbol{\xi}^{\mathbf{u}^*}$. Hence, if it is possible to compute $\boldsymbol{\xi}^{\mathbf{u}^*}$ directly from the knowledge of $\mathbf{u}^*$, then a very accurate approximation for $\tilde{\mathbf{u}}$ can be computed using (1.3) after neglecting the $O(\eta^2)$ terms, i.e., *without solving* the optimization problem (1.2).

The conditions under which the optimal solutions of parametric optimization problems are differentiable with respect to parameters and how to compute the first-order sensitivity information if the former hold for a given problem are studied under the *sensitivity analysis of parametric optimization problems.* Some other problems most commonly studied in sensitivity analysis are:

- Conditions for continuity, Lipschitz continuity and differentiability of *optimal cost* ($J(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}})$) with respect to parameters;[2]
- Conditions for continuity and Lipschitz continuity of *optimal inputs and associated Lagrange multipliers* ($\tilde{\mathbf{u}}, \tilde{\boldsymbol{\lambda}}$) with respect to parameters.

Various sub-cases of the above categories are studied by considering whether the underlying problem has cost and/or constraint functions convex or otherwise, whether there exist unique or multiple optimal inputs and/or associated Lagrange multipliers and so on.

A voluminous literature exists on the study of the sensitivity analysis of parametric NLP problems; see, for example, the classic references [4, 29] and the extensive literature cited therein. A more recent and more comprehensive reference, which

[2] The results dealing with continuity and Lipschitz continuity are sometimes labeled as *stability* results, in contrast with *sensitivity* results.

also addresses nonsmooth problems, is [65]. We also refer to the excellent survey articles [9, 61]. A more detailed description of a number of results from sensitivity analysis is deferred till Chapter 2 of the thesis, where they will be used to derive results on the performance of certain *adapted* solutions to the underlying parametric NLP. Not all of the aforementioned results in sensitivity analysis are needed however. The needed results can be divided in two categories: those implying Lipschitz continuity of *optimal cost* ($J(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}})$), and others dealing with Lipschitz continuity of *optimal inputs and associated Lagrange multipliers* ($\tilde{\mathbf{u}}, \tilde{\boldsymbol{\lambda}}$).

Extensive work has also been done on the sensitivity analysis of parametric optimal control problems; see, for example, [57, 69, 74, 75] and the numerous references cited therein. For a recent and comprehensive treatment, that also deals with nonsmooth problems, see [58] and other references it cites.

The main difficulty with the application of sensitivity analysis in practical RTO methods is that it is rarely possible to compute the (magnitude of) perturbed parameters for complex processes, as noted already.

Even if an estimate of parametric perturbations is available, closed form expressions for variations in optimal inputs are available only under restrictive assumptions. For example, for parametric NLP problems, closed form expressions for first-order variations in optimal inputs are available only if strict complementarity conditions hold [29]. Similarly, for parametric optimal control problems, first-order variations of the optimal inputs with respect to parametric perturbations can be computed [23, 86] only under the restrictive strict complementarity conditions for optimal control problems [74].

- Another approach to direct input adaptation is by transforming the optimization problem into a feedback control design problem such that the controller action generates the plant optimal inputs. The main idea is that [83, 99], the feedback controller should track such a *function of measured outputs* as will enforce optimal plant operation. Hence, these methods are sometimes commonly referred to as **reference tracking** methods.

  For example, in *self-optimizing control* for SRTO [99], the feedback controller is designed to track a linear combination of outputs. Similar ideas are applied to design self-optimizing controllers for DRTO problems involving polynomial systems in [59].

A more interesting *objective* to track using a feedback controller is the (full or partial) set of NCO of the plant. An early example of this idea is the *constraint control* method of [67]. More advanced methods based on this principle are: *extremum-seeking control* [3, 52, 64] and *NCO tracking* [37, 104].
Methods of extremum-seeking control need to compute experimental gradients using sinusoidal excitations. NCO tracking methods design a multivariable control strategy to track the NCO related to active constraints and to gradients (i.e., sensitivities). While the tracking of active constraints is quite straightforward using standard control tools [11, 102], the tracking of gradient terms involves more complicated techniques like neighboring-extremal control [51].
For application of NCO tracking framework to dynamic RTO (DRTO) problems, see [101, 103]. It is shown in [36, 101, 110] that the implementation of NCO-tracking controllers for enforcing active constraints using standard tools from control theory is fairly easy for DRTO problems also. This is especially true if the optimal active set remains unchanged after parametric perturbations. Furthermore, *neighboring-extremal control* techniques for tracking sensitivities of DRTO problems are developed in [51], though they are much difficult than the controllers tracking active constraints.

The main difference between reference tracking methods and methods based on sensitivity analysis is that the former typically do *not* need the knowledge of the parametric perturbations. As a result, the way the plant optimum is computed in the two types of methods is different. The exception to this observation is the neighboring-extremal control in which, the knowledge of the parametric perturbations is needed [51].

- Another group of direct input adaptation methods is the class of so-called **interpolation**-based methods [51] in which, the optimal input profiles are computed for different possible problem instances and are stored in look-up tables along with corresponding state and parameter instances. Using tools like search trees [50] or neural networks [63, 97], these methods compare the online measurements with stored instances and choose the input profiles corresponding to the closest match to apply to the process.

1.2.2 A Survey of Selected Analytical Results Relevant to RTO Methods

Let us recall that of all the optimization methods in the presence of uncertainty that were presented in the last section, only the methods that were clubbed under *modifier adaptation* and *direct input adaptation* are *fixed-model methods* [70]. Precisely these two groups of methods are shaded in Figure 1.1.

If we refer to various results on the different methods from these two groups, viz., bias update [32], constraint adaptation [16], (cost and/or constraint) gradient correction [12, 39, 72, 107], constraint control [67], self-optimizing control [99], extremum-seeking control [3, 52, 64], static and dynamic NCO tracking [11, 37, 101, 102, 103], we can realize that the results obtained by these methods, under different conditions, are quite impressive. That is to say that these methods are in many cases capable of converging (near) to plant optimum, and most of these methods have some or other features that are easy for implementation.

A little bit of thinking reveals that a common thread in all these diverse methods is that they are capable of operating in a *selective manner*, for example

- modifier adaptation methods choose to adapt part or all of the following:

  cost bias, constraint bias, cost-gradient correction, constraint-gradient correction, (1.4)

- direct input adaptation methods choose to track part or all of the following:

  active constraints, functions of outputs, sensitivities. (1.5)

What differs among the methods is how they achieve their aim. Also, note that the entities in (1.4) and (1.5) chosen selectively by the two types of methods are directly related to the components of the necessary conditions of optimality (NCO) for the plant [6, 89].

From these observations, we can abstract the following general conclusions:
The level of *selectivity* of the two types of methods affects their ease of implementation and also determines the *properties* of solutions they generate, viz., which components of the plant NCO the latter can satisfy. The last fact explains the general ability of these methods to converge (near) to the plant optimum.

At this point, the following question arises naturally:
What general analytical results exist to support the *selectivity* (or otherwise) of these RTO methods, from the point of view of optimality, and not just for the sake of ease of implementation?

An important result proved in [16] deals with the *variational analysis of cost* in static RTO (SRTO) problems. Under suitable constraint qualifications, it is possible to compute the singular value decomposition (SVD) of the Jacobian of the active constraints evaluated at the nominal optimal solution [16, 37]. The properties of the matrices that appear in the SVD [62] enable identification of two *orthogonal* sets of directions in input space such that small local variation of the model inputs ($\mathbf{u}^*$) along directions in one set does not affect the nominally active constraints, while variation along directions in the other set does [37]. The former are termed sensitivity-seeking (SS) directions and the latter constraint-seeking (CS) directions. Furthermore, the two sets of directions can be shown to span the entire input space.

The importance of the identification of the SS and CS directions in the input space is that, in case of small parametric perturbations, it is possible to define *selective* input adaptation strategies in which small local variation of nominal inputs along either set of directions are considered. Let the locally adapted inputs along the SS and CS directions be denoted by symbols $\mathbf{u}_s$ and $\mathbf{u}_c$, respectively. Thus, it is now possible to consider the effect of the following three strategies on cost in the presence of uncertainty:

1. no adaptation, i.e., applying the model inputs $\mathbf{u}^*$ as is to the plant,
2. applying $\mathbf{u}_s$ to the plant,
3. applying $\mathbf{u}_c$ to the plant.

The difference in costs resulting from the first two options can be considered as *cost variation due to SS adaptation* (δJ_s) over no adaptation. Similarly, the difference in costs resulting from the first and the third option can be considered as *cost variation due to CS adaptation* (δJ_c) over no adaptation.

The important result proved in [16] is that, for small parametric perturbations, the cost variation δJ_s is *significantly* smaller than δJ_c for any general parametric NLP problem. The implication of this result is that, if full adaptation is not possible, adaptation that favors meeting the active constraints should, in general, be preferred, provided the perturbations remain small.

Note, however, that the aforementioned arguments describe the situation *only* around the set of nominal optimal inputs, i.e., they do not take into account the set of plant optimal inputs. Indeed, the inputs $\mathbf{u}_s$ and $\mathbf{u}_c$ are not even guaranteed to be feasible under the perturbed parameters. Thus, in general, $\mathbf{u}_s$ and $\mathbf{u}_c$ cannot be treated as adapted solutions generated using some RTO method, neither is it possible to treat the aforementioned *cost variation* as a measure of performance of some RTO method. In particular, the absence of plant optimal inputs from the analysis means that practically important scenarios like change in optimal active set due to parametric perturbations cannot be addressed in this framework.

These results can be represented in a schematic diagram as shown in Figure 1.2. Recall that the results described above are derived only for SRTO problems.

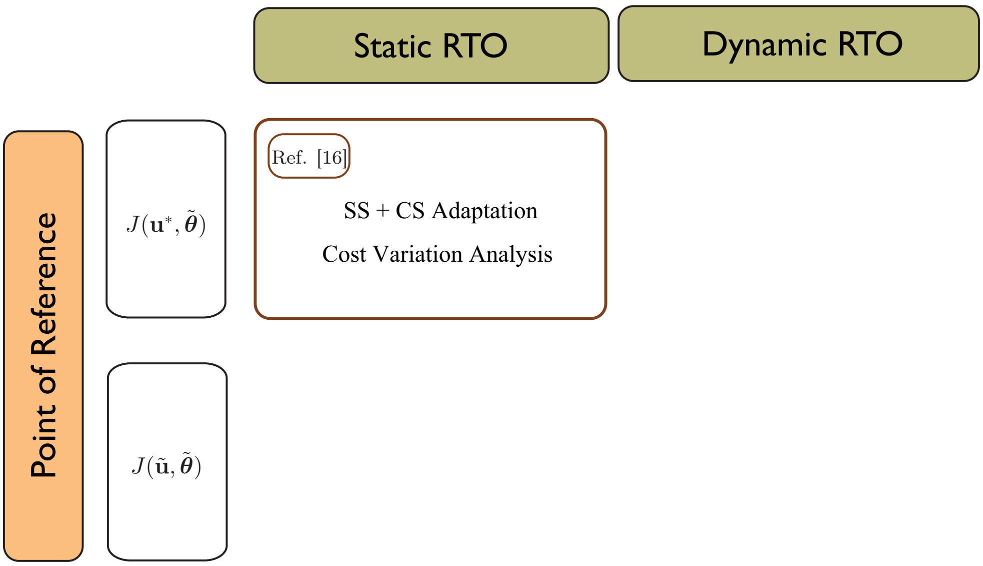

Figure 1.2 Existing analytical results relevant to (static) RTO methods under consideration before beginning of this thesis. $\tilde{\boldsymbol{\theta}}$ denotes the plant parameters while $\mathbf{u}^*$ and $\tilde{\mathbf{u}}$ denote, respectively, the model and plant optimal solutions, here of SRTO.

The term *Point of Reference* in Figure 1.2 is used to indicate the cost value used as reference for comparing the performance of adapted inputs under investigation. For example, the cost variation result in [16] described above deals with the difference between cost due to adaptation and that due to no adaptation of model optimal inputs $\mathbf{u}^*$. Hence, the *Point of Reference* for the block representing [16] is shown to be $J(\mathbf{u}^*, \tilde{\boldsymbol{\theta}})$. By analogy, if the *Point of Reference* for a block is $J(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}})$ (plant optimal cost), the block represents results of comparison of cost resulting from adapted inputs under consideration with that resulting from the *plant optimal inputs* $\tilde{\mathbf{u}}$.

1.3 Research Objectives

Figure 1.2 naturally gives rise to following questions:

- Is it possible – in SRTO problems – to move from a local variational analysis around the model-based optimum towards a more complete analysis that involves the plant optimum also? If yes, how exactly to do such an analysis and under what conditions?
- Is it possible to extend the local variational analysis of SRTO problems to dynamic RTO (DRTO) problems? If yes, what are the main challenges in doing so?

That these questions are not mere curiosities but have important implications for RTO methods will be clear from the discussion that follows.

In the remainder of the section, we denote the nominal and perturbed optimal inputs of the RTO under consideration by symbols $\mathbf{u}^*$ and $\tilde{\mathbf{u}}$, respectively.[3]

1. **SRTO**
   It is well known that parametric perturbations cause change in the optimal solutions of parametric NLP problems and possibly also in the optimal active set. Given the *tension* between feasibility and optimality discussed at the beginning of the chapter, what is the meaning of an active constraint becoming inactive, or vice versa, in the presence of uncertainty?
   Let us think again about the active constraints. Although general constraints define the feasibility requirements in the problem, the set of active constraints are actually part of the problem NCO. That is, active constraints contribute to the optimality of the problem while being *just feasible*.
   So, when the optimal active set changes in the presence of uncertainty, is it *only* to maintain the feasibility of the plant or *only* to contribute to its optimality? Or,

[3] If the problem under consideration is SRTO, the symbols need to be interpreted as *vectors*, whereas if the problem is DRTO, the symbols need to be interpreted as *vector functions*.

is it possible that some active constraints change owing to feasibility while others owing to optimality?

The importance of these questions to RTO methods designed for *selective* adaptation is evident. For example, we can ask the following questions:

when the active set changes not to maintain plant feasibility, but due to optimality, precisely how *important* is the contribution of its change to optimality? Or, thought differently, in which cases is the latter contribution not so important and hence the change can be practically ignored by an RTO method? How best to identify such conditions that help distinguish between changes that are due to optimality and others that are due to feasibility? Is it possible to develop such an analysis for as general a class of parametric NLP problems as possible?

These considerations give rise to the first research objective of the thesis:

> **Research Objective 1:**
>
> Under conditions as general as possible for SRTO problems, develop a joint analysis involving model optimal inputs $\mathbf{u}^*$, plant optimal inputs $\tilde{\mathbf{u}}$ and different sets of adapted solutions $\hat{\mathbf{u}}_i$ obtained from $\mathbf{u}^*$, such that different $\hat{\mathbf{u}}_i$ conserve different parts of the set of *nominally active constraints*. (1.6)

2. **DRTO**

In Section 1.2.2, we saw that the importance of a local variational analysis of cost due to selective adaptations along SS and CS directions is that it is possible to show clearly distinguishable cost variations for the two cases of adaptation. The result mainly implies a preference to active constraints over sensitivities in SRTO. If such a result were available for DRTO problems, it would have similar implications for its (active) constraints and sensitivities. This means that the first task for a similar analytical study of DRTO problems is to develop a characterization of the SS and CS directions.

Recall from Section 1.2.2 that the basic idea of these directions is such that a small variation of the model inputs $\mathbf{u}^*$ along an SS direction should not affect the nominally active constraints of the problem, whereas an input variation along a CS direction should. However, compared to SRTO problems, this task is more complicated in DRTO problems owing to the fundamentally different nature of constraints in them.

Consider, for example, the case of active path constraints in DRTO. By definition, a path constraint is an infinitude of constraints defined at each time instant. Recall again from Section 1.2.2 that the definition and all the *nice* properties of the SS and CS directions for SRTO problems followed from the properties of the SVD of the *Jacobian of active constraints of SRTO*. So, to attain the final aim of cost variational analysis of DRTO, should we consider the SVD of Jacobians of path constraints active at each instant? In other words, just as there is an infinitude of pointwise constraints in DRTO, should there be an infinitude of SS and CS directions in it? But what is the guarantee that an input variation along an SS direction *of* the *present* instant will *not* affect an active constraint in the future, given the fact that the underlying system in a DRTO problem is dynamic.

On the other hand, consider a DRTO problem having only terminal constraints. If we were to follow an SVD-based approach for the definition of SS and CS directions, we would only be able to define the directions at the final time. Would this mean that no SS and CS directions can be defined for intermediate time instants? But, we can certainly imagine changes in inputs during process operation propagating through the underlying dynamic system and changing the value of the terminal constraints. So, these changes should qualify – on the basis of the broad definition considered above – as changes along CS directions, which is absurd if the directions are defined only at the final time.

Thus, the main challenge in DRTO is to account for the fact that the definition of the input variation directions for time t requires that *all* past input variations up to and including time t need to be taken into account, not merely the input variations at time t.

Once such a *dynamic* characterization of the directions is available for a general DRTO problem, the next question to address is how to perform the local cost variational analysis for plant following selective input adaptation along each set of directions. The final objective is to see whether the characterization of SS and CS directions, and so of the local selective adaptation strategies, for the DRTO problems leads to clearly distinguishable cost variations over the case of no input adaptation.

If the sought cost variation result can be proved, then the relative importance of active constraints over sensitivities in DRTO problems can be inferred.
Thus, the second research objective of the thesis can be formulated:

Research Objective 2:

Extend the local variational analysis around $\mathbf{u}^*$
that exists for SRTO problems (Figure 1.2)
to DRTO problems under conditions as general as possible. (1.7)

These objectives can be represented in a schematic diagram as shown in Figure 1.3.

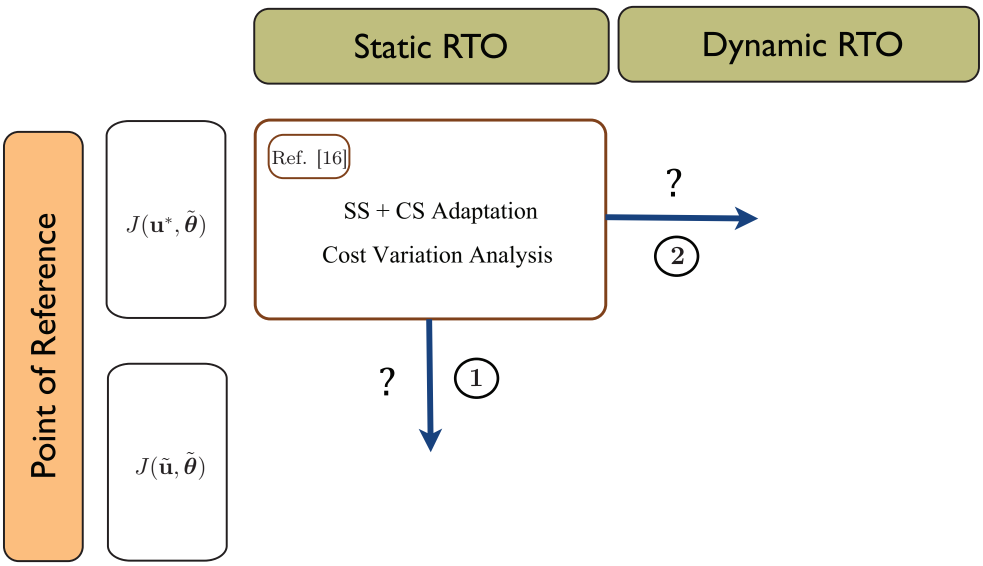

Figure 1.3 Questions that form the basis of the *Research Objectives* of the present thesis.

The results of these investigations directly depend on the *role* of constraints in RTO and so the investigations will, hopefully, yield an improved understanding of the latter.

1.4 Organization of the Thesis

This thesis deals with some key analytical aspects of the real-time optimization (RTO) in the presence of uncertainty. The type of static and dynamic RTO problems considered in the thesis are those in which, the uncertainty is represented by parametric perturbations.

Chapters 2 and 3 constitute the first part of the thesis that deals with static RTO (SRTO) problems.

Chapter 2 begins with a short survey of existing methods to SRTO problems and of available analytical results on the role of constraints in SRTO. The insights gained from this survey are discussed in Section 2.2, the main conclusion of which is the necessity of developing a *joint* analysis of the model optimal solution, the adapted solution generated by an SRTO method and the plant optimal solution while taking into account the possibility of change in optimal active set. Based on these insights, a precise mathematical formulation of the research objective for the SRTO is given in Section 2.3.

Chapter 3 accomplishes the research objective set forth in Chapter 2. Under suitable conditions on the underlying problem, viz., linear independence constraint qualification (LICQ) and strong second-order sufficient condition (SSOSC), the change in optimal active set is analyzed in Section 3.1. Using these insights, the optimality loss analysis is performed in Section 3.2. The main conclusion reached is that, under the assumed conditions, the detection of a change in the active set contributes only negligibly to optimality, as long as the adapted solution remains feasible. A numerical example illustrating the results is presented in Section 3.3.

The second part of the thesis deals with an analytical study of the dynamic RTO (DRTO) problems. It is divided in Chapters 4 and 5.

Chapter 4 begins with a short survey of existing DRTO methods and follows it up with a discussion of the challenges in an analytical study of role of constraints in DRTO, especially with reference to similar available results for SRTO. The precise mathematical formulation of the DRTO problem and the research objective for its analytical study is presented in Sections 4.3 and 4.4.

In Chapter 5, the research objective for the DRTO problem formulated in Chapter 4 is attained. First, a definition of sensitivity- and constraint-seeking (SS and CS) directions for the DRTO problem is developed in Section 5.1. The section also introduces the concept of local variation of model optimal inputs along each of the above set of directions and presents a numerical algorithm for computing SS and CS components of a given input variation direction.

Section 5.2.2 presents a variational analysis of cost due to small local variation of model optimal inputs along SS and CS directions. The main result of the analysis is that, for small parametric variations, the cost variation due to input variation along SS directions is negligible compared to that due to variation along CS directions. In other words, under small parametric variations, satisfaction of active constraints typically has more influence on cost than satisfaction of sensitivities. Section 5.3 presents two examples that demonstrate the results of Chapter 5.

Finally, Chapter 6 summarizes the main contributions of the thesis and results obtained in it and discusses some future perspectives.

Chapter 2

Static Real-Time Optimization

Many engineering processes are operated at steady state. Steady-state operation is attractive from point of view of implementation because the decision variables, or *inputs*, of a process need to be simply kept at constant values, called *operating set-points*, over long time-periods. There can be multiple set-points at which the system can operate in the steady-state and different choices of set-points can incur different operating costs or result in different profit levels. On the other hand, not all set-points can be attained owing to various operational limitations and some other set-points need to be avoided in order to obey various safety constraints. Hence, the choice of a particular set of inputs is based on whether or not it satisfies all process constraints and at the same time minimizes operational cost or maximizes operational profits, as the case may be.

If a mathematical model of steady-state operation is available, the problem of optimal selection of operating set-points can be formulated as a type of mathematical programming problem. For example, the most common formulations of such problems in chemical process industries are as nonlinear programming (NLP) and mixed-integer programming problems [27]. Owing to the advances in the theory and computational methods for these problems, it is not uncommon to encounter examples of steady-state, or *static*, optimization problems involving hundreds of decision variables and constraints. The optimal operating set-points can be computed using the model even before the start of operation and during actual operation, their stored values need to be simply maintained.

Unfortunately, highly accurate mathematical models are rarely available for industrial scale processes. Naturally, in real-time operation using model-based optimal set-points, both plant-model mismatch and process disturbances can lead to subopti-

mal operation or even infeasible operation. Hence, optimal steady-state operation in the presence of uncertainty is an important problem faced by the process industries. We refer to this problem as that of *static real-time optimization* (SRTO), which can be defined as:
online computation of feasible and near-optimal input values for a static optimization problem on the basis of the knowledge of nominal optimal solution and online measurement data.

It is thus clear that a study of SRTO problems entails the study of the interplay of the three main themes of the thesis, viz., uncertainty, feasibility and optimality.

2.1 A Short Survey of Existing Approaches for Static RTO Problems

A common practice of dealing with uncertainty is to represent it in the form of parametric perturbations. The optimal inputs are computed off-line for the nominal values of the parameters. Naturally, when some parameters deviate from their nominal values, a change in optimal inputs is required to maintain feasibility and optimality.

Ideally, one would need to repeat the computation with the modified values of the parameters to obtain the modified optimal inputs. A way to avoid re-solving the optimization problem is to quantify the parametric perturbations and *adapt* the nominal optimal inputs to maintain optimality. In theory, such an approach requires a *sensitivity analysis* of the parametric optimization problems, i.e., a study of the effect that parametric perturbations will have on the optimal inputs. Extensive work has been done regarding the stability and sensitivity analysis of parametric optimization problems; see, for example, the classic references [4, 29] and the extensive literature cited therein. A more recent and more comprehensive reference, which also addresses nonsmooth problems, is [65]. We also refer to the excellent survey articles [9, 61].

In practice, it may not be possible to quantify the parametric perturbations precisely. Even if an estimate of parametric perturbations is available, closed form expressions for first-order variations in optimal inputs are available only if strict complementarity and second-order sufficient conditions hold [29]. Thus, it may not always be possible to implement adaptation using first-order estimates in practice. Hence, real-time optimization (RTO) methods typically try to use the knowledge of the underlying system and adapt the nominal optimal inputs to obtain some set of feasible inputs. Numerous real-time optimization algorithms have been proposed in the literature. As noted in Introduction, these algorithms effect the input adaptation via different mechanisms. Recall some examples of the RTO methods most relevant to our investigations:

- some algorithms perform repeated optimization of fixed nominal model but with updating of constraints at each iteration using process measurements [17],
- some methods do repeated optimization of fixed nominal model but with updating of *both* cost function and constraints at each iteration using process measurements [39],
- some methods are based on repeated optimization of a process model that is updated at each iteration using process measurements [106],
- some algorithms are based on online control of active constraints [67] and sometimes, in addition, a provision of detecting the change in active set [111],
- some methods enforce the necessary conditions of optimality related to both constraints and sensitivities in a run-to-run fashion (NCO tracking for SRTO) [37].

For a more detailed survey of static RTO methods, refer to Section 1.2.1. As noted there, RTO methods based on enforcing of NCO related to constraints are typically simpler to implement than those based on enforcing of sensitivities.

Since the real-time adaptation may be sub-optimal, it becomes essential to be able to compare the performance of a given set of adapted inputs with that of the optimal inputs for the perturbed system.

2.1.1 Analytical Results on Role of Constraints

As mentioned in Section 1.2.2, for SRTO problems modeled in terms of parametric NLP, two sets of directions in input space can be identified such that small local adaptation of nominal inputs along directions in one set does not affect the nominally active constraints, while adaptation along directions in the other set does [37]. The former have been termed sensitivity-seeking (SS) directions while the latter constraint-seeking (CS) directions.

An important result proved in [16] is that, in case of small parametric perturbations, a small local variation of the nominal inputs along the constraint-seeking directions causes a larger *cost variation* over no input variation than does the variation along the sensitivity-seeking directions. To be more precise, consider parametric perturbations of form $\tilde{\boldsymbol{\theta}} = \boldsymbol{\theta}_0 + \eta\boldsymbol{\xi}^{\boldsymbol{\theta}}$, where $|\eta| \ll 1$ and $\boldsymbol{\xi}^{\boldsymbol{\theta}}$ is a given direction in the space of parameters. In case of such small parametric perturbations, let $\mathbf{u}_s$ and $\mathbf{u}_c$ denote the aforementioned small local variations of nominal optimal inputs along the SS and CS directions, respectively. If *cost variation* (δJ) over no adaptation due to a given set of inputs $\mathbf{u}$ is defined as

$$\delta J(\mathbf{u}) := J(\mathbf{u}, \tilde{\boldsymbol{\theta}}) - J(\mathbf{u}^*, \tilde{\boldsymbol{\theta}}), \tag{2.1}$$

then, the aforementioned result states that

$$\delta J(\mathbf{u}_s) = O(\eta^2), \quad \delta J(\mathbf{u}_c) = O(\eta).$$

The implication of this result is that, under small parametric variations, if full adaptation is not possible, adaptation that favors meeting the active constraints should be preferred.

Let us also recall from Section 1.2.2, that the aforementioned arguments describe *only* a local variational analysis around the set of nominal optimal inputs; i.e., they do not take into account the set of perturbed optimal inputs. Moreover, the inputs $\mathbf{u}_s$ and $\mathbf{u}_c$ are not even guaranteed to be feasible under the perturbed parameters $\tilde{\boldsymbol{\theta}}$. Thus, in general, $\mathbf{u}_s$ and $\mathbf{u}_c$ cannot be treated as adapted solutions generated using some RTO method, and so the *cost variation* (2.1) cannot be treated as a measure of performance of some RTO method. In particular, absence of perturbed optimal inputs from the analysis is a major shortcoming of this framework due to the fact that practically important scenarios like change in optimal active set due to parametric perturbations can also not be taken into account.

We have already represented these results in the schematic diagram in Figure 1.2 in Introduction.

2.2 Challenges in Analytical Studies

Let us abstract the main ideas scattered among the diversity of results surveyed in Section 2.1:

1. Different SRTO methods can result in different adapted solutions. Hence, performance measurement of an RTO method needs to compare the performance of the set of adapted inputs generated by it with that of the (unknown) perturbed optimal inputs.
2. Since an RTO algorithm will typically start from the nominal solution, the resulting adapted inputs might share only certain features with the perturbed optimal solution; moreover, different RTO algorithms will, typically, yield different adapted inputs.
3. Local analysis around nominal optimal solution of a general NLP implies that active constraints can influence cost more than can sensitivities.
4. SRTO methods based on enforcing of NCO related to constraints are quite simple to implement.

These observations naturally prompt the following questions:
Is it possible to develop a general analysis of performance loss due to a given set of adapted inputs based on the features it shares with the perturbed optimal inputs? What feature(s) might be most relevant for such an analysis to be most useful?

Observations (3) and (4) answer the last question:
the feature most important, from the point of view of optimality as well as practical relevance, is the set of constraints made active by a given set of inputs.

This combined with observation (2) answers the first question:
since the nominal active set is known and the adapted solutions are generated using the knowledge of nominal optimal solution, a general analysis of performance loss due to adapted inputs is possible, if we consider a different set of adapted inputs that conserve whole or part of the nominal active set and take into account the manner in which the optimal active set itself might possibly change.

In summary, it is essential to perform a *joint* analysis of the nominal optimal inputs ($\mathbf{u}^*$), the adapted inputs (say, $\hat{\mathbf{u}}$) and the optimal inputs for the perturbed system ($\tilde{\mathbf{u}}$) while taking into account the possibility of change in optimal active set as well as the fact the constraints kept active by the adapted solutions might be different from the perturbed optimal set.

In this spirit, we investigate the optimality loss due to different sets of adapted inputs that conserve some or other elements of the nominal active constraint set and thus share only a few features of the perturbed optimal solution. Naturally, the *optimality loss analysis* is more involved than the cost variation analysis, since the latter deals only with the nominal optimal ($\mathbf{u}^*$) and adapted ($\hat{\mathbf{u}}$) solutions. It is also different from the standard *sensitivity analysis* discussed in Section 1.2.1.3, since the latter deals only with the relation between nominal optimal and perturbed optimal *entities* (i.e., inputs: $\mathbf{u}^*, \tilde{\mathbf{u}}$, associated Lagrange multipliers: $\boldsymbol{\lambda}^*, \tilde{\boldsymbol{\lambda}}$, cost: $J(\mathbf{u}^*, \boldsymbol{\theta}_0), J(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}})$), while there is, typically, no notion of *adapted* solutions involved. However, as noted in Section 1.2.1.3, we will need to make use of various results from sensitivity analysis in investigations of optimality loss.

These investigations will, hopefully, help understand in more detail the importance of the active constraints in designing RTO schemes for static optimization.

2.3 Research Objective for Static RTO Problems

In this section, we give the precise mathematical formulation for the ideas mentioned in the previous section. We will be dealing with SRTO problems modeled as general parametric nonlinear programming (pNLP) problems. First, we present the mathematical formulation, various assumptions and the form of necessary conditions of optimality for the pNLP problems considered. Then, we discuss the effect of parametric uncertainty on the optimal solution of the problem.

Finally, we define the concept of optimality loss and present some results on the optimality loss due to no adaptation, assuming it is feasible. The discussion of the results leads to the precise research objective for SRTO problems.

2.3.1 Problem Formulation and Optimality Conditions

We consider the following parametric nonlinear programming (pNLP) problem (NP($\boldsymbol{\theta}$)):

$$
\begin{aligned}
\min_{\mathbf{u}} \quad & J(\mathbf{u}, \boldsymbol{\theta}) \\
\text{s.t.} \quad & G_i(\mathbf{u}, \boldsymbol{\theta}) \leq 0, \quad i = 1, \ldots, n_{\mathbf{G}}, \\
& \mathbf{u} \in \mathbb{R}^{n_{\mathbf{u}}}, \quad \boldsymbol{\theta} \in \mathbb{R}^{n_{\boldsymbol{\theta}}},
\end{aligned}
\tag{2.2}
$$

where $\mathbf{u}$ is the input vector, J the cost function and G_i the i^{th} constraint. The nominal value of the parameters is $\boldsymbol{\theta}_0$. We assume that the functions J and G_i are twice continuously differentiable in all arguments, i.e.,

Assumption 2.1 (Differentiability of J and G_i)

$$
J \in \mathcal{C}^2(\mathbb{R}^{n_{\mathbf{u}}} \times \mathbb{R}^{n_{\boldsymbol{\theta}}}, \mathbb{R}), \quad G_i \in \mathcal{C}^2(\mathbb{R}^{n_{\mathbf{u}}} \times \mathbb{R}^{n_{\boldsymbol{\theta}}}, \mathbb{R}), \quad \forall\, i = 1, \ldots, n_{\mathbf{G}}. \tag{2.3}
$$

Henceforth, we will be dealing with the *global* optimum solution(s) of the pNLP (2.2). Let $\mathbf{u}^*$ denote the nominal global optimal solution of (2.2).

The active set at $\mathbf{u}^*$ is defined as [84]:

$$
\mathcal{A}^* := \{ i \mid G_i(\mathbf{u}^*, \boldsymbol{\theta}_0) = 0 \}. \tag{2.4}
$$

We assume constraint qualification of the linear independence of the gradients of the active constraints (LICQ) at the nominal solution $\mathbf{u}^*$. In terms of the notation of active set, we have[1]

Assumption 2.2 (LICQ)

$$
\textit{Column vectors of } \frac{\partial \mathbf{G}_{\mathcal{A}^*}}{\partial \mathbf{u}}(\mathbf{u}^*, \boldsymbol{\theta}_0) \textit{ are independent.} \tag{2.5}
$$

Under the assumption of LICQ, the Karush-Kuhn-Tucker NCO hold for NP($\boldsymbol{\theta}$) [5, 84, 88]:

$$
\begin{aligned}
\frac{\partial J}{\partial \mathbf{u}} + \boldsymbol{\lambda}^T \frac{\partial \mathbf{G}}{\partial \mathbf{u}} &= \mathbf{0}, \\
\lambda_i G_i(\mathbf{u}, \boldsymbol{\theta}) &= 0, \\
\lambda_i &\geq 0, \quad i = 1, \ldots, n_{\mathbf{G}}, \\
G_i(\mathbf{u}, \boldsymbol{\theta}) &\leq 0, \quad i = 1, \ldots, n_{\mathbf{G}}.
\end{aligned}
\tag{2.6}
$$

[1] Henceforth, we use the following notation: given an index set $\mathcal{I} = \{m_1, \ldots, m_p\}$ and variables/functions $f_1, \ldots, f_k$, $\mathbf{F}_{\mathcal{I}} := \begin{bmatrix} f_{m_1} \\ \vdots \\ f_{m_p} \end{bmatrix}$. A vector (function) without an index-subscript will indicate, as usual, the vector (function) of all underlying elements, the total number of elements being clear from the context.

Let the nominal solution $(\mathbf{u}^*, \boldsymbol{\lambda}^*)$ be such that:

$$\begin{aligned} &\lambda_i^* > 0 \quad \& \quad G_i(\mathbf{u}^*, \boldsymbol{\theta}_0) = 0, \quad i \in \mathcal{I}^*, \\ &\lambda_i^* = 0 \quad \& \quad G_i(\mathbf{u}^*, \boldsymbol{\theta}_0) = 0, \quad i \in \mathcal{J}^*, \\ &\lambda_i^* = 0 \quad \& \quad G_i(\mathbf{u}^*, \boldsymbol{\theta}_0) < 0, \quad i \in \mathcal{K}^*, \\ &\mathcal{I}^* \cup \mathcal{J}^* \cup \mathcal{K}^* = \{1, \ldots, n_{\mathbf{G}}\}. \end{aligned} \tag{2.7}$$

In practice, knowledge of (2.7) is available via off-line numerical optimization. Note that there are no elements common in $\mathcal{I}^*, \mathcal{J}^*$ and $\mathcal{K}^*$ and that $\mathcal{A}^* = \mathcal{I}^* \cup \mathcal{J}^*$. In literature [31, 84], $\mathcal{I}^*$ is called the index set of *strongly active* constraints, $\mathcal{J}^*$ that of *weakly active* constraints, and $\mathcal{K}^*$ that of inactive constraints. Strongly and weakly active constraints have been called nondegenerate and degenerate constraints, respectively, in [60].

The main difference between the two parts $\mathcal{I}^*$ and $\mathcal{J}^*$ of the active set is that non-satisfaction of the strongly active constraints in $\mathcal{I}^*$ has a more significant impact on the cost function than non-satisfaction of the weakly active constraints in $\mathcal{J}^*$. This aspect will be quantified later.

2.3.2 Uncertainty Description

The following type of parametric variations is considered:

$$\tilde{\boldsymbol{\theta}} = \boldsymbol{\theta}_0 + \eta\, \boldsymbol{\xi}^{\boldsymbol{\theta}}, \quad \eta \in \mathcal{B}_0, \tag{2.8}$$

where $\boldsymbol{\xi}^{\boldsymbol{\theta}}$ is a vector – of unit Euclidean norm – in the parameter space $\mathbb{R}^{n_{\boldsymbol{\theta}}}$, and $\mathcal{B}_0$ is a small interval around zero that will be specified later.

Let $\tilde{\mathbf{u}}$ denote the *global* optimal inputs for the perturbed system, which are, typically, different from the nominal inputs. It is important to note that an additional complexity for a general pNLP of type (2.2) is that there can exist multiple perturbed optimal solutions $\tilde{\mathbf{u}}_i$ for some $\eta \in \mathcal{B}_0$.

Henceforth, we will assume that a perturbed optimal solution $(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\lambda}})$ also satisfies the NCO (2.6) for each η. Hence, the perturbed optimal solution for a given η satisfies:

$$\begin{aligned}
&\tilde{\lambda}_i > 0 \quad \& \quad G_i(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}}) = 0, \quad i \in \tilde{\mathcal{I}}, \\
&\tilde{\lambda}_i = 0 \quad \& \quad G_i(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}}) = 0, \quad i \in \tilde{\mathcal{J}}, \\
&\tilde{\lambda}_i = 0 \quad \& \quad G_i(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}}) < 0, \quad i \in \tilde{\mathcal{K}}, \\
&\tilde{\mathcal{I}} \cup \tilde{\mathcal{J}} \cup \tilde{\mathcal{K}} = \{1, \ldots, n_{\mathbf{G}}\}.
\end{aligned} \tag{2.9}$$

The index sets $\tilde{\mathcal{I}}, \tilde{\mathcal{J}}$ and $\tilde{\mathcal{K}}$ can, in general, be different from $\mathcal{I}^*, \mathcal{J}^*$ and $\mathcal{K}^*$.

2.3.3 Optimality Loss

Recall from Section 2.2 that the research objective for the SRTO problems is to develop a general analysis that will enable comparison of the performance of a given set of adapted inputs with that of perturbed (global) optimal inputs. To this end, we introduce a generic measure for the aforementioned comparison called *optimality loss*:

Definition 2.1 (Optimality Loss)
For NP($\tilde{\boldsymbol{\theta}}$) (2.2) *and for parametric variations given by* (2.8), *the difference between the cost resulting from a given set of* feasible *inputs* $\mathbf{u}$ *and the perturbed optimal cost is called* optimality loss *and is denoted by* δJ:

$$\delta J(\mathbf{u}) := J(\mathbf{u}, \tilde{\boldsymbol{\theta}}) - J(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}}), \tag{2.10}$$

where $\tilde{\mathbf{u}}$ *denotes the optimal inputs for the perturbed system.*

Remarks:

1. Note that although the cost difference in (2.10) can be computed for *any* set of inputs, the *optimality loss* is defined *only* for feasible inputs since it is pointless to compare performance of infeasible inputs with perturbed optimal inputs.
2. When there is a set of multiple (global) optimal inputs $\{\tilde{\mathbf{u}}_i\}$ for some $\eta \in \mathcal{B}_0$, the definition (2.10) of optimality loss is valid for each of $\tilde{\mathbf{u}}_i$. This is because, by definition of a global optimal solution, the perturbed optimal cost is a unique number, i.e.
$$J(\tilde{\mathbf{u}}_i, \tilde{\boldsymbol{\theta}}) = J(\tilde{\mathbf{u}}_j, \tilde{\boldsymbol{\theta}}), \quad \tilde{\mathbf{u}}_i \neq \tilde{\mathbf{u}}_j.$$

Note, in particular, that while computing the optimality loss due to a given set of adapted inputs, no attention is given to how exactly the latter are (or can be) generated. For example, one can imagine a given set of adapted inputs as an outcome of a particular RTO method. But, while computing the optimality loss, other performance features, e.g., rate of convergence, of the RTO method are not given any consideration. Thus, the approach here is conceptually different from other existing approaches in literature, notably [115, 116].

In other words, what we will be analyzing is the performance of a set of adapted inputs and not the underlying RTO method, per se. The advantage of this approach is that it will, hopefully, enable us to derive results that are fairly general, i.e., tied not to the exact workings of different RTO methods, but solely to *properties* of their outcomes. Also, as noted in Section 2.2, we will be considering such properties of the adapted solutions as will make the analysis most relevant for the workings of a large class of RTO methods.

2.3.3.1 The Basic Approach to Optimality Loss Analysis

In order to keep the optimality loss analysis amenable, we need to impose certain conditions on the underlying problem. These conditions will ensure that the pNLPs under consideration, and their solutions, have certain regularity properties and so will help rule out cases of less practical importance. As mentioned in Section 1.2.1.3, the most widely studied regularity properties of the solutions – inputs and Lagrange multipliers – of pNLPs in the literature on sensitivity analysis of pNLP are continuity, Lipschitz continuity and differentiability.

We would be dealing with systems in which the perturbed optimal inputs $\tilde{\mathbf{u}}(\eta)$ are, at least, Lipschitz continuous with respect to the nominal optimal inputs $\mathbf{u}^*$, so that $\tilde{\mathbf{u}}(\eta) - \mathbf{u}^* = O(\eta)$. Following is a very short summary of the most relevant results from the literature on sensitivity analysis about the Lipschitz continuity of solutions of a pNLP that exhibit *presence of weakly active constraints*. Note that most of the results treat more general pNLP that also includes nonlinear equality constraints.

1. [93] defines a property called *strong regularity* for so called *generalized equations* and proves in Corollary 2.2 that strong regularity of a generalized parametric

equation implies the Lipschitz continuity of its solutions with respect to parametric perturbations.

Further, Theorem 4.1 of [93] proves the strong regularity of the KKT system (2.6) (expressed as a generalized equation) associated with a given pNLP, and by implication the Lipschitz continuity of optimal inputs and associated Lagrange multipliers, under assumptions (2.3), LICQ (2.5) and the following *strong second-order sufficient condition* (SSOSC) for problem NP($\boldsymbol{\theta}_0$):

Assumption 2.3 (SSOSC)

$$\mathbf{v}^T \left\{ \frac{\partial^2 J}{\partial \mathbf{u}^2}(\mathbf{u}^*, \boldsymbol{\theta}_0)\,\mathbf{v} + \boldsymbol{\lambda}^{*T} \frac{\partial^2 \mathbf{G}}{\partial \mathbf{u}^2}(\mathbf{u}^*, \boldsymbol{\theta}_0)\,\mathbf{v} \right\} > 0, \quad \forall\, \mathbf{v} \in \mathcal{N}^s \setminus \{\mathbf{0}\}, \tag{2.11}$$

where $\quad \mathcal{N}^s := \left\{ \mathbf{v} \in \mathrm{IR}^{n_\mathbf{u}} \;\middle|\; \frac{\partial \mathbf{G}_{\mathcal{I}^*}}{\partial \mathbf{u}}(\mathbf{u}^*, \boldsymbol{\theta}_0)\mathbf{v} = 0 \right\}.$

Remarks:

a. It is easy to verify that the set $\mathcal{N}^s$ in the SSOSC (2.11) is a vector space. Thus, it is the null space of the Jacobian of the strongly active constraints at the nominal solution $\mathbf{u}^*$.

   If *strict complementarity condition* holds at the nominal solution, viz. the absence of weakly active constraints ($\mathcal{J}^* = \emptyset$), then $\mathcal{N}^s$ is the same as the *sensitivity-seeking subspace* of NP($\boldsymbol{\theta}$) defined in [37, 16].

b. Identifying

$$\mathcal{L}(\mathbf{u}, \boldsymbol{\lambda}, \boldsymbol{\theta}) = J(\mathbf{u}, \boldsymbol{\theta}) + \boldsymbol{\lambda}^T \mathbf{G}(\mathbf{u}, \boldsymbol{\theta}), \tag{2.12}$$

   as the Lagrangian for NP($\boldsymbol{\theta}$), the SSOSC (2.11) amounts to the *positive definiteness* of the Hessian of the Lagrangian on the null space of the Jacobian of the strongly active constraints at the nominal solution.

   This sufficient condition is called *strong* because there exists a weaker second-order sufficient condition for optimality (WSOSC), which requires the positive definiteness of the Hessian of the Lagrangian *only* on the following *subset* of $\mathcal{N}^s$:

$$\mathcal{C}^w = \left\{ \mathbf{v} \in \mathcal{N}^s \;\middle|\; \frac{\partial \mathbf{G}_{\mathcal{J}^*}}{\partial \mathbf{u}}(\mathbf{u}^*, \boldsymbol{\theta}_0)\mathbf{v} \le 0 \right\}. \tag{2.13}$$

   It is easy to see that $\mathcal{C}^w$ is a *cone*, not a vector space. For a proof that the aforementioned WSOSC condition, viz.,

$$\mathbf{v}^T \left\{ \frac{\partial^2 J}{\partial \mathbf{u}^2}(\mathbf{u}^*, \boldsymbol{\theta}_0)\, \mathbf{v} + \boldsymbol{\lambda}^{*T} \frac{\partial^2 \mathbf{G}}{\partial \mathbf{u}^2}(\mathbf{u}^*, \boldsymbol{\theta}_0)\, \mathbf{v} \right\} > 0, \quad \forall\, \mathbf{v} \in \mathcal{C}^w \setminus \{\mathbf{0}\}, \tag{2.14}$$

is a sufficient condition of optimality for NP($\boldsymbol{\theta}_0$), see Theorem 12.6 in [84]. If *strict complementarity condition* holds at the nominal solution, viz. the absence of weakly active constraints ($\mathcal{J}^* = \emptyset$), then, naturally, the two conditions SSOSC and WSOSC coincide.

2. Theorem 2 in [60] proves the Lipschitz continuity of optimal inputs and associated Lagrange multipliers of a pNLP under the assumption of LICQ and SSOSC. For the sake of completeness, we reproduce the theorem in our notation below:

Theorem 2.1 (Theorem 2 in [60])
At a local solution $\mathbf{u}^*$ of NP($\boldsymbol{\theta}_0$) satisfying (2.3), assume that LICQ (2.5) and SSOSC (2.11)[2] are satisfied, then

a. *$\mathbf{u}^*$ is a local isolated minimizer of NP($\boldsymbol{\theta}_0$) and the associated Lagrange multipliers $\boldsymbol{\lambda}^*$ are unique;*

b. *for $\eta \in \mathcal{B}_0$, there exists a unique continuous vector function $\left[\tilde{\mathbf{u}}(\eta)\ \tilde{\boldsymbol{\lambda}}(\eta)\right]^T$ satisfying the SSOSC for a local minimum for NP($\tilde{\boldsymbol{\theta}}(\eta)$) such that $\left[\tilde{\mathbf{u}}(0)\ \tilde{\boldsymbol{\lambda}}(0)\right]^T = \left[\mathbf{u}^*\ \boldsymbol{\lambda}^*\right]^T$ and, hence $\tilde{\mathbf{u}}(\eta)$ is the locally unique minimizer of NP($\tilde{\boldsymbol{\theta}}(\eta)$) with associated unique Lagrange multipliers $\tilde{\boldsymbol{\lambda}}(\eta)$;*

c. *LICQ holds at $\tilde{\mathbf{u}}(\eta)$ for $\eta \in \mathcal{B}_0$;*

d. *there exist $0 < \alpha, \beta < \infty$ and $\eta_0 > 0$ such that, $\forall\, \eta$ with $|\eta| < \eta_0$,*

$$\begin{aligned} ||\tilde{\mathbf{u}}(\eta) - \mathbf{u}^*|| &\leq \alpha|\eta|, \\ \left|\left|\tilde{\boldsymbol{\lambda}}(\eta) - \boldsymbol{\lambda}^*\right|\right| &\leq \beta|\eta|, \end{aligned} \tag{2.15}$$

e. *optimal cost function $J^o(\eta) := J(\tilde{\mathbf{u}}(\eta), \tilde{\boldsymbol{\theta}}(\eta))$ is differentiable with respect to η at $\eta = 0$:*

$$\frac{d}{d\eta} J^o(0) = \frac{\partial J}{\partial \eta}(\mathbf{u}^*, \boldsymbol{\theta}_0) + \{\boldsymbol{\lambda}^*\}^T \frac{\partial \mathbf{G}}{\partial \eta}(\mathbf{u}^*, \boldsymbol{\theta}_0).$$

Remarks:

[2] It is easy to see that the form of SSOSC in [60] is equivalent to (2.11).

a. Recall that we have already assumed LICQ (2.5) for the NCO (2.6) to hold. Thus, the main additional condition needed for the Lipschitz continuity of the optimal solution (relation (2.15)) is the SSOSC (2.11).
b. Result 2b of the theorem implies that the variation in $\mathbf{u}^*$, i.e., the entity denoted by symbol $\tilde{\mathbf{u}}(\eta)$, is (only) a *local* optimal solution of NP($\tilde{\boldsymbol{\theta}}(\eta)$). In some cases, the said entity can also be a *global* optimal solution of NP($\tilde{\boldsymbol{\theta}}(\eta)$), as seen in Example 2.4 later. However, in general, it need not be a global optimal solution, as can be seen from Example 2.3. Thus, result (2.15) (Lipschitz continuity of $\tilde{\mathbf{u}}(\eta)$) is applicable *only* for $\tilde{\mathbf{u}}(\eta)$ as a *local* optimal solution of NP($\tilde{\boldsymbol{\theta}}(\eta)$).
   Since, we had remarked earlier that the symbol $\tilde{\mathbf{u}}$ would be used to denote a perturbed global optimal solution of NP($\boldsymbol{\theta}$), its use in the theorem above is a slight abuse of notation. Later, we will assume condition (2.21) to remove this ambiguity.

Since the conditions of this theorem will be used subsequently, it is interesting to see implications of these conditions using some simple examples. The first (counter-)example demonstrates the necessity of SSOSC for Lipschitz continuity of a local optimal solution.[3]

Example 2.1

$$\min_u \quad J(u,\theta) = \{\tanh(u-1)\}^2 + (1+\theta)\{\tanh(u+1)\}^2$$

$$\theta_0 = -0.576, \quad \xi^\theta = 1.$$

It is easy to verify that $J(u,\theta)$ above satisfies the differentiability assumption (2.3). Since the problem has no constraints, the LICQ condition (2.5) is satisfied everywhere, whereas the NCO (2.6) reduce to $\frac{\partial J}{\partial u}(u^*,\theta_0) = 0$ and the SSOSC (2.11) reduces to $\frac{\partial^2 J}{\partial u^2}(u^*,\theta_0) > 0$.

In Figure 2.1, plots of J, $\frac{\partial J}{\partial u}$ and $\frac{\partial^2 J}{\partial u^2}$ at $\theta = \theta_0$ are shown.

It can be seen that the NCO $\frac{\partial J}{\partial u} = 0$ is satisfied at two points marked u_A^* and u_B^*, but the SSOSC is *not* satisfied at u_A^* while it is satisfied at u_B^*. Strictly speaking, the former is only a stationary point while the latter is a local (and, in this case, global) minimum.

[3] The author is grateful to Prof. Nicolas Petit for providing the interesting problem.

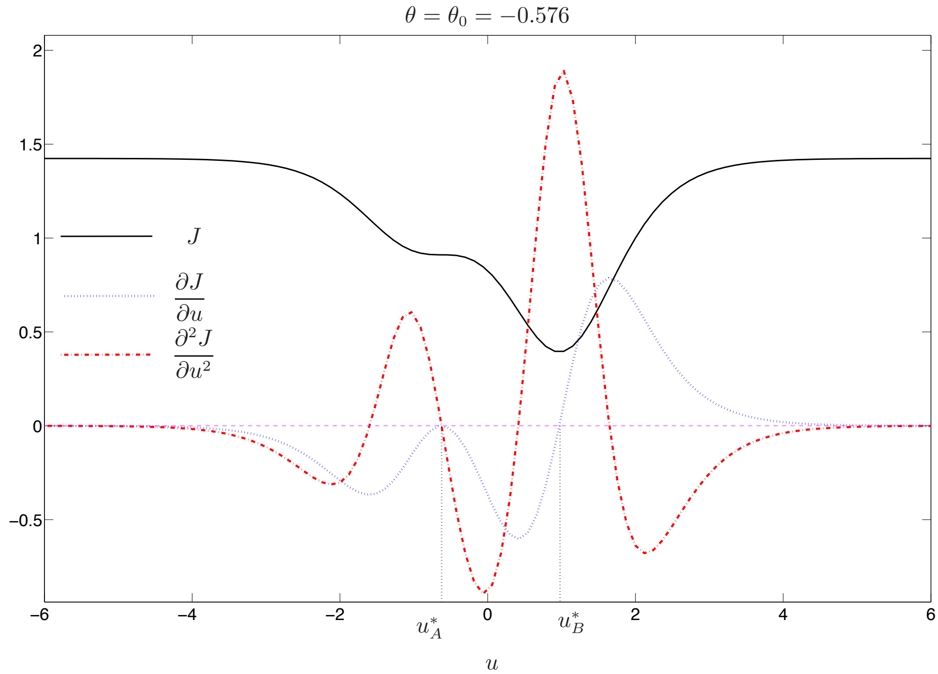

Figure 2.1 Plots of J, $\dfrac{\partial J}{\partial u}$ and $\dfrac{\partial^2 J}{\partial u^2}$ for Example 2.1 at $\theta = \theta_0$.

Next, in Figure 2.2, plots of $J(u, \theta_0 + \eta)$ are shown for three different values of $\eta \in \mathcal{B}_0$. It is clear from it that there is only one minimum for $\eta \leq 0$, but two (local) minima for $\eta > 0$, the *new* minimum arising close to u_A^*. Naturally, the results of Theorem 2.1 cannot hold at u_A^*. On the other hand, the local minimum u_B^*, at which the SSOSC holds, is Lipschitz continuous with respect to η as can seen from Figure 2.3.

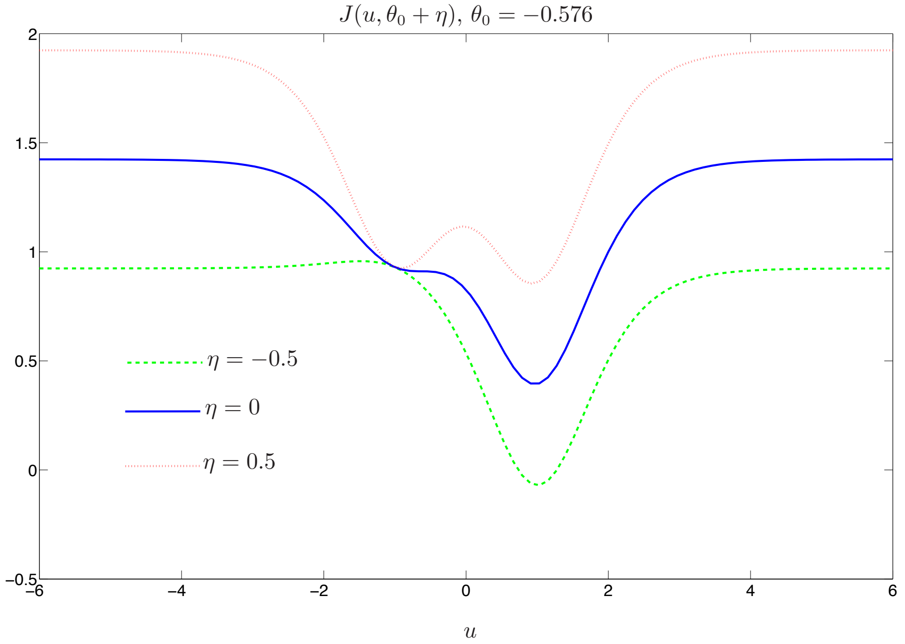

Figure 2.2 Plots of $J(u, \theta(\eta))$ in Example 2.1 for three different values of η.

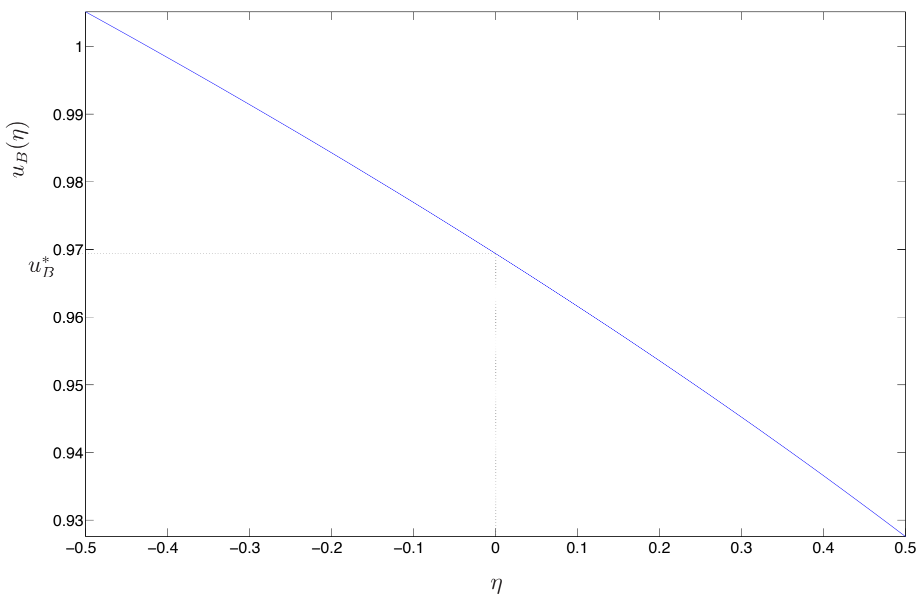

Figure 2.3 Plot of the variation of the local optimal solution u_B^* with respect to η in Example 2.1.

The second (counter-)example to demonstrate the necessity of SSOSC is the following parametric Linear Program (pLP):

Example 2.2

$$
\begin{aligned}
\min_{\mathbf{u}=\left[x_1\ x_2\right]} \quad & J(\mathbf{u},\theta) = x_1 + \theta x_2, \quad \theta_0 = 1, \quad \xi^{\theta} = 1 \\
s.t. \quad & G_1: \quad x_1 + x_2 \geq 1, \\
& G_2: \quad x_1 \geq 0, \\
& G_3: \quad x_2 \geq 0.
\end{aligned}
\tag{2.16}
$$

The feasibility region for this problem is shown in Figure 2.4. For $\eta = 0$, each

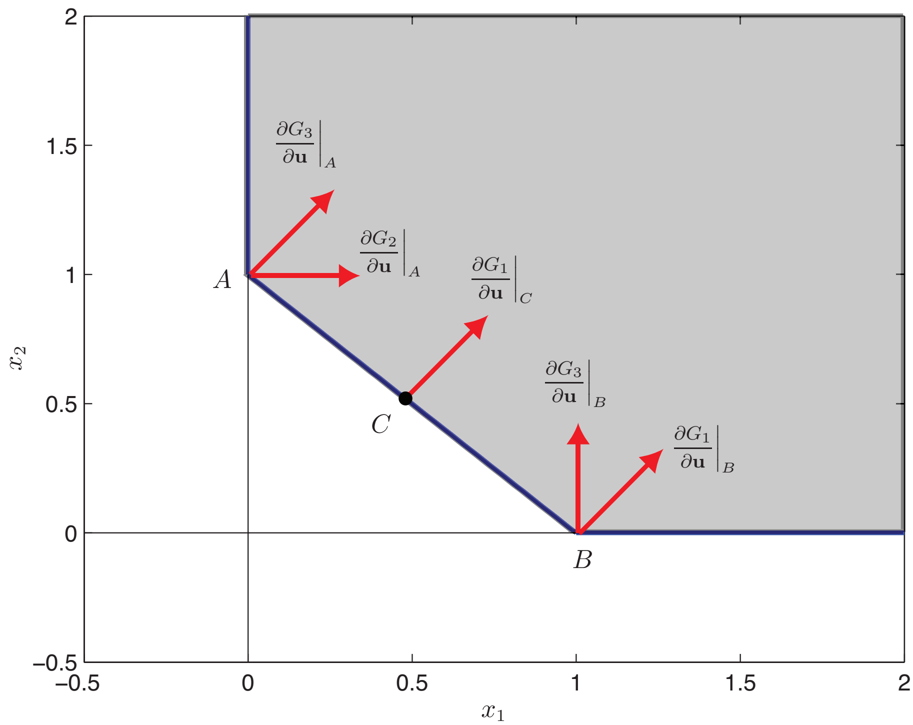

Figure 2.4 The shaded open region is the feasibility region for Problem (2.16).

point on the entire segment AB is an optimal solution.

Consider the optimal solutions A, B and C shown in Figure 2.4. The active sets at these points are $\mathcal{A}_A^* = \{1, 2\}$, $\mathcal{A}_B^* = \{1, 3\}$, $\mathcal{A}_C^* = \{1\}$. Gradients of active constraints with respect to $\mathbf{u}$ at these three points are also shown in Figure 2.4. It can be easily verified that the LICQ is satisfied at each point of AB.
On the other hand, since the cost and constraints are linear in inputs, the SSOSC *cannot* be satisfied at any optimal solution. As a consequence, the variation in optimal solutions is *not* Lipschitz continuous as can be seen from Figure 2.5.

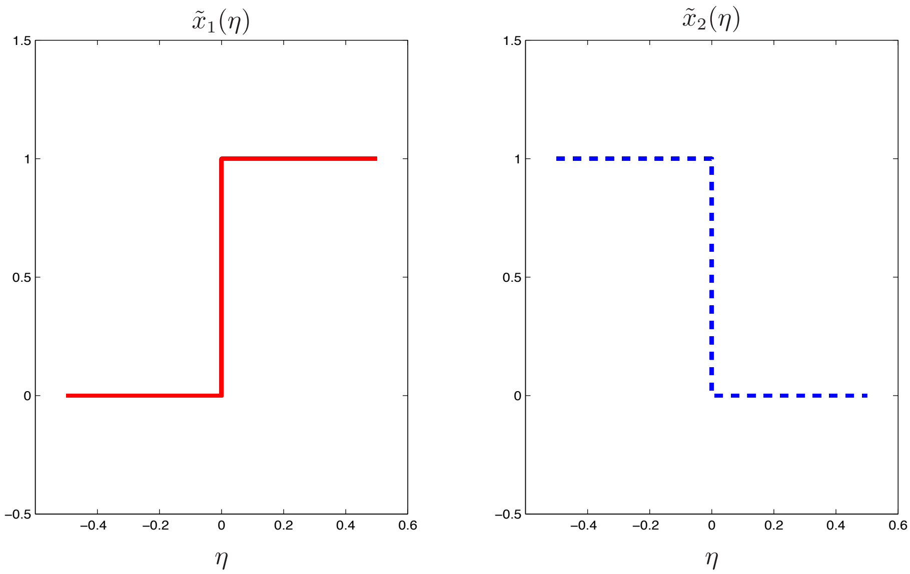

Figure 2.5 The variation in the optimal solution of Problem (2.16) with respect to $\eta \in [-0.5, 0.5]$. $\tilde{\mathbf{u}}(\eta) = [\tilde{x}_1(\eta) \quad \tilde{x}_2(\eta)]$ denotes the optimal solution at $\theta = \theta_0 + \eta$.

The next example shows that the results of Theorem 2.1 are valid only for local optimal solutions (Remark 2b after the said theorem).

Example 2.3

$$\min_u \quad J(u, \theta) = \{\tanh(u-1)\}^2 + (1+\theta)\{\tanh(u+1)\}^2$$
$$\theta_0 = 0, \quad \xi^\theta = 1.$$

In this case, it can be seen that the SSOSC $\left(\dfrac{\partial^2 J}{\partial u^2}(u^*, \theta_0) > 0\right)$ is satisfied at both (local) minimum solutions marked u_1^* and u_2^* in Figure 2.6. Hence, as a result of Theorem 2.1, the corresponding perturbed local optima $\tilde{u}_1(\eta)$ and $\tilde{u}_2(\eta)$ are

Lipschitz continuous with respect to η in a neighborhood of $\eta = 0$, as can be seen from Figure 2.7.

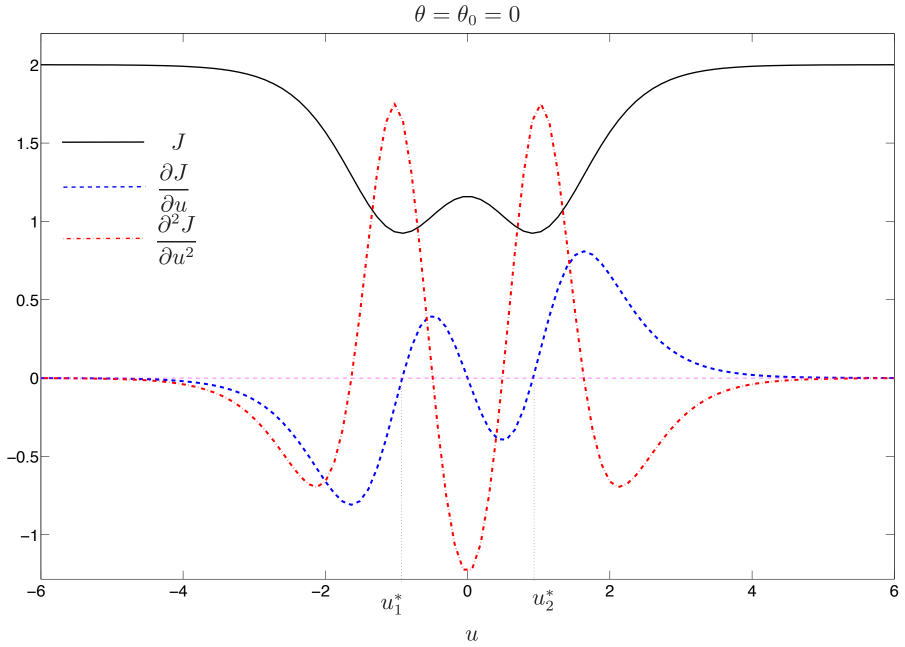

Figure 2.6 Plots of $J, \dfrac{\partial J}{\partial u}$ and $\dfrac{\partial^2 J}{\partial u^2}$ for Example 2.3 at $\theta = \theta_0$.

We can also see that both local minima are also global minima at $\eta = 0$. However, as η crosses 0 from a negative to a positive value, the global minimum solution, say $\tilde{u}^g(\eta)$, changes abruptly from a positive value to a negative value. This can be seen from Figures 2.8 and 2.9.

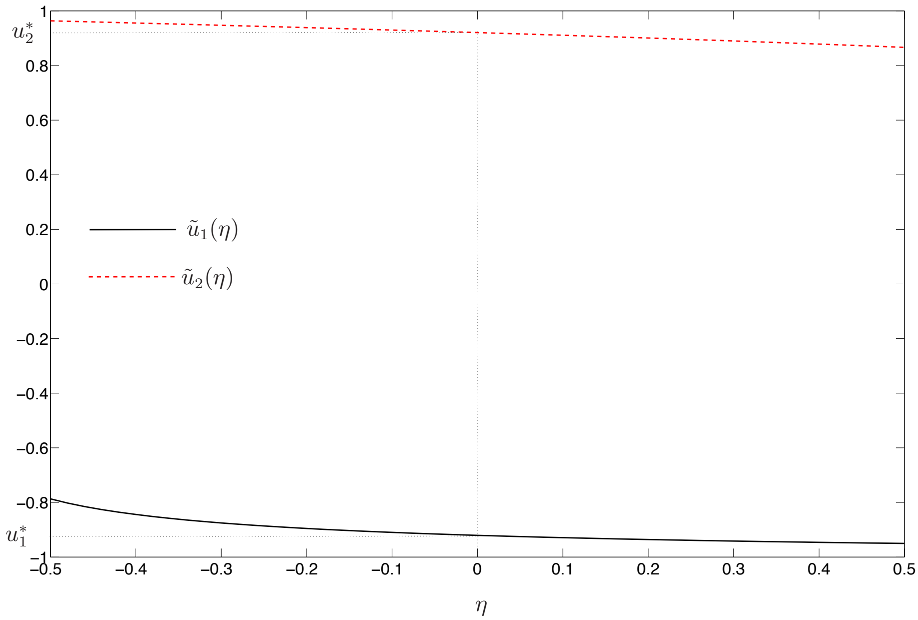

Figure 2.7 Variation of the (local) optimal solutions u_1^* and u_2^* in Example 2.3 with respect to η.

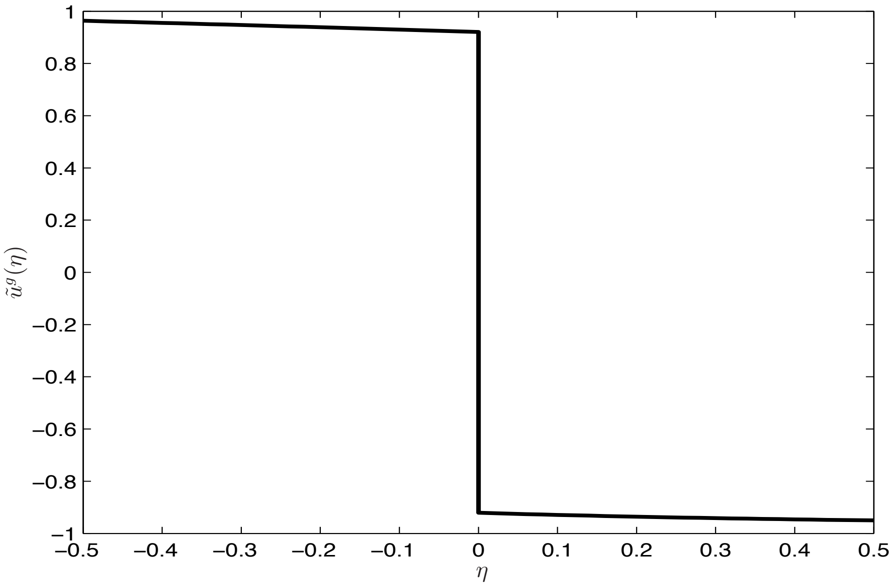

Figure 2.8 Variation of the global optimal solution of Example 2.3 with respect to η.

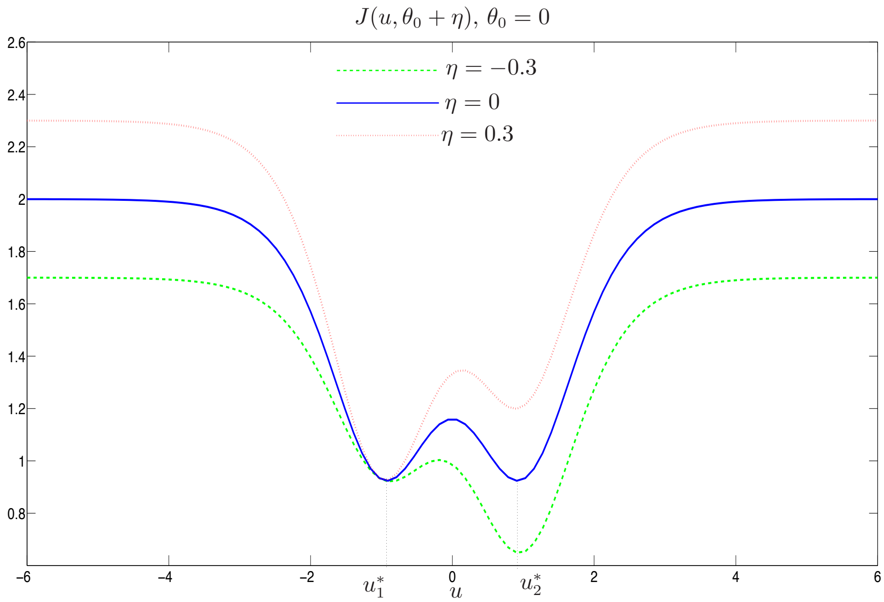

Figure 2.9 Plots of $J(u, \theta(\eta))$ in Example 2.3 for three different values of η.

Based on the result of Theorem 2.1, let us now define the interval $\mathcal{B}_0$ as follows:

$$\mathcal{B}_0 := [-\eta_0, \eta_0] \bigcap [-\eta_1, \eta_1], \tag{2.17}$$

for some η_1 chosen such that $0 < \eta_1 \ll 1$ and where η_0 is as defined in result 2d of Theorem 2.1 for $\mathbf{u}^*$ under consideration. Hence, one can also write

$$\begin{aligned} \mathcal{B}_0 := [-\eta_0, \eta_0], &\quad \text{if} \quad \eta_0 < \eta_1 \ll 1, \\ [-\eta_1, \eta_1], &\quad \text{if} \quad \eta_0 > \eta_1. \end{aligned} \tag{2.18}$$

A *schematic* representation of $\mathcal{B}_0$ is shown in Figure 2.10.

Definition (2.17) simply ensures that $\mathcal{B}_0$ is a *small* interval (length of $\mathcal{B}_0 \ll 1$) around 0 on which the relations (2.15) hold, if the conditions of Theorem 2.1 hold at the optimum solution $\mathbf{u}^*$.

Theorem 3 in [60] further proves the existence of the directional derivatives of $\tilde{\mathbf{u}}(\eta)$ and $\tilde{\boldsymbol{\lambda}}(\eta)$ with respect to η for a given the direction of parametric perturbations $\boldsymbol{\xi}^{\boldsymbol{\theta}}$, under conditions of Theorem (2.1) and shows that these derivatives are (unique) solutions of an associated system of equalities and inequalities.

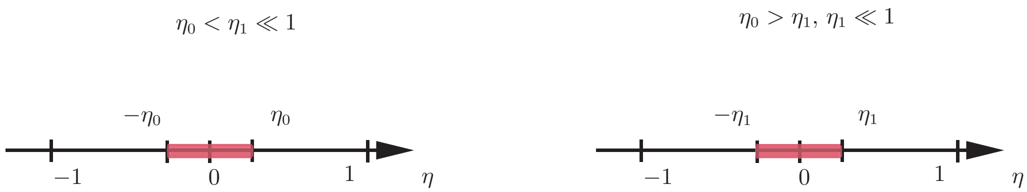

Figure 2.10 Schematic representation of $\mathcal{B}_0$ (the shaded band).

3. Corollary 2.3 in [21] proves the same result as Theorem (2.1) above. Under similar assumptions, viz. LICQ and SSOSC, Theorem 2.2 (in combination with Proposition 2.1) in [20] also proves the Lipschitz continuity of the optimal inputs $\tilde{\mathbf{u}}(\eta)$ with respect to parameters.
4. Similar, but less general, result on Lipschitz continuity of optimal solutions of NP($\boldsymbol{\theta}$) using SSOSC is also proved in Theorem 4.3 [43] assuming a restriction on $\boldsymbol{\xi}^{\boldsymbol{\theta}}$, but under regularity assumptions somewhat less restrictive than LICQ. Theorem 5.1 in [43] also proves the existence of directional derivative of $\tilde{\mathbf{u}}(\eta)$ with respect to η under certain restrictions on $\boldsymbol{\xi}^{\boldsymbol{\theta}}$.

The following two results deal directly with the stronger property of (one-sided) differentiability of $(\tilde{\mathbf{u}}(\eta), \tilde{\boldsymbol{\lambda}}(\eta))$ and so, automatically, imply (one-sided) Lipschitz continuity of the same.

1. Theorem 3.3.4 in [53] proves the piecewise differentiability of $\tilde{\mathbf{u}}(\eta)$ and $\tilde{\boldsymbol{\lambda}}(\eta)$ under similar assumptions, viz., (2.3), LICQ, SSOSC and an additional technical condition, which restricts the number of changes in the active set of NP($\boldsymbol{\theta}$) to be finite as η varies over $\mathcal{B}_0^+$, a small interval on the right(positive) side of 0. It shows that the right-hand derivatives of $\tilde{\mathbf{u}}(\eta)$ and $\tilde{\boldsymbol{\lambda}}(\eta)$ with respect to η at $\eta = 0$, i.e.,

$$\begin{aligned} \dot{\mathbf{u}}(0_+) &:= \lim_{\eta \to 0_+} \frac{\tilde{\mathbf{u}}(\eta) - \mathbf{u}^*}{\eta}, \\ \dot{\boldsymbol{\lambda}}(0_+) &:= \lim_{\eta \to 0_+} \frac{\tilde{\boldsymbol{\lambda}}(\eta) - \boldsymbol{\lambda}^*}{\eta}, \end{aligned} \tag{2.19}$$

are, respectively, the (unique) solutions ($\mathbf{w}^*$) and associated Lagrange multipliers ($\boldsymbol{\mu}^*$) of the following quadratic program:

$$\begin{aligned}
\min_{\mathbf{w}\in\mathbb{R}^{n_\mathbf{u}}} \quad & \frac{1}{2}\mathbf{w}^T \frac{\partial^2 \mathcal{L}}{\partial \mathbf{u}^2}(\mathbf{u}^*, \boldsymbol{\lambda}^*, \boldsymbol{\theta}_0)\mathbf{w} + \frac{\partial \mathcal{L}}{\partial \mathbf{u}\partial \eta}(\mathbf{u}^*, \boldsymbol{\lambda}^*, \boldsymbol{\theta}_0)\mathbf{w}, \\
\text{s.t.} \quad & \frac{\partial \mathbf{G}_{\mathcal{I}^*}}{\partial \eta}(\mathbf{u}^*, \boldsymbol{\theta}_0) + \frac{\partial \mathbf{G}_{\mathcal{I}^*}}{\partial \mathbf{u}}(\mathbf{u}^*, \boldsymbol{\theta}_0)\mathbf{w} = 0, \\
& \frac{\partial \mathbf{G}_{\mathcal{J}^*}}{\partial \eta}(\mathbf{u}^*, \boldsymbol{\theta}_0) + \frac{\partial \mathbf{G}_{\mathcal{J}^*}}{\partial \mathbf{u}}(\mathbf{u}^*, \boldsymbol{\theta}_0)\mathbf{w} \leq 0,
\end{aligned} \tag{2.20}$$

where $\mathcal{L}$ is the same as in (2.12).

Remark: For a given direction $\boldsymbol{\xi}^{\boldsymbol{\theta}}$, the directional derivatives in Theorem 3 of [60] mentioned above are the same as (2.19). It is indeed easy to check that the system of equalities and inequalities satisfied by these derivatives in [60] is the same as the KKT NCO for the quadratic program (2.20).

2. Theorem 3.4 in [24] is very similar to Theorem 3.3.4 in [53] in that it proves the piecewise differentiability of $(\tilde{\mathbf{u}}(\eta), \tilde{\boldsymbol{\lambda}}(\eta))$ in terms of the (unique) solutions of the same quadratic program (2.20) under similar assumptions (2.3), LICQ, SSOSC and an additional technical assumption of strict complementarity for the quadratic program (2.20).

   As mentioned in Remark 2 following the above theorem in [24], the purpose of the technical condition is to guarantee the constancy of the active set of NP($\boldsymbol{\theta}$) for small variations in η and thus, it is somewhat similar in spirit to the technical condition in Theorem 3.3.4 in [53].

   [24] also mentions an additional technical condition, viz., strict complementarity for an *inverted* version of the quadratic program (2.20), for existence of two-sided derivatives of $(\tilde{\mathbf{u}}(\eta), \tilde{\boldsymbol{\lambda}}(\eta))$.

Since, as mentioned at the beginning of the survey above, we would like NP($\boldsymbol{\theta}$) to be regular enough as to have Lipschitz continuous optimal solutions, we would henceforth impose conditions of Theorem 2.1, viz., (2.3), LICQ (2.5) and SSOSC (2.11) on NP($\boldsymbol{\theta}$), unless stated otherwise.

Let us also recall that we are interested in global optimum solutions $\mathbf{u}^*$ and $\tilde{\mathbf{u}}$ whereas Theorem 2.1 (point *b.*) ensures the Lipschitz continuity only of local optimum solutions. In other words, the theorem only ensures that the entity denoted by the symbol $\tilde{\mathbf{u}}(\eta)$, which satisfies the relation (2.15), is a *local* optimal solution of the perturbed problem NP($\tilde{\boldsymbol{\theta}}(\eta)$) for each $\eta \in \mathcal{B}_0$. Hence, as mentioned in Remark 2b after the said theorem, it is necessary to be more precise while using the notation $\tilde{\mathbf{u}}(\eta)$ for a global optimal solution of NP($\tilde{\boldsymbol{\theta}}(\eta)$).

For example, as seen in Figure 2.8 of Example (2.1), in some problems, there is a possibility that one local optimum solution takes over the other as the global optimum as η changes, even if conditions of Theorem 2.1 hold at each local solution. That is, there is a possibility of discontinuity in variation of global optimum solution with respect to η. Hence, to avoid such scenarios and to make sure that the use of notation $\tilde{\mathbf{u}}(\eta)$ is not ambiguous, we make the following additional assumption:

Assumption 2.4
For given pNLP (2.2) *satisfying the conditions of Theorem 2.1, viz.,* (2.3), *LICQ* (2.5) *and SSOSC* (2.11), *and for corresponding $\mathcal{B}_0$ as defined by* (2.17),

$$\begin{aligned}&\textit{the (local) variation in } \mathbf{u}^* \textit{ given by (2.15), i.e., } \tilde{\mathbf{u}}(\eta),\\ &\textit{is a global minimum solution for the corresponding}\\ &\textit{perturbed problem NP}(\tilde{\boldsymbol{\theta}}(\eta)) \textit{ for each } \eta \in \mathcal{B}_0.\end{aligned} \tag{2.21}$$

Since $\tilde{\mathbf{u}}(\eta)$ is defined by the Lipschitz continuity relation (2.15) and since it is also a global optimal solution of NP($\boldsymbol{\theta}$) over $\mathcal{B}_0$ by assumption (2.21), the said global optimal solution itself is Lipschitz continuous over $\mathcal{B}_0$. Hence, for the said *global* optimal solution $\tilde{\mathbf{u}}(\eta)$, we can write:

$$\tilde{\mathbf{u}}(\eta) - \mathbf{u}^* = O(\eta), \quad \eta \in \mathcal{B}_0. \tag{2.22}$$

This is illustrated in the following example:

Example 2.4

$$\begin{aligned}\min_u \quad & J(u,\theta) = \{\tanh(u-1)\}^2 + (1+\theta)\{\tanh(u+1)\}^2\\ & \theta_0 = -1.5, \quad \xi^\theta = 1, \mathcal{B}_0 = [-0.5, 0.5].\end{aligned}$$

In this example, the variation in u^* can be seen to be the global optimal solution, say $\tilde{u}^g(\eta)$, of NP($\tilde{\theta}(\eta)$) for each $\eta \in \mathcal{B}_0 = [-0.5, 0.5]$ (Figure 2.11). Thus, assumption (2.21) is satisfied in this example. As in Examples 2.1 and 2.3, it is easy to verify that the conditions of Theorem 2.1 hold at $u^* = \tilde{u}^g(0)$, i.e., the nominal global optimal solution.

Hence, $\tilde{u}^g(\eta)$ can be seen to be Lipschitz continuous with respect η over $\mathcal{B}_0$ (Figure 2.12).

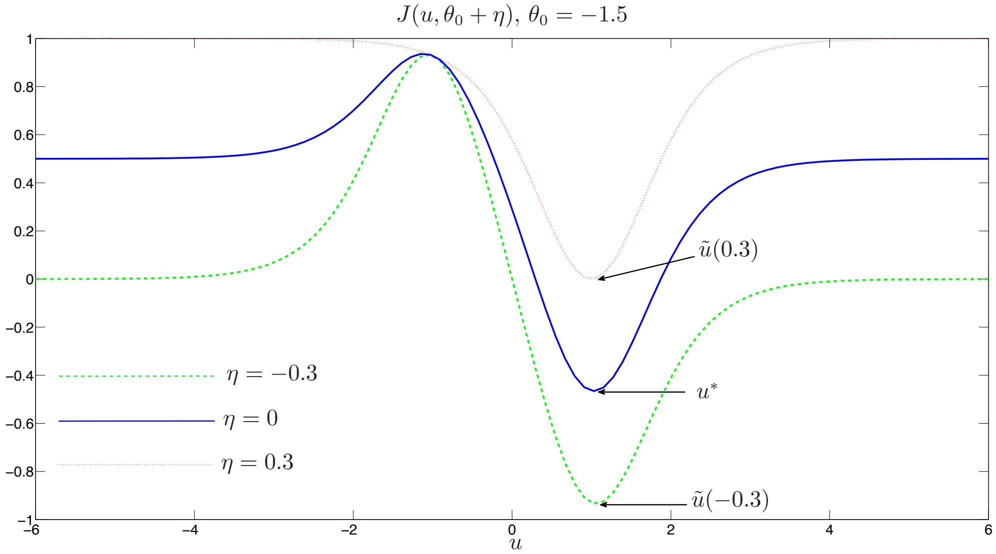

Figure 2.11 Plots of $J(u, \theta(\eta))$ in Example 2.4 for three different values of η. $\tilde{u}(\eta)$ denotes the local variation in u^* with respect to η (as in (2.15)). It is also a global minimum for $J(u, \theta(\eta))$ for each $\eta \in \mathcal{B}_0$, thus satisfying condition (2.21).

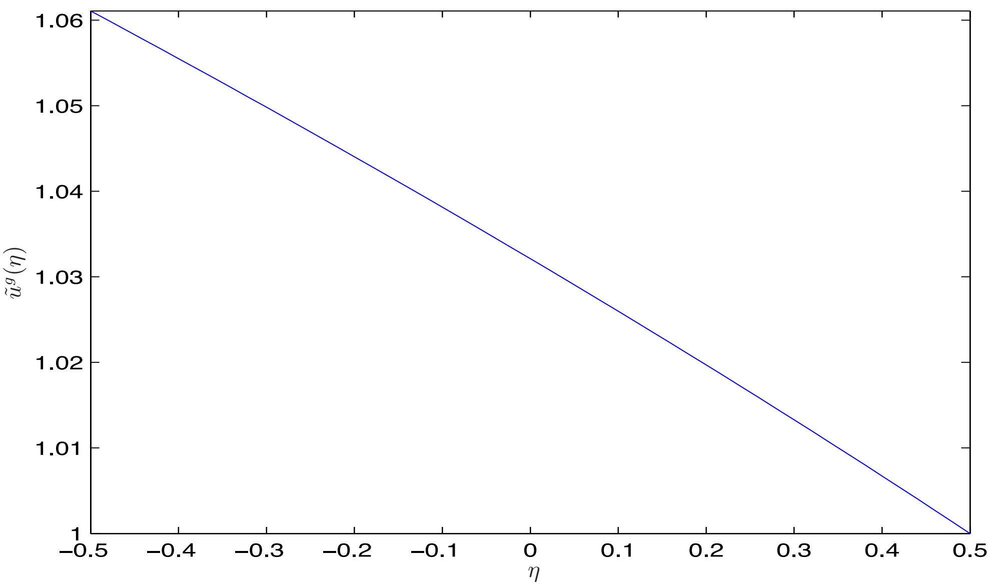

Figure 2.12 Variation of the global optimal solution of Example 2.4 with respect to η.

As already remarked earlier, an example in which assumption (2.21) is not satisfied is Example 2.3 at $\eta = 0$ (Figures 2.7 and 2.9). In this example, $\tilde{u}_2(\eta)$ is not a global optimal solution for $\eta \in (0, 0.5]$ while $\tilde{u}_1(\eta)$ is not a global optimal solution for $\eta \in [-0.5, 0)$, although both are local optimal solutions and are local variations of u_1^* and u_2^* respectively. Hence, the variation in the global optimal solution is not Lipschitz continuous at $\eta = 0$ (Figure 2.8).

Equipped with suitable regularity conditions on the underlying pNLP, we are now ready to demonstrate the general approach for analysis of optimality loss using the following theorem. It will also clarify the exact research question we will be dealing with.

Theorem 2.2 (Optimality Loss due to No Adaptation)
Consider the pNLP (2.2) *satisfying* (2.3)*, for which conditions* (2.5) *(LICQ) and* (2.11) *(SSOSC) and* (2.21) *hold at the nominal optimal input* $\mathbf{u}^*$*. If* $\mathbf{u}^*$ *remains feasible under parametric perturbations* (2.8)*, then the optimality loss without adaptation is* $O(\eta)$*.*

Proof: Using the differentiability properties of J with respect to $\mathbf{u}$, it is possible to consider the first-order Taylor series expansion of $J(\mathbf{u}, \tilde{\boldsymbol{\theta}})$ around $(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}})$:

$$\delta J(\mathbf{u}) = \frac{\partial J}{\partial \mathbf{u}}(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}}) \{\mathbf{u} - \tilde{\mathbf{u}}\} + O(||\mathbf{u} - \tilde{\mathbf{u}}||^2), \tag{2.23}$$

where $||\ ||$ denotes the Euclidean norm on $\mathbb{R}^{n_\mathbf{u}}$. From the NCO (2.6) written for the perturbed optimal solution and (2.9), one can write:

$$\frac{\partial J}{\partial \mathbf{u}}(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}}) + \tilde{\boldsymbol{\lambda}}_{\tilde{\mathcal{I}}}^T \frac{\partial \mathbf{G}_{\tilde{\mathcal{I}}}}{\partial \mathbf{u}}(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}}) = \mathbf{0}. \tag{2.24}$$

Using (2.24) in (2.23), gives:

$$\delta J(\mathbf{u}) = -\tilde{\boldsymbol{\lambda}}_{\tilde{\mathcal{I}}}^T \frac{\partial \mathbf{G}_{\tilde{\mathcal{I}}}}{\partial \mathbf{u}}(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}}) \{\mathbf{u} - \tilde{\mathbf{u}}\} + O(||\mathbf{u} - \tilde{\mathbf{u}}||^2). \tag{2.25}$$

Without adaptation, i.e. when $\mathbf{u} = \mathbf{u}^*$, following results of Theorem 2.1 and assumption (2.21), we have $\mathbf{u}^* - \tilde{\mathbf{u}} = O(\eta)$ (as in (2.22)).

This implies $\delta J(\mathbf{u}^*) = O(\eta)$. □

Remarks:

1. Note that for a general pNLP (2.2), there is no guarantee that the nominal optimal solution will remain feasible after parametric perturbations, in which case, adaptation becomes *necessary*. The theorem above says that, when input adaptation is *not necessary* to maintain *feasibility*, the optimality loss due to no adaptation is of the order of $O(\eta)$.
2. Instead of assuming (2.21), by assuming that the conditions of Theorem 2.1 hold at *each* global optimal solution $\mathbf{u}_i^*$ of pNLP (2.2), the same result as Theorem 2.2 can be obtained.[4]

   Under these conditions, all corresponding perturbed local minimum solutions $\tilde{\mathbf{u}}_i(\eta)$ are Lipschitz continuous with respect to η. Hence, due to assumption (2.3), the corresponding cost values $J(\tilde{\mathbf{u}}_i(\eta), \tilde{\boldsymbol{\theta}}(\eta))$ are also Lipschitz continuous. Let $J^\circ(\eta)$ denote the perturbed global optimal cost, i.e., $J(\tilde{\mathbf{u}}^g(\eta), \tilde{\boldsymbol{\theta}}(\eta))$ at any perturbed global optimal input $\tilde{\mathbf{u}}^g(\eta)$. Hence, by definition

$$\begin{aligned} J^\circ(\eta) &= \min_i \{\text{cost due to each perturbed local minimum } \tilde{\mathbf{u}}_i(\eta)\}, \\ &= \min_i \{J(\tilde{\mathbf{u}}_k(\eta), \tilde{\boldsymbol{\theta}}(\eta))\}. \end{aligned}$$

   Hence, $J^\circ(\eta)$ is Lipschitz continuous, since the minimum of a set of Lipschitz continuous functions is itself Lipschitz continuous. Thus, $J^\circ(\eta) - J(\mathbf{u}_i^*, \boldsymbol{\theta}_0) = O(\eta)$. Now, optimality loss due to (non adaptation of) any nominal optimal input $\mathbf{u}_k^*$, assuming it remains feasible, is

$$\begin{aligned} \delta J(\mathbf{u}_k^*) &= J(\mathbf{u}_k^*, \tilde{\boldsymbol{\theta}}(\eta)) - J^\circ(\eta), \\ &= J(\mathbf{u}_k^*, \tilde{\boldsymbol{\theta}}(\eta)) - J(\mathbf{u}_k^*, \boldsymbol{\theta}_0) + J(\mathbf{u}_k^*, \boldsymbol{\theta}_0) - J^\circ(\eta), \\ &= \frac{\partial J}{\partial \mathbf{u}}(\mathbf{u}^*, \boldsymbol{\theta}_0)\, \eta\, \boldsymbol{\xi}^{\boldsymbol{\theta}} + O(\eta^2) + O(\eta), \\ &= O(\eta). \quad \square \end{aligned} \tag{2.26}$$

   Note that the importance of derivation (2.26) is that it shows that the *Lipschitz continuity of global optimal cost* ($J^\circ(\eta)$) is sufficient to obtain the result of optimality loss due to no adaptation of order $O(\eta)$ and that *Lipschitz continuity of global optimal solution* (2.22) is *not* necessary. In other words, the assumption (2.21) is *not necessary* for the above result to hold.

[4] The author is grateful to Prof. Dr. Moritz Diehl for pointing out the possibility of such a result.

This can be illustrated using Example (2.3) seen earlier, in which the global optimal solution is not Lipschitz continuous on $\mathcal{B}_0 = [-0.5, 0.5]$ (Figures 2.8 and 2.9). For this example, the variation of global minimum cost $J^\circ(\eta)$ with respect to η is plotted in Figure 2.13 below. Evidently, $J^\circ(\eta)$ is Lipschitz continuous over $\mathcal{B}_0$.

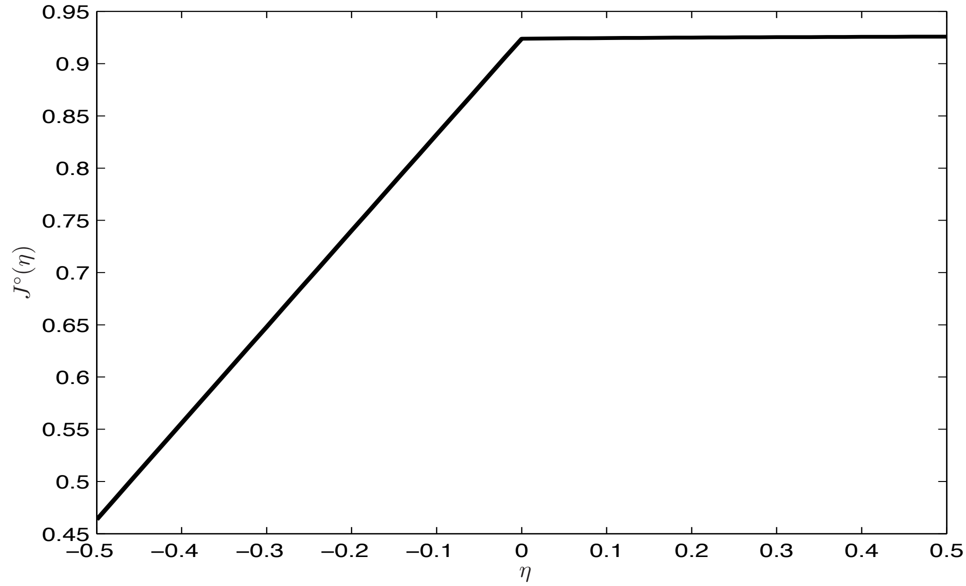

Figure 2.13 Variation of the (global) minimum *cost* $J^\circ(\eta)$ in Example 2.3 with respect to η.

In summary, the result (2.26) is applicable even when the global minimizer changes discontinuously with respect to η and so is more general than that of Theorem 2.2.

2.3.3.2 Optimality Loss Analysis due to No Adaptation under Weaker Conditions

Before moving on to optimality loss analysis due to adaptation, it would be interesting to discuss a stronger version of Theorem 2.2 that can be proved by assuming weaker conditions on NP($\boldsymbol{\theta}$).[5]

[5] The author is grateful to Prof. Dr. Moritz Diehl for pointing out the possibility of such a result.

Recall from Remark 2 after Theorem 2.2 of the last subsection that to obtain the result of optimality loss due to no adaptation of order $O(\eta)$, what is more important is the *Lipschitz continuity of global optimal cost* ($J^\circ(\eta) = J(\tilde{\mathbf{u}}(\eta), \tilde{\boldsymbol{\theta}}(\eta))$) and *not* that of *global optimal solution*. Also recall from Theorem 2.1 and the illustrative Examples 2.1 and 2.2 that the role of the assumption of SSOSC (2.11) was to ensure the Lipschitz continuity of a given *(local) optimal solution*.

Combining these observations, it might be further asked whether even the strong condition of SSOSC is *necessary* to ensure the Lipschitz continuity of *optimal cost*. It turns out that it is not. For example, consider again the pLP in Example 2.2 in which the SSOSC *cannot* be satisfied at any optimal solution. However, the variation of *optimal cost* ($J^\circ(\eta)$) with respect to η for this example can be seen to be Lipschitz continuous (Figure 2.14 below).

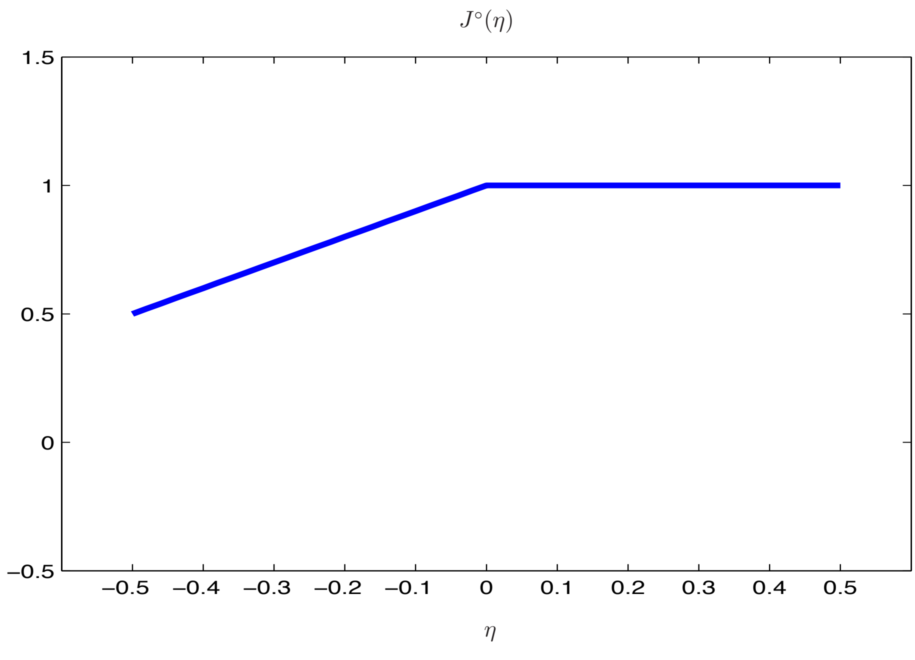

Figure 2.14 Variation of the *optimal cost* $J^\circ(\eta)$ in Example 2.16 with respect to η. The SSOSC *cannot* hold at any optimal solution of this example.

There exist a number of results in the literature on sensitivity analysis that ensure Lipschitz continuity of the *optimal cost* $J^\circ(\eta)$ with respect to parametric perturbations without assuming SSOSC. Following is a short list of such results relevant to pNLP (2.2). Almost all the results assume some basic *regularity* conditions on the feasible set mapping, viz.,

$$\mathcal{F}(\eta) := \left\{ \mathbf{u} \in \mathrm{I\!R}^{n_\mathbf{u}} \;\middle|\; G_i(\mathbf{u}, \tilde{\boldsymbol{\theta}}(\eta)) \le 0, \quad i = 1, \ldots, n_\mathbf{G} \right\}. \tag{2.27}$$

Most of the said results are applicable to more general pNLPs that involve equality constraints also.

1. Theorem 5.1 in [42] proves the Lipschitz continuity of optimal cost under the Mangasarian-Fromovitz constraint qualification (MFCQ) [5, 88]:

$$\exists \text{ a direction } \mathbf{d} \in \mathrm{I\!R}^{n_\mathbf{u}} \text{ such that } \mathbf{d}^T \frac{\partial \mathbf{G}_i}{\partial \mathbf{u}}(\mathbf{u}^*, \boldsymbol{\theta}_0) < 0, \quad i \in \mathcal{A}^*. \tag{2.28}$$

   We reproduce the theorem below in our notation.

   Theorem 2.3 (Theorem 5.1 of [42])
   For pNLP (2.2), *suppose* $\mathcal{F}(\eta)$ *is nonempty for* $\eta \in \mathcal{B}_0$, $\mathcal{F}(\eta)$ *is uniformly compact near* $\eta = 0$ *and MFCQ holds at* each *nominal optimal solution* $\mathbf{u}^*$, *then the optimal cost is locally Lipschitz continuous near* $\eta = 0$.

   Remarks:

   a. The theorem admits the possibility of multiple optimal solutions $\mathbf{u}^*$. Thus, the optimal cost is Lipschitz continuous despite the multiplicity of optimal solutions under the assumed conditions.
   b. It is well-known that MFCQ is a weaker condition than LICQ [5, 88]. Further, in contrast to Theorem 2.1, there are no second-order conditions in the theorem above and so the functions f, G_i can be $\mathcal{C}^1$, rather than $\mathcal{C}^2$, in their arguments. Thus, the conditions of the theorem above are much weaker than that of Theorem 2.1.
   c. The uniform compactness of the feasible set mapping $\mathcal{F}(\eta)$ is a technical regularity condition, which ensures that for small variations in η, any sequence of feasible $\mathbf{u}$ converges within the closure of $\mathcal{F}(\eta)$; for more details, see [42, 56].

2. Corollary 4.1 in [44] proves the directional differentiability (and by implication Lipschitz continuity) of optimal cost with respect to η for a given $\boldsymbol{\xi}^{\boldsymbol{\theta}}$ under conditions of Theorem 2.3 and the additional condition of WSOSC at any one nominal optimal solution $(\mathbf{u}^*, \boldsymbol{\lambda}^*)$. The last condition, of course, necessitates f, G_i to be at least $\mathcal{C}^2$ in their arguments.

3. Corollary 1 (in view of Definition 1) in [78] is essentially the same result as Theorem (2.3) above.

For the special type of pNLPs having only the so called *right hand side (RHS) perturbations*, results on Lipschitz-continuity of optimal cost are derived in a number of publications. For the sake of completeness, we list a few of these results below: Theorem 4.1 and its corollaries in [105], Theorem 3.3 in [45], Theorem 2 in [41], Theorem 3.2 of [48] and Theorem 3.2 of [43].

As remarked in [43] and [44], a general pNLP (2.2) can always be transformed into a problem with RHS perturbations (with equality constraints). Based on the equivalence of the two formulations, the results on Lipschitz continuity of optimal cost for the latter can be easily extended to the former.

Earlier results on Lipschitz continuity of optimal cost for a special case of the aforementioned problems in which there is no parametric perturbation in cost are Theorem 3 of [38] and Theorem 1 of [46].

Under conditions of Theorem 2.3 above, it is easy to show that the optimality loss due to no adaptation, if it remains feasible, is $O(\eta)$:

Theorem 2.4
(Optimality Loss due to No Adaptation under Weak Conditions)
For pNLP (2.2)*, suppose the feasible set mapping $\mathcal{F}(\eta)$ is nonempty for $\eta \in \mathcal{B}_0$, $\mathcal{F}(\eta)$ is uniformly compact near $\eta = 0$ and MFCQ holds at* each *nominal optimal solution. If any nominal optimal solution $\mathbf{u}^*$ remains feasible under parametric perturbations* (2.8)*, then the optimality loss without adaptation is $O(\eta)$.*

Proof: The derivation is similar to (2.26). Starting from the general expression for optimality loss (2.10), we get

$$\begin{aligned}
\delta J(\mathbf{u}^*) &= J(\mathbf{u}^*, \tilde{\boldsymbol{\theta}}(\eta)) - J(\tilde{\mathbf{u}}(\eta), \tilde{\boldsymbol{\theta}}(\eta)), \\
&= J(\mathbf{u}^*, \tilde{\boldsymbol{\theta}}(\eta)) - J(\mathbf{u}^*, \boldsymbol{\theta}_0) + J(\mathbf{u}^*, \boldsymbol{\theta}_0) - J(\tilde{\mathbf{u}}(\eta), \tilde{\boldsymbol{\theta}}(\eta)), \\
&= \frac{\partial J}{\partial \eta}(\mathbf{u}^*, \boldsymbol{\theta}_0)\eta \boldsymbol{\xi}^{\boldsymbol{\theta}} + O(\eta^2) + J(\tilde{\mathbf{u}}(0), \tilde{\boldsymbol{\theta}}(0)) - J(\tilde{\mathbf{u}}(\eta), \tilde{\boldsymbol{\theta}}(\eta)),
\end{aligned} \tag{2.29}$$

the last step owing to continuity of J in its $\boldsymbol{\theta}$-argument. (Recall: J is, at least, continuously differentiable in its $\boldsymbol{\theta}$-argument.) Since results on Lipschitz continuity of optimal cost of Theorem 2.3 hold under the assumed conditions, we have

$$J(\tilde{\mathbf{u}}(0), \tilde{\boldsymbol{\theta}}(0)) - J(\tilde{\mathbf{u}}(\eta), \tilde{\boldsymbol{\theta}}(\eta)) = O(\eta),$$

using which in (2.29) proves the result. □

Remarks:

1. A special feature of this theorem is that it admits cases in which the pNLP (2.2) has multiple optimal solutions (recall Remark 1a after Theorem 2.3), in contrast to Theorem 2.2, in which the optimal solutions happen to be unique under the assumed strong conditions.
   The possibility of multiple optimal solutions means that there can be a jump in optimal solution for some values of η. The theorem above implies that irrespective of the possibility of jump in solutions in a pNLP that satisfies the stated conditions, the non adaptation – as long as it can remain feasible – results in optimality loss of the order of $O(\eta)$.
   As a special case, consider parametric linear programming (pLP) problems, i.e. when cost J and constraints G_i are linear functions of their arguments. It is well known that a pLP can have multiple optimal solutions for some values of η. This means that there can be a jump in optimal solution of a pLP for some values of η. Recall, for example, Figure 2.5 of Example 2.2.
   The theorem above implies that irrespective of the possibility of jump in solutions in a pLP, even the non adaptation – as long as it can remain feasible – prevents a jump in optimality loss. Moreover, *any Lipschitz continuous feasible* adaptation $\hat{\mathbf{u}}$ of a nominal optimal solution $\mathbf{u}^*$ of a pLP (i.e., $\hat{\mathbf{u}} - \mathbf{u}^* = O(\eta)$) will also result in an optimality loss of $O(\eta)$. This is easy to check by simply replacing the term $J(\mathbf{u}^*, \tilde{\boldsymbol{\theta}}(\eta))$ by $J(\hat{\mathbf{u}}, \tilde{\boldsymbol{\theta}}(\eta))$ in (2.29) in the derivation above. In summary, for a pLP that satisfies conditions of Theorem 2.4, *no* feasible adaptation of a nominal optimal solution can bring any significant benefit, in terms of optimality loss, over non adaptation, as long as the latter is feasible.
2. Note that the restrictive condition (2.21) assumed for Theorem 2.2 is not assumed for Theorem 2.4 above. As observed in Remark 1b after Theorem 2.3, other conditions assumed for Theorem 2.4 are also weaker than those assumed for Theorem 2.2, making the former a strong version of the latter. Remark 1 above can be seen as an example of this fact.

The results of Theorems 2.2 and 2.4 above naturally raise the following question:

for an SRTO problem expressed as a general pNLP, if no adaptation, in general, cannot reduce the optimality loss below $O(\eta)$, can some type of (feasible) adaptation that is based on the knowledge of nominal solution, reduce it below $O(\eta)$? If yes, what type of adaptation can achieve this and under what conditions?

In other words, we want to compare the performance of adapted inputs with that of nominal inputs; although, not in the manner of the local cost-variation (2.1), but with the perturbed optimal cost $J(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}})$ as a *point of reference*.

Hence, the research objective for the SRTO problem can be schematically represented as in Figure 2.15:

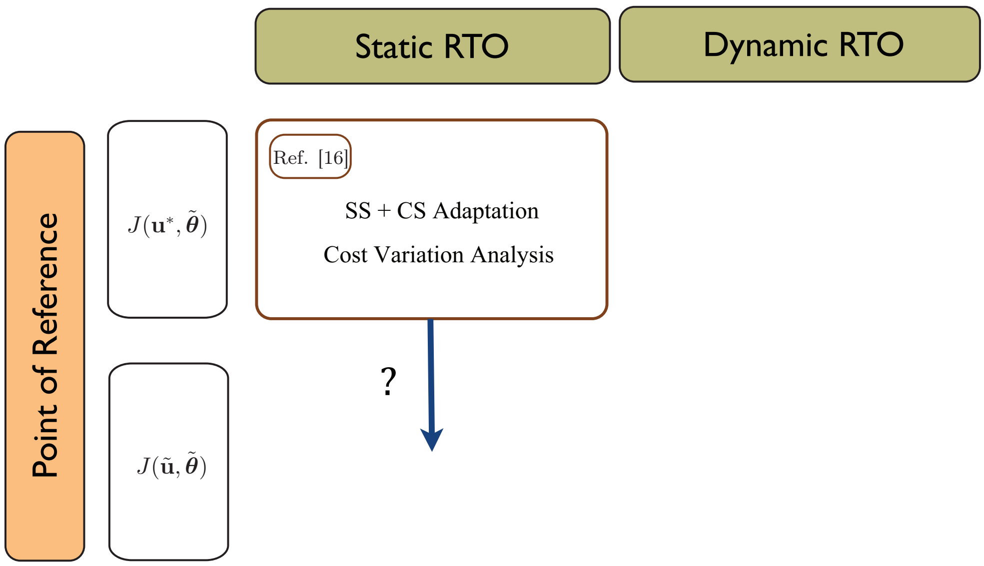

Figure 2.15 Research objective for the analytical study of SRTO.

Chapter 3

Role of Constraints in Optimality of Parametric Nonlinear Programs

In this chapter, we perform a joint analysis of nominal optimal, perturbed optimal and feasible adapted solutions that conserve part or whole of the nominal active set. As explained in Chapter 2, the motivation behind such a characterization of adapted inputs, viz., the one that is based on their *properties* common with nominal solution, is to *imagine* that the adapted inputs are generated by some RTO method that makes use of the knowledge of the nominal optimal solution.

Recall also from Section 2.3.3 that the aim here is *not* to study how such an RTO method is to be designed; but, to *assume* that such adapted inputs are available. The main goal is to develop an analysis to quantify the optimality loss incurred due to such – possibly *insufficient* – adaptation, especially when the nominal and perturbed active sets are different.

It is hoped that the results of the analysis in turn will help shed some light on the relative importance of RTO methods, when they exist, that are capable of generating the concerned adapted inputs and might provide some insights in simplifying the design of such RTO methods.

We perform the said analysis using the following two-step approach:

Step 1 Characterize the change in the optimal active set resulting from small parametric perturbations.

Step 2 Use the information about the change in active set in combination with the information about the set of constraints kept active by the adapted solution to quantify the optimality loss suffered by the adapted solution.

Thus, it is evident that to perform a quantitative analysis of the optimality loss resulting from a given set of adapted inputs, it is first necessary to impose certain conditions on the underlying pNLP so as to ensure a sufficiently *regular behavior* of the optimal inputs for the perturbed system, $\tilde{\mathbf{u}}(\eta)$. A number of such conditions were discussed in Section 2.3.3. Let us recall the role of the main conditions:

- LICQ (2.5) ensures that the KKT NCO hold at the nominal optimal solution $\mathbf{u}^*$,
- the combination of LICQ (2.5) and SSOSC (2.11) ensures Lipschitz continuity of a local optimal solution of NP($\boldsymbol{\theta}$) and of its associated Lagrange multipliers (relation (2.15)),
- the combination of LICQ (2.5), SSOSC (2.11) and assumption (2.21) ensures Lipschitz continuity of a global optimal solution of NP($\boldsymbol{\theta}$) and of its associated Lagrange multipliers (relation (2.22)).

Under the last set of assumptions, we will use the same symbol $\tilde{\mathbf{u}}(\eta)$ to denote a global optimal solution of NP($\tilde{\boldsymbol{\theta}}(\eta)$) that is also the local variation in the (global) optimal solution $\mathbf{u}^*$ of NP($\boldsymbol{\theta}_0$).

In the next two sections, we present the optimality loss analysis under these assumptions. We prove the important result that the optimality loss associated with adaptation that conserves the nominal active set is $O(\eta^2)$, *even when there is a change in the set of active constraints.* In addition, we show that conserving only a particular *subset* of nominal active set, viz., the nominal *strong* active set, is sufficient to limit the optimality loss to the order of O(η^2). In Section 3.3, an example is presented to illustrate the results and in Section 3.4 the results are summarized.

3.1 Change in Active Set due to Parametric Perturbation

As mentioned at beginning of the chapter, Step 1 is to analyze how the active set for Problem (2.2) changes as a result of the parametric perturbations (2.8).

Without loss of generality, suppose that there is a change in active set around $\eta = 0$. In terms of the notation introduced in (2.7) and (2.9), we need to deal with three triplets of sets: At $\eta = 0$, the strongly active, weakly active and inactive sets correspond to $\mathcal{I}^*$, $\mathcal{J}^*$, and $\mathcal{K}^*$, respectively; at $\eta = 0_+$, these sets are $\tilde{\mathcal{I}}_+$, $\tilde{\mathcal{J}}_+$, and $\tilde{\mathcal{K}}_+$, while at $\eta = 0_-$, these sets are $\tilde{\mathcal{I}}_-$, $\tilde{\mathcal{J}}_-$, and $\tilde{\mathcal{K}}_-$. The relationship between them is studied next.

Recall from Section 2.3.3, that conditions (2.3), (2.5) (LICQ), (2.11) (SSOSC) and (2.21) on NP($\boldsymbol{\theta}$) ensure Lipschitz continuity of $(\tilde{\mathbf{u}}(\eta), \tilde{\boldsymbol{\lambda}}(\eta))$. As a straightforward consequence of it, we can derive the following relation between the sets $\mathcal{K}^*$ and $\tilde{\mathcal{K}}$:

Lemma 3.1 (Constancy of inactive set under $\tilde{\boldsymbol{\theta}}(\eta)$)
For pNLP (2.2) *satisfying assumption* (2.3)*, if conditions* (2.5) *(LICQ),* (2.11) *(SSOSC) and* (2.21) *hold at the nominal optimal solution* $\mathbf{u}^*$*, then under parametric perturbations* (2.8)*,* $\mathcal{K}^* \subseteq \tilde{\mathcal{K}}$*.*

Proof: For $\eta = 0_+$, let us assume the contrary, namely, that there exists an index $i \in \mathcal{K}^* \cap (\tilde{\mathcal{I}}_+ \cup \tilde{\mathcal{J}}_+)$. Hence,

$$G_i(\mathbf{u}^*, \boldsymbol{\theta}_0) < 0; \quad \text{with} \quad G_i(\tilde{\mathbf{u}}(0_+), \tilde{\boldsymbol{\theta}}(0_+)) = 0.$$

The last statement, however, is a contradiction since $\tilde{\mathbf{u}}(\eta)$ is continuous as a result of Theorem 2.1 and G_i is continuous in both its arguments by assumption (2.3). Hence, it must be that $\mathcal{K}^* \cap (\tilde{\mathcal{I}}_+ \cup \tilde{\mathcal{J}}_+) = \emptyset$. The same argument holds for $\eta = 0_-$. □

Lemma 3.1 implies that it is not possible for inactive constraints to become (strongly/weakly) active after small parametric perturbations.

Next, we prove that strongly active constraints at the nominal solution remain strongly active after parametric perturbations.

Lemma 3.2 (Constancy of strongly active set under $\tilde{\boldsymbol{\theta}}(\eta)$)
For pNLP (2.2) *satisfying assumption* (2.3)*, if conditions* (2.5) *(LICQ),* (2.11) *(SSOSC) and* (2.21) *hold at the nominal optimal solution* $\mathbf{u}^*$*, then under parametric perturbations* (2.8)*,* $\mathcal{I}^* \subseteq \tilde{\mathcal{I}}$*.*

Proof: Let us assume the contrary, viz., some nominal strongly active constraints do not remain strongly active after parametric perturbations so that only a (strict) subset of $\mathcal{I}^*$ belongs to $\tilde{\mathcal{I}}$. Next, we will show, for $\eta = 0_+$, that this leads to contradiction.

In general, there can be some new indices in $\tilde{\mathcal{I}}_+$ that are not present in $\mathcal{I}^*$. Thus, we have:

$$\mathcal{I}^* = \mathcal{C} \cup \mathcal{Z}_1, \quad \tilde{\mathcal{I}}_+ = \mathcal{C} \cup \mathcal{Z}_2, \quad \mathcal{Z}_1 \neq \emptyset, \quad \mathcal{C} \cap \mathcal{Z}_1 \cap \mathcal{Z}_2 = \emptyset. \tag{3.1}$$

Thus, $\mathcal{Z}_2$ represents the new strongly active constraints after perturbation. Since result of Lemma 3.1 holds under the assumed conditions, $\mathcal{Z}_2$ *cannot* be part of $\mathcal{K}^*$. Hence, from the last relation in (3.1), we can infer that

$$\mathcal{Z}_2 \subseteq \mathcal{J}^*, \tag{3.2}$$

i.e. the constraints in the strict active set of perturbed solution that are not present in the strict active set of nominal solution must have come from the marginal active set of the nominal solution.

The KKT NCO (2.6) for NP($\boldsymbol{\theta}$) at $\eta = 0$ and (2.9) $\eta = 0_+$ read:

$$\begin{aligned}
\mathbf{0} &= \frac{\partial J}{\partial \mathbf{u}}(\mathbf{u}^*, \boldsymbol{\theta}^*) + \boldsymbol{\lambda}_{\mathcal{I}^*}^{*\,T} \frac{\partial \mathbf{G}_{\mathcal{I}^*}}{\partial \mathbf{u}}(\mathbf{u}^*, \boldsymbol{\theta}^*), \\
\mathbf{0} &= \left. \frac{\partial J}{\partial \mathbf{u}}(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}}) \right|_{\eta=0_+} + \tilde{\boldsymbol{\lambda}}_{\tilde{\mathcal{I}}_+}^{T}(\eta = 0_+) \left. \frac{\partial \mathbf{G}_{\tilde{\mathcal{I}}_+}}{\partial \mathbf{u}}(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}}) \right|_{\eta=0_+},
\end{aligned} \tag{3.3}$$

respectively. Using (3.1) and (3.2), the above system can be rewritten as:

$$\begin{aligned}
\mathbf{0} &= \frac{\partial J}{\partial \mathbf{u}}(\mathbf{u}^*, \boldsymbol{\theta}^*) + \boldsymbol{\lambda}_{\mathcal{C}}^{*T} \frac{\partial \mathbf{G}_{\mathcal{C}}}{\partial \mathbf{u}}(\mathbf{u}^*, \boldsymbol{\theta}^*) + \boldsymbol{\lambda}_{\mathcal{Z}_1}^{*\,T} \frac{\partial \mathbf{G}_{\mathcal{Z}_1}}{\partial \mathbf{u}}(\mathbf{u}^*, \boldsymbol{\theta}^*), \\
\mathbf{0} &= \left\{ \frac{\partial J}{\partial \mathbf{u}}(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}}) + \tilde{\boldsymbol{\lambda}}_{\mathcal{C}}^{T} \frac{\partial \mathbf{G}_{\mathcal{C}}}{\partial \mathbf{u}}(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}}) + \tilde{\boldsymbol{\lambda}}_{\mathcal{Z}_2}^{T} \frac{\partial \mathbf{G}_{\mathcal{Z}_2}}{\partial \mathbf{u}}(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}}) \right\}_{\eta=0_+}.
\end{aligned} \tag{3.4}$$

Under the assumed conditions on NP($\boldsymbol{\theta}$), results of Theorem 2.1 hold implying the Lipschitz continuity of $\tilde{\mathbf{u}}(\eta)$. Owing to continuity of the derivatives of J and $\mathbf{G}$ with respect to $\mathbf{u}$ and $\boldsymbol{\theta}$, and that of $\tilde{\mathbf{u}}$ and $\tilde{\boldsymbol{\theta}}$ with respect to η, (3.4) implies

$$\begin{aligned}
\mathbf{0} = {} & \left\{ \tilde{\boldsymbol{\lambda}}_{\mathcal{C}}(\eta = 0_+) - \boldsymbol{\lambda}_{\mathcal{C}}^* \right\}^T \frac{\partial \mathbf{G}_{\mathcal{C}}}{\partial \mathbf{u}}(\mathbf{u}^*, \boldsymbol{\theta}^*) + \tilde{\boldsymbol{\lambda}}_{\mathcal{Z}_2}^{T}(\eta = 0_+) \frac{\partial \mathbf{G}_{\mathcal{Z}_2}}{\partial \mathbf{u}}(\mathbf{u}^*, \boldsymbol{\theta}^*) \\
& - \boldsymbol{\lambda}_{\mathcal{Z}_1}^{*\,T} \frac{\partial \mathbf{G}_{\mathcal{Z}_1}}{\partial \mathbf{u}}(\mathbf{u}^*, \boldsymbol{\theta}^*),
\end{aligned}$$

which, owing to the (Lipschitz) continuity of $\tilde{\boldsymbol{\lambda}}(\eta)$, reduces to:

$$\mathbf{0} = \tilde{\boldsymbol{\lambda}}_{\mathcal{Z}_2}^{T}(\eta = 0_+) \frac{\partial \mathbf{G}_{\mathcal{Z}_2}}{\partial \mathbf{u}}(\mathbf{u}^*, \boldsymbol{\theta}^*) - \boldsymbol{\lambda}_{\mathcal{Z}_1}^{*\,T} \frac{\partial \mathbf{G}_{\mathcal{Z}_1}}{\partial \mathbf{u}}(\mathbf{u}^*, \boldsymbol{\theta}^*). \tag{3.5}$$

Next, we make two important observations.

Observation 1: $\boldsymbol{\lambda}_{\mathcal{Z}_1}^* \neq \mathbf{0}$.

The reason is that the first relation in (3.1) implies that $\mathcal{Z}_1 \subset \mathcal{I}^*$.

Observation 2: From **Observation 1** and (3.5), we can infer that the column vectors of

$$\frac{\partial \mathbf{G}_{\mathcal{Z}_2}}{\partial \mathbf{u}}(\mathbf{u}^*, \boldsymbol{\theta}^*) \quad \text{and} \quad \frac{\partial \mathbf{G}_{\mathcal{Z}_1}}{\partial \mathbf{u}}(\mathbf{u}^*, \boldsymbol{\theta}^*)$$

cannot all be independent.

But, the last observation is a contradiction, since (3.2) implies that $\mathcal{Z}_2$ is a part of $\mathcal{J}^*$ and LICQ (2.5) implies that the the column vectors of $\dfrac{\partial \mathbf{G}_{\mathcal{J}^*}}{\partial \mathbf{u}}(\mathbf{u}^*, \boldsymbol{\theta}^*)$ *must* be *independent of* those of $\dfrac{\partial \mathbf{G}_{\mathcal{I}^*}}{\partial \mathbf{u}}(\mathbf{u}^*, \boldsymbol{\theta}^*)$.

Hence, it is not possible that some nominal strongly active constraints do not remain strongly active for $\eta = 0_+$.

Since the same arguments can be applied for the case $\eta = 0_-$, the same result also holds for $\tilde{\mathcal{I}}_-$. □

As a consequence of the above two lemmas, the following theorem describing possible change in *all* index sets due to parametric perturbations can be proved:

Theorem 3.1 (Relation between $\mathcal{I}^*, \mathcal{J}^*, \mathcal{K}^*, \mathcal{A}^*$ and $\tilde{\mathcal{I}}, \tilde{\mathcal{J}}, \tilde{\mathcal{K}}, \tilde{\mathcal{A}}$)
For pNLP (2.2) *satisfying assumption* (2.3), *if conditions* (2.5) *(LICQ),* (2.11) *(SSOSC) and* (2.21) *hold at the nominal optimal solution* $\mathbf{u}^*$, *then under parametric perturbations* (2.8), *the following relations hold:*

$$\mathcal{I}^* \subseteq \tilde{\mathcal{I}}, \quad \mathcal{K}^* \subseteq \tilde{\mathcal{K}}, \quad \tilde{\mathcal{J}} \subseteq \mathcal{J}^*, \quad \tilde{\mathcal{A}} \subseteq \mathcal{A}^*. \tag{3.6}$$

Proof: Since results of Lemmas 3.1 and 3.2 hold, the strict active set will remain strongly active, and the inactive set will remain inactive, after parametric perturbations. Only the elements in the weakly active set can change sides, i.e., they can either stay weakly active, become strongly active or become inactive, proving the result. □

Remark: Note that $\mathcal{I}^*$ is the minimal strict active set, i.e. smaller than or equal to $\tilde{\mathcal{I}}_+$ and $\tilde{\mathcal{I}}_-$, while $\mathcal{A}^*$ is the maximal active set, i.e., larger than or equal to $\tilde{\mathcal{A}}_+$ and $\tilde{\mathcal{A}}_-$.

A *schematic* representation of these results is shown in Figures 3.1 to 3.3.

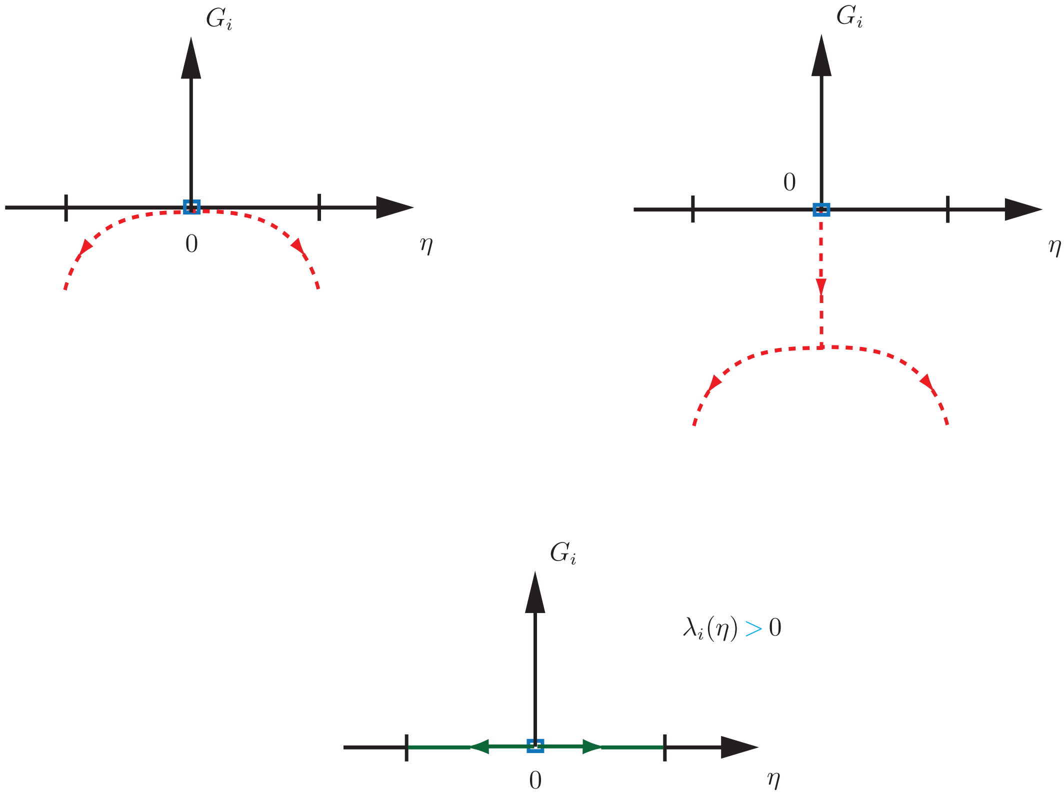

Figure 3.1 Effect of parametric variation on the strongly active constraint G_i, $i \in \mathcal{I}^*$. The rectangle denotes G_i^*. The dashed lines with arrows show the impossible change in value of G_i. The solid lines with arrows show the possible change in G_i. The reason for the impossible change in the top-left figure is the LICQ, while that in the top-right figure is the continuity of G_i and $\tilde{\mathbf{u}}$ with respect to η. The reason for the corresponding Lagrange multiplier $\lambda_i(\eta)$ being strictly greater than zero (bottom figure) is again LICQ.

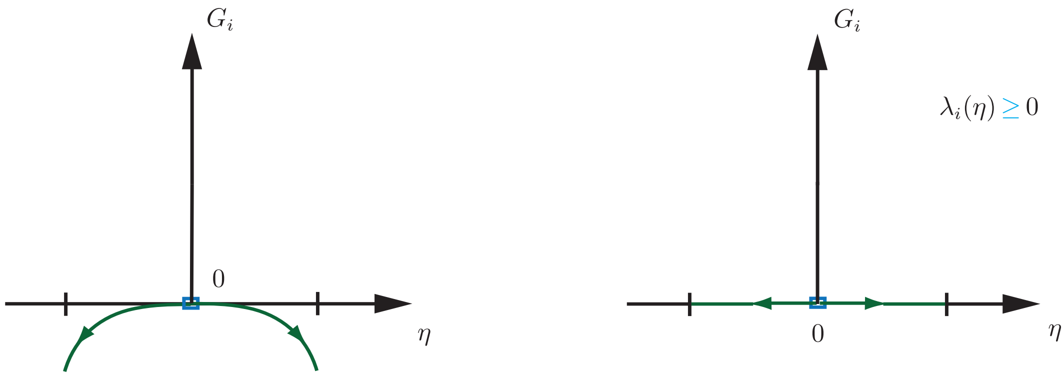

Figure 3.2 Effect of parametric variation on the weakly active constraint G_i, $i \in \mathcal{J}^*$. The rectangle denotes G_i^*. The solid lines with arrows show the possible change in G_i, which can become inactive (left figure), remain weakly active or become active (right figure).

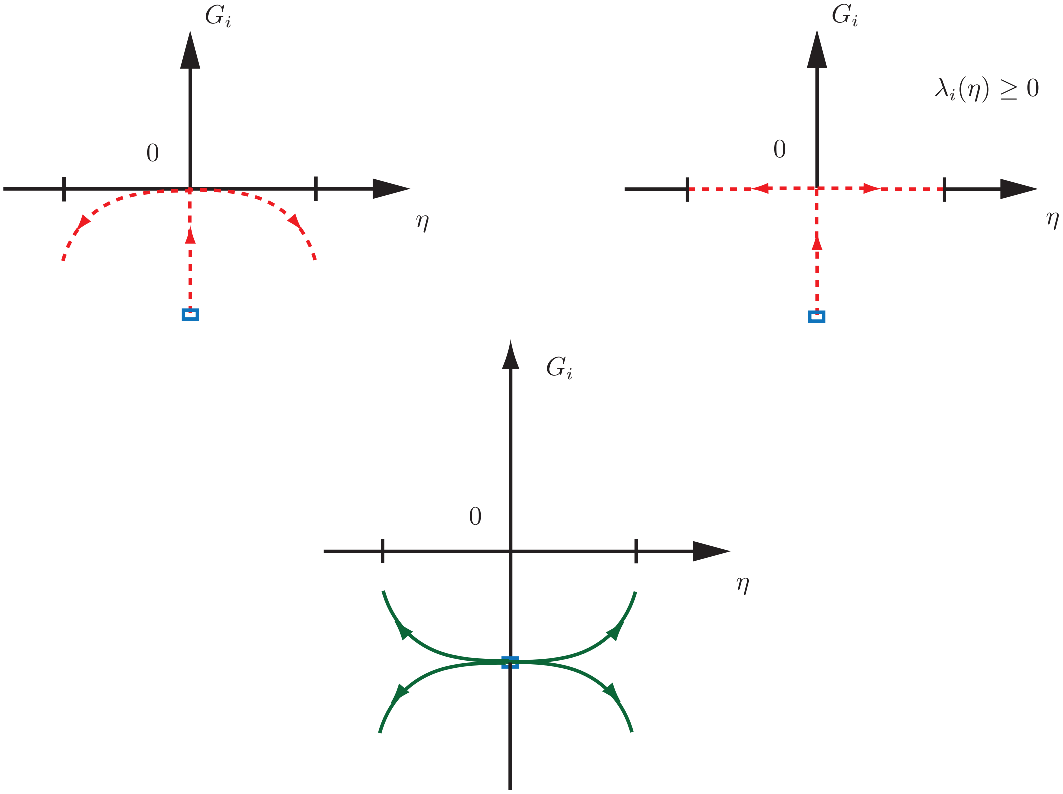

Figure 3.3 Effect of parametric variation on the inactive constraint G_i, $i \in \mathcal{K}^*$. The rectangle denotes G_i^*. The dashed lines with arrows show the impossible change in value of G_i. The solid lines with arrows show the possible change in G_i. The reason for the impossible changes in G_i is the continuity of G_i and $\tilde{\mathbf{u}}$ with respect to η.

3.2 Optimality Loss Analysis

This section accomplishes the task of Step 2, viz. it investigates the optimality loss when the nominal active constraints are kept active using input adaptation. To be precise, let $\hat{\mathbf{u}}$ denote adapted inputs that satisfy

$$\hat{\mathbf{u}} - \mathbf{u}^* = O(\eta) \tag{3.7}$$

and keep the set $\mathcal{A}^*$ active *without violating any other constraint*, i.e., the adapted inputs $\hat{\mathbf{u}}$ satisfy the following conditions for the perturbed system:[1]

$$\begin{aligned} G_i(\hat{\mathbf{u}}, \tilde{\boldsymbol{\theta}}) &= 0, \quad \forall\, i \in \mathcal{I}^*, \\ G_i(\hat{\mathbf{u}}, \tilde{\boldsymbol{\theta}}) &= 0, \quad \forall\, i \in \mathcal{J}^*, \\ G_i(\hat{\mathbf{u}}, \tilde{\boldsymbol{\theta}}) &\leq 0, \quad \forall\, i \in \mathcal{K}^*. \end{aligned} \tag{3.8}$$

We assume that, for the pNLP (2.2) and $\tilde{\boldsymbol{\theta}}$ under consideration, there exist solution(s) to the system of equations (3.8) that satisfy (3.7).

We start with the case when there is no change in the active sets of constraints.

3.2.1 Optimality Loss with Same Index Sets of Constraints

The simplest case is when there is no change in the index sets of constraints after parametric perturbations, i.e. $\mathcal{I}^* = \tilde{\mathcal{I}}$, $\mathcal{J}^* = \tilde{\mathcal{J}}$, and $\mathcal{K}^* = \tilde{\mathcal{K}}$.

Theorem 3.2
For pNLP (2.2) *satisfying assumption* (2.3), *if conditions* (2.5) *(LICQ),* (2.11) *(SSOSC) and* (2.21) *hold at the nominal optimal solution* $\mathbf{u}^*$, *and the active index sets* $\mathcal{I}^*$ *and* $\mathcal{J}^*$ *do not change under parametric perturbations* (2.8), *then the optimality loss associated with any input adaptation that satisfies* (3.7) *and* (3.8) *(keeping the constraints* $\mathcal{A}^*$ *active while being feasible) is* $O(\eta^2)$.

Proof: The Taylor series expansion of $\mathbf{G}_{\tilde{\mathcal{I}}}(\hat{\mathbf{u}}, \tilde{\boldsymbol{\theta}})$ around $(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}})$ yields:

$$\mathbf{G}_{\tilde{\mathcal{I}}}(\hat{\mathbf{u}}, \tilde{\boldsymbol{\theta}}) = \mathbf{G}_{\tilde{\mathcal{I}}}(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}}) + \frac{\partial \mathbf{G}_{\tilde{\mathcal{I}}}}{\partial \mathbf{u}}(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}})\, \{\hat{\mathbf{u}} - \tilde{\mathbf{u}}\} + O(\{\hat{\mathbf{u}} - \tilde{\mathbf{u}}\}^2). \tag{3.9}$$

Note that $\mathbf{G}_{\tilde{\mathcal{I}}}(\hat{\mathbf{u}}, \tilde{\boldsymbol{\theta}}) = \mathbf{0}$ by the definition of $\hat{\mathbf{u}}$ since $\tilde{\mathcal{I}} = \mathcal{I}^*$. Also, $\mathbf{G}_{\tilde{\mathcal{I}}}(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}}) = \mathbf{0}$ by definition of the active set of the perturbed optimum.

$\hat{\mathbf{u}} - \mathbf{u}^* = O(\eta)$ by construction as given by (3.7) and $\tilde{\mathbf{u}} - \mathbf{u}^* = O(\eta)$ since (2.22) holds under the assumed conditions. Hence, $\hat{\mathbf{u}} - \tilde{\mathbf{u}} = O(\eta)$.

Using all these facts, (3.9) gives:

$$\frac{\partial \mathbf{G}_{\tilde{\mathcal{I}}}}{\partial \mathbf{u}}(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}})\, \{\hat{\mathbf{u}} - \tilde{\mathbf{u}}\} = O(\eta^2), \tag{3.10}$$

[1] Note that the value of η used to specify the difference between $\hat{\mathbf{u}}$ and $\mathbf{u}^*$ in (3.7) is the same as the magnitude of parametric variations in (2.8).

which, when combined with (2.25), leads to $\delta J(\hat{\mathbf{u}}) = O(\eta^2)$. $\square$

Remark: Note that keeping $\mathbf{G}_{\mathcal{J}^*}(\hat{\mathbf{u}}, \tilde{\boldsymbol{\theta}}) = \mathbf{0}$ does not help toward optimality since the corresponding Lagrange multipliers are zero, i.e., these constraints though active do not contribute to the cost. Hence, they could indeed be relaxed to become inactive.

3.2.2 Optimality Loss with Change in Optimal Active Set

For this scenario, several possibilities need to be considered. One could use input adaptation to keep either $\mathcal{A}^*$ or $\tilde{\mathcal{A}}$ active over the interval $\mathcal{B}_0$. Alternatively, as noted in the remark above, it is sufficient to keep the smallest of these sets, namely either $\mathcal{I}^*$ or $\tilde{\mathcal{I}}$ active. Of course, in all these adaptation strategies, it is assumed that feasibility of the other constraints is guaranteed. Also recall that we are not concerned with how exactly can the strategies that produce said adapted inputs be designed; we are concerned with analysis of such adapted inputs, if they are available.

The next result proves that all these strategies are equivalent.

Theorem 3.3
Let pNLP (2.2) *satisfy assumption* (2.3) *and let conditions* (2.5) *(LICQ),* (2.11) *(SSOSC) and* (2.21) *hold at its nominal optimal solution* $\mathbf{u}^*$*. In case of parametric perturbations* (2.8)*, consider Strategy (i) that adapts the inputs to keep the constraints* $\mathcal{A}^*$ *active, Strategy (ii) that keeps the constraints* $\tilde{\mathcal{A}}$ *active, Strategy (iii) that keeps the constraints* $\mathcal{I}^*$ *active, and Strategy (iv) that keeps the constraints* $\tilde{\mathcal{I}}$ *active. The optimality loss associated with all these adaptation strategies, assuming they are feasible, is* $O(\eta^2)$*.*

Proof: Let $\mathcal{S}$ be the set of constraints enforced by the adopted strategy. It follows from (2.25) that the constraints to be enforced for the sake of optimality are only $\mathcal{C} = \mathcal{S} \cap \tilde{\mathcal{I}}$. Although other constraints are enforced, they do not have a first-order effect on the cost. Also note that all strategies ensure that $\mathcal{I}^* \subseteq \mathcal{C}$.

On the other hand, there are other elements in $\tilde{\mathcal{I}}$ that are not forced to zero. Let us denote them by $\mathcal{D}$, i.e. $\mathcal{D} = \tilde{\mathcal{I}} \setminus \mathcal{C}$. Note that $\mathcal{D}$ does not contain any elements of $\mathcal{I}^*$. From $\tilde{\mathcal{I}} = \mathcal{C} \cup \mathcal{D}$, (2.25) can be written as

$$\delta J(\hat{\mathbf{u}}) = -\tilde{\boldsymbol{\lambda}}_{\mathcal{C}}^T \frac{\partial \mathbf{G}_{\mathcal{C}}}{\partial \mathbf{u}}(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}}) \{\hat{\mathbf{u}} - \tilde{\mathbf{u}}\} - \tilde{\boldsymbol{\lambda}}_{\mathcal{D}}^T \frac{\partial \mathbf{G}_{\mathcal{D}}}{\partial \mathbf{u}}(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}}) \{\hat{\mathbf{u}} - \tilde{\mathbf{u}}\} + O(\eta^2). \tag{3.11}$$

Since results of Theorem 2.1 and relation (2.22) hold under assumed conditions, the first term of the expression above can be shown to be $O(\eta^2)$ following the same arguments as in the proof of Theorem 3.2. Results of Theorem 2.1 also imply Lipschitz continuity of Lagrange multipliers associated with $\tilde{\mathbf{u}}(\eta)$, so that $\tilde{\boldsymbol{\lambda}}_{\mathcal{D}} - \boldsymbol{\lambda}^*_{\mathcal{D}} = O(\eta)$. However, since $\mathcal{D}$ does not contain any elements of $\mathcal{I}^*$, $\boldsymbol{\lambda}^*_{\mathcal{D}} = 0$, which results in $\tilde{\boldsymbol{\lambda}}_{\mathcal{D}} = O(\eta)$. Also, $\hat{\mathbf{u}} - \tilde{\mathbf{u}} = O(\eta)$ as discussed in the proof of Theorem 3.2, and thus (3.11) becomes:

$$\delta J(\hat{\mathbf{u}}) = O(\eta^2) + O(\eta)\frac{\partial \mathbf{G}_{\mathcal{D}}}{\partial \mathbf{u}}(\tilde{\mathbf{u}}, \tilde{\boldsymbol{\theta}})O(\eta) + O(\eta^2) = O(\eta^2). \tag{3.12}$$

□

Remark: As noted earlier, $\mathcal{I}^*$ is the minimal set characterizing the four strategies under consideration in Theorem 3.3. The implication of all strategies being equal in terms of optimality loss is the following: $\mathcal{I}^*$ is the constraint set that needs to be kept active under parametric variations to guarantee an optimality loss of *no more* than O(η^2), even when the perturbed active set is different from the nominal one.

In summary, when LICQ and SSOSC hold for the pNLP NP($\boldsymbol{\theta}$), the optimality loss associated with conserving the nominal active set is *always* $O(\eta^2)$, regardless of whether or not the active set for the plant, which is unknown in practice, is the same as that of the model. The practical implication of this result is that, at least locally, static RTO methods are better off in terms of cost by *simply* striving to maintain the active set found with the nominal model. As long as the adapted solution remains feasible, *there is no need for any mechanism to detect the constraints that become active.*[2] On the other hand, failure to maintain the active set in RTO can, in general, result in an optimality loss of the order of $O(\eta)$.

3.3 Illustrative Example

This section illustrates the results of Section 3.1 via the optimization of a chemical process. The alkylation process is taken from Example 14.3 in [27] and modified slightly for the purpose of this illustration.

[2] Note, however, that such a mechanism might be necessary to ensure feasibility.

Mathematically, the optimization problem is formulated as the following parametric NLP:

$$
\begin{aligned}
\max_{\mathbf{u}=\{x_1,x_3\}} \quad & J(x_1,x_3,\boldsymbol{\theta}) = C_1x_4x_7 - C_2x_1 - C_3x_2 \\
& \qquad - C_4(x_3 - x_3^{\text{mean}} - \theta_4)^2 - C_5x_5, \\
\text{s.t.} \quad & G_1 : -x_1(1.12 + 0.13167x_8 - 0.00667x_8^2) \\
& \qquad + k_1x_4 \leq 0, \\
& G_2 : x_1(1.12 + 0.13167x_8 - 0.00667x_8^2) \\
& \qquad - k_2x_4 \leq 0, \\
& G_3 : k_3x_7 - 86.35 - 1.098x_8 + \theta_2x_8^2 \\
& \qquad - 0.325(x_6 - 89) \leq 0, \\
& G_4 : -k_4x_7 + 86.35 + 1.098x_8 - \theta_2x_8^2 \\
& \qquad + 0.325(x_6 - 89) \leq 0, \\
& G_5 : L_1 - x_5 \leq 0, \\
& G_6 : x_5 - U_1 \leq 0, \\
& G_7 : L_2 - x_6 \leq 0, \\
& G_8 : x_6 - U_2 \leq 0, \\
& G_9 : L_3 - x_8 \leq 0, \\
& G_{10} : x_8 - U_3 \leq 0, \\
& 0 \leq x_1 \leq 2000, \\
& 0 \leq x_3 \leq 120,
\end{aligned}
\tag{3.13}
$$

where

$$
\begin{aligned}
x_5 &:= \theta_1x_4 - x_1, \\
x_6 &:= \frac{98000x_3}{x_4x_9 + 1000x_3}, \\
x_7 &:= \frac{x_{10} + 133}{\theta_3}, \\
x_8 &:= \frac{x_2 + x_5}{x_1}, \\
x_9 &:= 35.82 - 0.222x_{10},
\end{aligned}
$$

and x_2, x_4 and x_{10} are kept at the following constant values:

$$x_2 = 16000 \quad \text{barrels/day},$$
$$x_4 = 3049 \quad \text{barrels/day},$$
$$x_{10} = 149.598.$$

Parameters θ_1 to θ_4 are uncertain. Two different sets of nominal parameters $\boldsymbol{\theta}_0$ and of directions of parametric variations $\boldsymbol{\xi}^{\boldsymbol{\theta}}$ will be chosen to illustrate the two cases mentioned in Section 3.2, namely no change and change in optimal active set after parametric variations.

Table 3.1 Set of values for $\boldsymbol{\theta}_0$ and $\boldsymbol{\xi}^{\boldsymbol{\theta}}$ in the chemical process optimization problem.

	$\boldsymbol{\theta}_0$	$\boldsymbol{\xi}^{\boldsymbol{\theta}}$
Case 1:	$\boldsymbol{\theta}_{0,1} = \begin{bmatrix} 1.2225 \\ 0.0355 \\ 2.9975 \\ 2.9975 \end{bmatrix}$	$\boldsymbol{\xi}^{\boldsymbol{\theta}}_1 = \begin{bmatrix} -0.5 \\ 0.5 \\ 0.5 \\ 0.5 \end{bmatrix}$
Case 2:	$\boldsymbol{\theta}_{0,2} = \begin{bmatrix} 1.2200 \\ 0.0394 \\ 3.0000 \\ 2.9986 \end{bmatrix}$	$\boldsymbol{\xi}^{\boldsymbol{\theta}}_2 = \dfrac{-1}{\sqrt{3}} \begin{bmatrix} 1 \\ -1 \\ 0 \\ 1 \end{bmatrix}$

The values of other parameters in the problem are given in Table 3.2.

Table 3.2 Values of parameters in the chemical process optimization problem.

Parameter	Value	Unit	Parameter	Value
C_1	0.063	\$/octane-barrel	k_1	99/100
C_2	5.04	\$/barrel	k_2	100/99
C_3	0.035	\$/barrel	k_3	99/100
C_4	0.1	\$ day/$(10^3$ lbs$)^2$	k_4	100/99
C_5	3.36	\$/barrel	L_3	3.0
x_3^{mean}	65	10^3 lbs/day	U_3	12.0
L_1	0.0	barrels/day		
U_1	2000.0	barrels/day		
L_2	85.0	weight %		
U_2	93.0	weight %		

The problem encompasses lower and upper bounds on the decision variables x_1 and x_3 as well as the constraints G_1 to G_{10} that are (nonlinear) functions of x_1, x_3 and $\boldsymbol{\theta}$.

3.3.1 Case 1: No Change in Active Set

Consider $\boldsymbol{\theta}_{0,1}$, $\boldsymbol{\xi}_1^{\boldsymbol{\theta}}$ and the range of uncertainty $\mathcal{B}_\eta = [-0.005, 0.005]$. The nominal optimal solution is $(x_1^*, x_3^*) = (1727.4, 68.0)$, for which the constraint G_6 is active.

For $\eta = -0.0044$, Figure 3.4 shows the iso-cost contours, the nominal optimal solution $\mathbf{u}^*$, the perturbed optimal inputs $\tilde{\mathbf{u}}$, and the adapted inputs $\hat{\mathbf{u}}$ generated by constraint control that conserves the nominal active set. One sees that $\hat{\mathbf{u}}$ and $\tilde{\mathbf{u}}$ are very close to each other. The legend for all contour plots is given in Table 3.3.

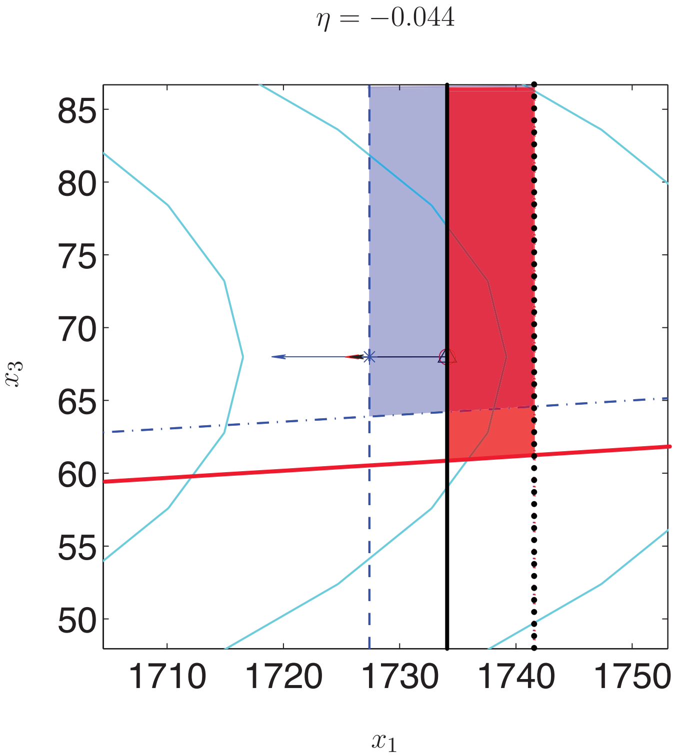

Figure 3.4 Iso-cost contours for Case 1 for $\eta = -0.0044$ depicting the nominal optimal inputs (star), the perturbed optimal inputs (circle), and the adapted inputs generated by constraint control (triangle). The triangle and circle appear to be almost overlapped. Refer to Table 3.3 for a complete legend.

Table 3.3 Legend for the contour plots in Problem (3.13)

Thin solid curves	iso-cost contours for $\tilde{\boldsymbol{\theta}}$
Thin dotted line	$G_2(\mathbf{u}, \boldsymbol{\theta}_0) = 0$ curve
Thick dotted line	$G_2(\mathbf{u}, \tilde{\boldsymbol{\theta}}) = 0$ curve
Dash-dotted curve	$G_3(\mathbf{u}, \boldsymbol{\theta}_0) = 0$ curve
Thick solid curve	$G_3(\mathbf{u}, \tilde{\boldsymbol{\theta}}) = 0$ curve
Dashed vertical line	$G_6(\mathbf{u}, \boldsymbol{\theta}_0) = 0$ curve
Thick solid vertical line	$G_6(\mathbf{u}, \tilde{\boldsymbol{\theta}}) = 0$ curve
Arrow at a point $\mathbf{u}^\circ = [x_1^\circ, x_3^\circ]$	direction of $J_\mathbf{u}$ at $\mathbf{u}^\circ$
Star	$\mathbf{u}^*$
Triangle	$\hat{\mathbf{u}}$
Circle	$\tilde{\mathbf{u}}$
Dark shaded region	nominal feasible region
Light shaded region	perturbed feasible region

Note that it is difficult to distinguish between the loci of $G_2(\mathbf{u}, \boldsymbol{\theta}_0) = 0$ (thin dotted line) and $G_2(\mathbf{u}, \tilde{\boldsymbol{\theta}}) = 0$ (thick dotted line).

Figure 3.4 shows that the nominal optimal inputs are on the $G_6(\mathbf{u}, \boldsymbol{\theta}_0) = 0$ curve and the perturbed optimal inputs are on the $G_6(\mathbf{u}, \tilde{\boldsymbol{\theta}}) = 0$ curve. Hence, the active set remains unchanged under parametric variations. The same is verified for all $\eta \in \mathcal{B}_\eta$.

Figure 3.5 shows the optimality loss associated with input adaptation as a function of η (Theorem 3.2). The $\mathrm{O}(\eta^2)$ fit of the plot agrees with the result of Theorem 3.2.

3.3.2 Case 2: Change in Active Set

Consider $\boldsymbol{\theta}_{0,2}$, $\boldsymbol{\xi}_2^{\boldsymbol{\theta}}$ and $\mathcal{B}_\eta = [-0.005, 0.005]$. The nominal optimal solution is $(u_1^*, u_2^*) = (1719.8, 71.4)$, for which the constraints G_3 and G_6 are active. Note that, for $\eta \leq -0.0023$, the constraint G_3 is no longer active and thus the active set is smaller.

For $\eta = 0.0029$, Figure 3.6 shows the iso-cost contours, the nominal optimal solution $\mathbf{u}^*$, the perturbed optimal inputs $\tilde{\mathbf{u}}$, and the adapted inputs $\hat{\mathbf{u}}$ generated by constraint control that conserves the nominal active set. The nominal optimal inputs are at the intersection of the $G_3(\mathbf{u}, \boldsymbol{\theta}_0) = 0$ and $G_6(\mathbf{u}, \boldsymbol{\theta}_0) = 0$ curves and,

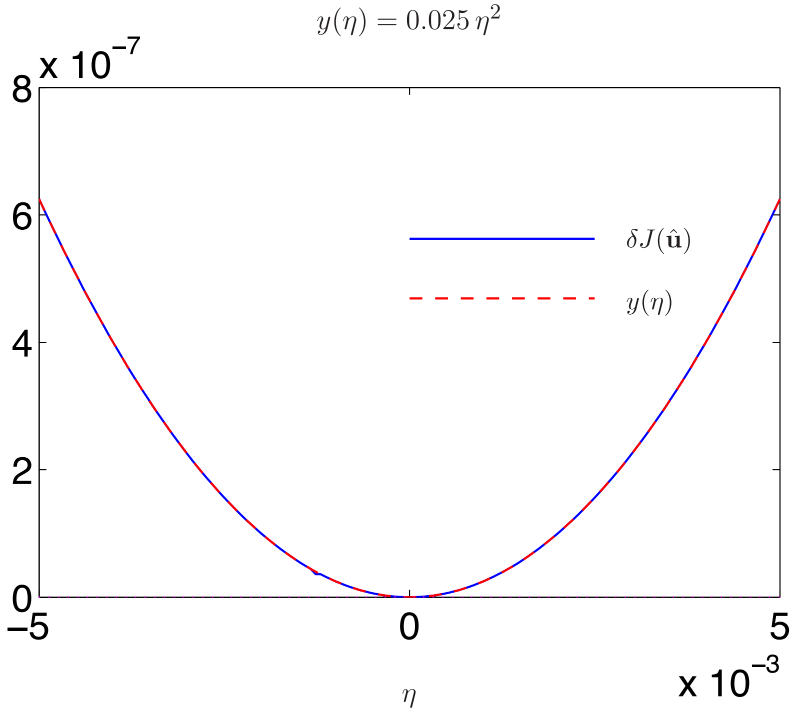

Figure 3.5 Optimality loss associated with the adapted inputs $\hat{\mathbf{u}}$ that keep the nominal active set active when there is no change in optimal active set. $y(\eta)$ is the best quadratic fit.

similarly, the perturbed optimal inputs are at the intersection of the $G_3(\mathbf{u}, \tilde{\boldsymbol{\theta}}) = 0$ and $G_6(\mathbf{u}, \tilde{\boldsymbol{\theta}}) = 0$ curves. Here again, one sees that $\hat{\mathbf{u}}$ and $\tilde{\mathbf{u}}$ are very close to each other.

Figure 3.7 shows the same information for $\eta = -0.0044$. Since the perturbed optimal inputs are *only* on the $G_6(\mathbf{u}, \tilde{\boldsymbol{\theta}}) = 0$ curve, the adapted inputs $\hat{\mathbf{u}}$, which lie at the intersection of the $G_3(\mathbf{u}, \tilde{\boldsymbol{\theta}}) = 0$ and $G_6(\mathbf{u}, \tilde{\boldsymbol{\theta}}) = 0$ curves, deviate significantly from $\tilde{\mathbf{u}}$.

Finally, Figure 3.8 shows the optimality loss associated with input adaptation that conserves the nominal active set as a function of η (Theorem 3.3). Note that the adapted inputs coincide with the perturbed optimal solution for $\eta > -0.0023$, which results in zero optimality loss.

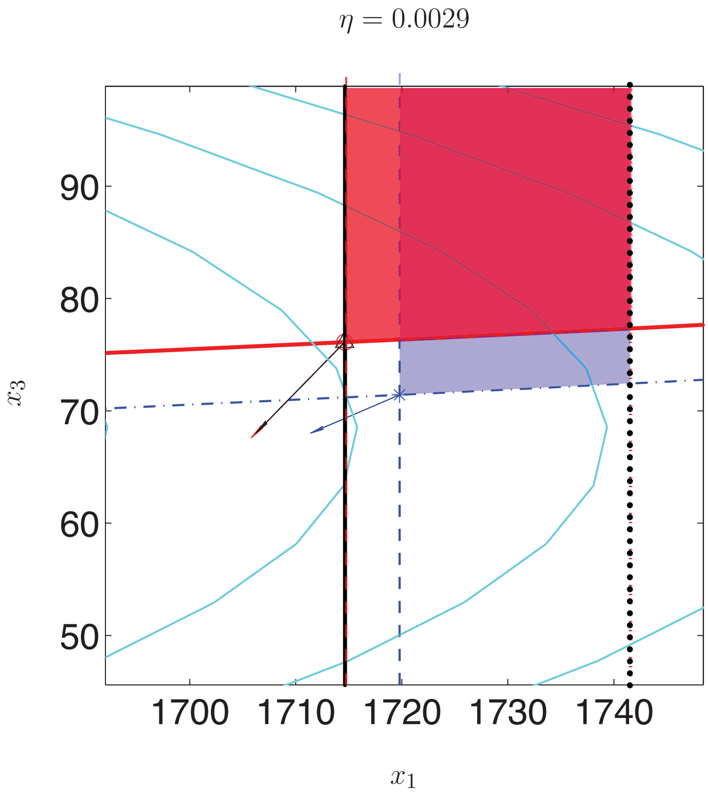

Figure 3.6 Iso-cost contours for Case 2 for $\eta = 0.0029$ depicting the nominal optimal inputs (star), the perturbed optimal inputs (circle) and the adapted inputs generated by constraint control (triangle). The circle and triangle appear to be almost overlapped. Refer to Table 3.3 for a complete legend.

3.4 Summary

Input adaptation methods have become the cornerstone of static RTO. The performance of these methods can be enhanced by consideration of how the optimal active set changes under parametric perturbations and what effect does the said change have on optimality.

We have studied input-adaptation strategies that compensate the effect of parametric variations by keeping the nominal active set active, under the assumption that the problem remains feasible. For small parametric variations, the difference between the cost associated with adaptation and the perturbed optimal cost can be expressed as a function of η, the magnitude of the parametric variations. Under conditions that are standard for parametric NLP, the following important result has been proved: the optimality loss associated with adaptation that keeps the nominal

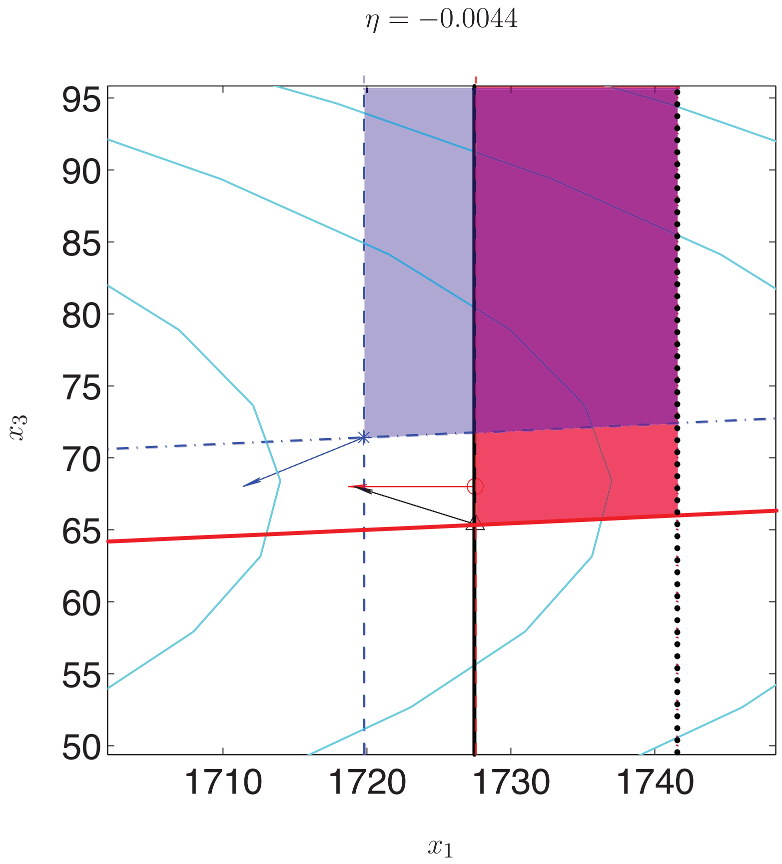

Figure 3.7 Iso-cost contours for Case 2 for $\eta = -0.0044$ depicting the nominal optimal inputs (star), the perturbed optimal inputs (circle) and the adapted inputs generated by constraint control (triangle). Refer to Table 3.3 for a complete legend.

active set is $O(\eta^2)$, *even when there is a change in the set of active constraints*. In addition, it has been shown that keeping only the *strict* nominal active set is what really matters to limit the optimality loss to the order of $\mathrm{O}(\eta^2)$.

The practical implication of this result is that static RTO methods are sub-optimal by order of only $O(\eta^2)$ by *simply* striving to maintain the nominally active set. On the other hand, failure to maintain the strict active set in an RTO will certainly result in a larger optimality loss – at least of the order of $O(\eta)$.

Thus, we have accomplished the task set at the end of Chapter 2 and the results obtained can be represented in the following schematic diagram:

It is hoped that the results presented here will help analyze and compare the performance of existing static RTO methods and will also inspire the design of alternative RTO schemes.

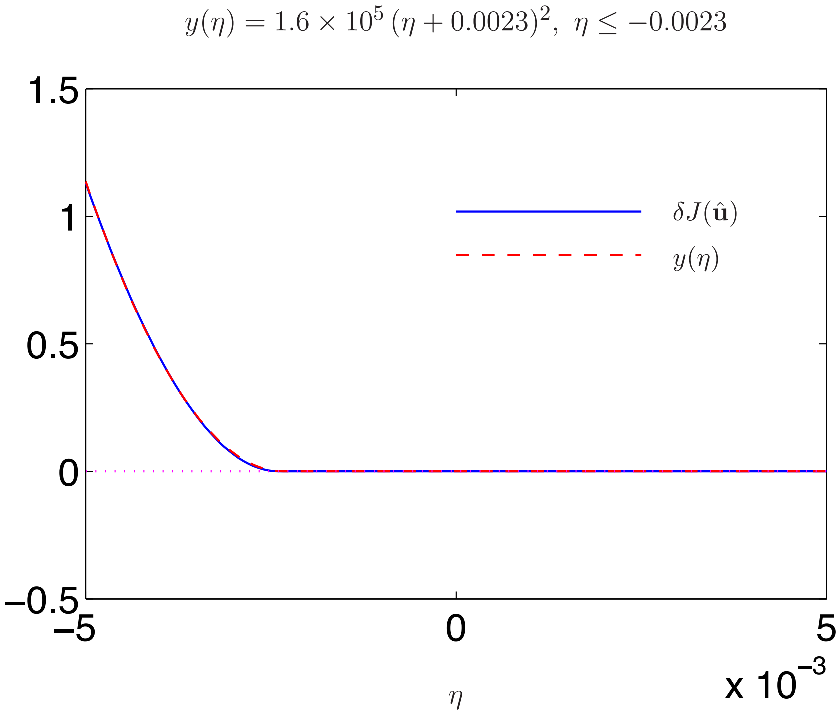

Figure 3.8 Optimality loss associated with the adapted inputs $\hat{\mathbf{u}}$ that conserve the nominal active set when there is a change in the optimal active set. $y(\eta)$ is the best quadratic fit.

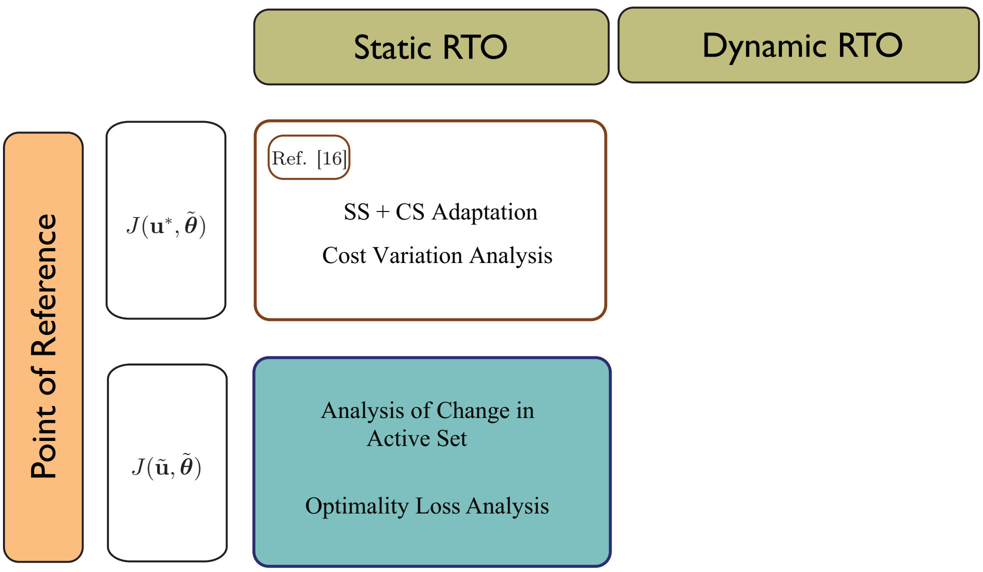

Figure 3.9 Contributions of this thesis to the analytical study of SRTO.

Chapter 4

Dynamic Real-Time Optimization

Transient processes represent an important class of industrial processes. For example, many processes in the resource industries are either inherently transient or operated in an unsteady-state manner. Batch and semi-batch processes in the chemical process industry are other examples of processes that are characterized by the absence of a steady state. Many alternative technologies in the energy sector also exhibit discontinuous operation, and transient energy-generation systems are expected to play a key role in future years.

The optimization of transient processes, in contrast to that of processes operated at steady-state, necessitates computation of *time profiles* of certain process variables so as to reduce production costs or improve product quality, while meeting strict safety requirements and environmental regulations. Similar to static optimization problems, aforementioned dynamic optimization problems are generally solved by computing optimal input profiles off-line on the basis of a process model and applying these profiles open-loop to the process. However, the off-line computation of the input profiles involves solving an optimal control problem as opposed to solving nonlinear or mixed-integer programming problems that arise in static optimization. However, in real-time operation, both plant-model mismatch and process disturbances can result in suboptimal process operation or, worse, infeasible operation. This gives rise to the problem of *dynamic real-time optimization* (DRTO), which can be defined as:

online computation of feasible and near-optimal input profiles for a dynamic optimization problem on the basis of the knowledge of nominal optimal solution and online measurement data.

Thus, the three main themes of the thesis, viz., uncertainty, feasibility and optimality, are already evident in a study of DRTO problems also.

4.1 A Short Survey of Existing Approaches for Dynamic RTO Problems

A common practice of dealing with uncertainty in transient processes is to represent it in the form of parametric perturbations. The optimal input profiles are computed off-line for the nominal values of the parameters. Naturally, when some parameters deviate from their nominal values, a change in optimal input profiles is required to maintain feasibility and optimality.

The ideal way to compute the plant optimal input profiles is to repeat the computation with the modified values of the parameters. Given the complexity of solving realistic optimal control problems [8, 87, 108], re-solving the problem in real-time can be a challenging task in many practical cases. Another point of view is to avoid re-solving the optimal control problem by quantifying the parametric perturbations and by *adapting* the nominal optimal inputs accordingly to maintain optimality. In theory, such an approach requires a *sensitivity analysis* of the parametric optimal control problems, i.e., a study of the effect that parametric perturbations will have on the optimal input profiles. The sensitivity analysis of parametric optimal control problems has been studied in a number of publications; see, for example, [57, 69, 74, 75] and the numerous references cited therein. For a recent and comprehensive treatment, that also deals with nonsmooth problems, see [58] and other references it cites. See also [23] for a derivation, based on the theory of neighboring extremals [13, 86], of the first-order variations of the optimal input profiles with respect to parametric perturbations in optimal control problems with mixed control-state constraints.

In practice, it may not be possible to quantify the parametric perturbations precisely. Even if an estimate of parametric perturbations is available, closed form expressions for first-order variations in optimal input profiles are available only if strict complementarity conditions and strong second-order sufficient conditions hold [74]. Thus, it may not always be possible to implement adaptation using first-order estimates in practice. Hence, real-time optimization (RTO) methods typically try to use the knowledge of the underlying system and adapt the nominal optimal input profiles to obtain some set of feasible input profiles. Numerous real-time optimization algorithms for dynamic optimization problems have been proposed in the literature. As noted in Introduction, these algorithms effect the input adaptation via different mechanisms. Recall some examples of the dynamic RTO methods most relevant to our investigations:

- some methods are based on repeated optimization of a process model that is updated using process measurements either within run [1, 95] or in a run-to-run manner [19, 100], as the case may be,
- some methods enforce the necessary conditions of optimality related to both constraints and sensitivities (NCO tracking for DRTO) [101],
- some algorithms addressed to polynomial systems involve a self-optimizing controller to track a linear combination of outputs [59],
- some algorithms perform repeated optimization of the fixed nominal model but after adding correction terms to constraint functions at each iteration using process measurements [71],
- some methods do repeated optimization of fixed nominal model but after adding correction terms to either dynamics or constraint functions and cost function [22] at each iteration using process measurements.

For a more detailed survey of static RTO methods, refer to Section 1.2.1.

4.2 Challenges in Analytical Study of Dynamic RTO Problems

As mentioned above, the quantification of parametric perturbations may not be possible in most practical processes that exhibit complex dynamics. Thus, adapting all parts of the model optimal input profiles to compensate for the effect of parametric perturbations is rarely possible in practice. Partial or selective input adaptation scenarios that result in sub-optimal process operation with acceptable performance loss are therefore worth analyzing. Recall from the survey of DRTO methods in Section 1.2.1 that, the direct input adaptation methods for DRTO problems typically enforce the constraints or sensitivities *selectively* and the particular choice can affect significantly the complexity of implementation. For example, enforcing of NCO related to constraints are typically simpler to implement than those based on enforcing of sensitivities since the latter involves more complicated techniques like neighboring-extremal control.

Following the example of the *selective adaptation* approach for static RTO problems as explained in Chapter 2, it is natural to ask if a similar approach can be developed for DRTO problems. We know that the implication of results concerning selective adaptation is that *full* knowledge of the change in optimal inputs is not needed to achieve *effective* input adaptation and that one component of optimality (viz., constraints) needs to be given *more importance* over the other (viz., sensitivities). From the experience of the static case, we know that the first step in this direction is to identify *sensitivity- and constraint-seeking directions* for local variation of nominal optimal inputs and the effect of such directional variations on cost.

Hence, the research objective for the DRTO problem is as shown in Figure 4.1

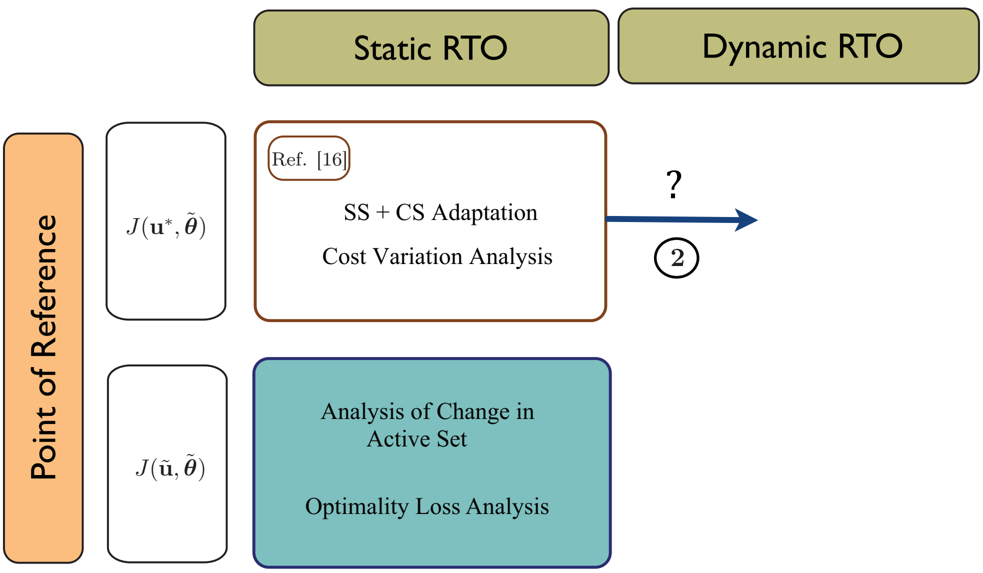

Figure 4.1 Research objective for the analytical study of DRTO.

Specifically, the first objective is to develop a characterization for the sensitivity- and constraint-seeking directions in DRTO such that a small variation of nominal optimal inputs along any of the sensitivity-seeking directions will not affect the active terminal and path constraints, whereas such an input variation along a constraint-seeking direction will. Note that this task is much more complicated than in the SRTO owing to the different nature of DRTO problems.

Consider, for example, the case of active path constraints. By their definition, the latter are functional constraints, i.e. they represent a continuum of constraints. So, when we talk of an input variation that does not cause change in an active path constraint, we are referring to no change in an infinitude of pointwise constraints. On the other hand, active terminal constraints are finite in number; but, by their definition, effect of any of the input variations, which occur within the process duration, on the the former needs to be *anticipated*. Indeed, a variation in input at a given instant is also going to affect the value of an active path constraint at any future instant. To summarize, the main challenge here is that the definition of the input variation directions for time t requires that *all* past input variations up to and including time t need to be taken into account, not merely the input variations at time t.

Once such a *dynamic* characterization of the directions is available, the next challenge is to analyze the effect of selective input adaptation along each set of directions on cost in the presence of parametric perturbations. The final objective is to see if the aforementioned characterization of selective adaptation strategies leads to clearly distinguishable cost variations over the case of no input adaptation. Only in the latter case can we be assured about the relative importance of the corresponding components of the NCO in DRTO.

4.3 Problem Formulation and Assumptions

In this section, the precise mathematical formulation for the general parametric optimal control problem involving both terminal and mixed control-state path constraints is given, along with a summary of the necessary conditions of optimality (NCOs) and of the corresponding assumptions.

The following parametric optimal control problem in the parameters $\boldsymbol{\theta}$, subject to the terminal inequality constraints $\mathbf{T} \leq \mathbf{0}$ and the mixed control-state inequality constraints $\boldsymbol{\Omega} \leq \mathbf{0}$, with given initial time t_0 and terminal time t_f, is considered

(OC($\boldsymbol{\theta}$)):

$$\min_{\mathbf{u}} \; J(\mathbf{u}) = \varphi(\mathbf{x}(t_\mathrm{f}), \boldsymbol{\theta}) + \int_{t_0}^{t_\mathrm{f}} \phi(t, \mathbf{x}(t), \mathbf{u}(t), \boldsymbol{\theta})\, dt, \tag{4.1}$$

$$\dot{\mathbf{x}}(t) = \mathbf{f}(t, \mathbf{x}(t), \mathbf{u}(t), \boldsymbol{\theta}); \quad \mathbf{x}(t_0) = \mathbf{h}(\boldsymbol{\theta}), \tag{4.2}$$

$$T_i(\mathbf{x}(t_\mathrm{f}), \boldsymbol{\theta}) \leq 0, \quad i = 1, \ldots, n_{\mathbf{T}}, \tag{4.3}$$

$$\Omega_i(t, \mathbf{x}(t), \mathbf{u}(t), \boldsymbol{\theta}) \leq 0, \quad i = 1, \ldots, n_{\boldsymbol{\Omega}}, \tag{4.4}$$

where $t \in [t_0, t_\mathrm{f}]$, $\mathbf{u}(t) \in \mathbb{R}^{n_\mathbf{u}}$, $\mathbf{x}(t) \in \mathbb{R}^{n_\mathbf{x}}$ and $\boldsymbol{\theta} \in \Theta$, where Θ is a compact subset of $\mathbb{R}^{n_{\boldsymbol{\theta}}}$. Moreover, the functions $\mathbf{f}$, $\mathbf{T}$, $\boldsymbol{\Omega}$, φ 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 OC($\boldsymbol{\theta}_0$). We assume that the following two constraint qualifications hold [74][1]:

1. $\operatorname{rank}\left(\{\mathbf{T}^a_\mathbf{x}(\mathbf{x}^*(t_\mathrm{f}), \theta_0)\}\right) = n_{\mathbf{T}^a}$,
2. $\operatorname{rank}\left(\{\boldsymbol{\Omega}^a_\mathbf{u}(t, \mathbf{x}^*(t), \mathbf{u}^*(t), \theta_0)\}\right) = n_{\boldsymbol{\Omega}^a}(t), \quad \forall\, t \in [t_0, t_\mathrm{f}]$,

where $n_{\mathbf{T}^a}$ and $n_{\boldsymbol{\Omega}^a}(t)$ denote the numbers of active terminal constraints and the number of active path constraints at time t, respectively. Introducing the Hamiltonian function $\mathcal{H}$,

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

and assuming that the problem OC($\boldsymbol{\theta}_0$) is not abnormal, the following first-order necessary conditions of optimality must hold almost everywhere in $[t_0, t_\mathrm{f}]$ [54]:

[1] The notation $\mathbf{y}_\mathbf{z}$ is used for the Jacobian matrix of the vector $\mathbf{y}$ with respect to the vector $\mathbf{z}$ [68].

$$\mathbf{0} = \mathcal{H}_{\mathbf{u}}(t, \mathbf{x}^*(t), \mathbf{u}^*(t), \boldsymbol{\lambda}^*(t), \boldsymbol{\theta}_0), \tag{4.5}$$

$$\dot{\boldsymbol{\lambda}}^*(t) = -\mathcal{H}_{\mathbf{x}}(t, \mathbf{x}^*(t), \mathbf{u}^*(t), \boldsymbol{\lambda}^*(t), \boldsymbol{\theta}_0), \tag{4.6}$$

$$\begin{aligned} \boldsymbol{\lambda}^*(t_\mathrm{f}) &= \varphi_{\mathbf{x}}(\mathbf{x}^*(t_\mathrm{f}), \boldsymbol{\theta}_0) + \mathbf{T}_{\mathbf{x}}(\mathbf{x}^*(t_\mathrm{f}), \boldsymbol{\theta}_0)^T \boldsymbol{\rho}^*, \\ 0 &= \rho_i^* T_i(\mathbf{x}^*(t_\mathrm{f}), \boldsymbol{\theta}_0), \quad \forall\, i = 1, \ldots, n_{\mathbf{T}}, \\ 0 &\leq \rho_i^*, \quad \forall\, i = 1, \ldots, n_{\mathbf{T}}, \end{aligned} \tag{4.7}$$

$$\begin{aligned} 0 &= \mu_i^*(t) \Omega_i(t, \mathbf{x}^*(t), \mathbf{u}^*(t), \boldsymbol{\theta}_0), \quad \forall\, i = 1, \ldots, n_{\boldsymbol{\Omega}}, \\ 0 &\leq \mu_i^*(t), \quad \forall\, i = 1, \ldots, n_{\boldsymbol{\Omega}}, \end{aligned} \tag{4.8}$$

for some $\boldsymbol{\lambda}^*(t) \in \mathrm{I\!R}^{n_{\mathbf{x}}}$, $\boldsymbol{\mu}^*(t) \in \mathrm{I\!R}^{n_{\boldsymbol{\Omega}}}$, $t \in [t_0, t_\mathrm{f}]$, and $\boldsymbol{\rho}^* \in \mathrm{I\!R}^{n_{\mathbf{T}}}$.

The vectors of multipliers corresponding to active terminal constraints and active path constraints will be denoted by $\boldsymbol{\rho}^a$ and $\boldsymbol{\mu}^a(t)$, respectively.

Two additional assumptions are made in the analysis that follows in Chapter 5:

1. Strict complementarity slackness holds, i.e.,
   a. the multipliers $\boldsymbol{\rho}^a$ are strictly nonzero, and
   b. if $[a_{ik}, b_{ik}] \subset [t_0, t_\mathrm{f}]$ is an interval of maximal length on which the path constraint Ω_i^* is active, then the corresponding multiplier function $\mu_i^*(t)$ is strictly nonzero for each $t \in (a_{ik}, b_{ik})$ [74].
2. The Hamiltonian function is *regular*, which implies that the optimal inputs $\mathbf{u}^*(t)$ are continuous in $[t_0, t_\mathrm{f}]$ [74].

4.4 Details of the *Nature* of Nominal Optimal Solution

Since the subsequent analysis of the DRTO problem is based on the knowledge of nominal optimal solution, it is necessary to characterize the *nature* of the latter in detail. To this end, the terminology of *switching times* of mixed control-state constraints and related notation are formalized in the following.

For problems having mixed control-state constraints, a constraint can be active over a number of different time intervals, meaning that the number of active constraints may fluctuate over time. To describe this situation, let the structure of the nominal optimal inputs be such that the constraint Ω_i is active on N_i disjoint intervals $[a_{ik}, b_{ik}] \subset [t_0, t_\mathrm{f}]$. Therefore,

$$\Omega_i(t, \mathbf{x}^*(t), \mathbf{u}^*(t), \boldsymbol{\theta}_0) = 0,$$

for each $i = 1, \ldots, n_{\boldsymbol{\Omega}}$ and at each $t \in \{[a_{i1}, b_{i1}], \ldots, [a_{iN_i}, b_{iN_i}]\}$.

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 $\boldsymbol{\Omega}^a(t, \mathbf{x}^*(t), \mathbf{u}^*(t), \boldsymbol{\theta}_0)$. Let the set of all switching times for the nominal solution, together with the initial time t_0 and final time t_f, be denoted by $\mathcal{T}$,

$$\mathcal{T} := \bigcup_{i \in \{1,\ldots,n_{\boldsymbol{\Omega}}\}} \{a_{i1}, b_{i1}, \ldots, a_{iN_i}, b_{iN_i}\} \bigcup \{t_0, t_\mathrm{f}\} \, .$$

Henceforth, the set $\mathcal{T}$ will simply be 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 $[t_k^*, t_{k+1}^*]$ is constant, while the sets of active constraints in different subintervals $[t_k^*, t_{k+1}^*]$ and $[t_l^*, t_{l+1}^*]$ of $[t_0, t_\mathrm{f}]$ are generally different. That is, $\boldsymbol{\Omega}^a(t, \mathbf{x}^*(t), \mathbf{u}^*(t), \boldsymbol{\theta}_0)$ will typically be a different vector function on different subintervals $[t_k^*, t_{k+1}^*]$ and $[t_l^*, t_{l+1}^*]$. To keep notations simple, we still choose to keep the generic notation $\boldsymbol{\Omega}^a$ for vector of active constraints on any subinterval of $[t_0, t_\mathrm{f}]$. In the sequel, care will be taken to associate each vector function $\boldsymbol{\Omega}^a$ with its corresponding subinterval.

Chapter 5

A Directional Variational Analysis of Parametric Optimal Control Problems

In this chapter, we accomplish the task of the directional variational analysis of DRTO problems modeled as parametric optimal control problems (4.1) – (4.4) subject to parametric uncertainty.

The analysis is performed in two steps.

The first step begins with the identification of selective input adaptation directions around the nominal optimal solution. Specifically, the space of input variation functions is split into two orthogonal subsets of directions, namely the sensitivity- and constraint-seeking directions, with the following property:
An input variation along any of the sensitivity-seeking directions will not affect the active terminal and path constraints, whereas an input variation along a constraint-seeking direction will.

In the second step, the effect of different selective input adaptation strategies on cost is analyzed in case of small parametric perturbations. Using the sets of input directions defined previously, it is possible to propose two selective adaptation strategies, for which the *cost variation* obtained with either strategy compared to no adaptation can be quantified.

The important contribution of this chapter will be to establish that, for small parametric perturbations, the cost variation resulting from input adaptation along the sensitivity-seeking directions is typically smaller than that resulting from adaptation along the constraint-seeking directions.

Finally, the results are demonstrated using two real-life optimal control examples.

5.1 Sensitivity- and Constraint-Seeking Directions

The purpose of this section is to introduce the concepts of sensitivity- and constraint-seeking directions in the space of input variation functions. To characterize these directions, small variations of the optimal inputs around their nominal optimal values $\mathbf{u}^*$ are considered and their effect on active terminal and path constraints is studied. As mentioned in the previous chapter, the main challenge here is that the definition of these directions for time t requires that *all* past input variations up to and including time t be taken into account, not merely the input variations at time t.

After defining the directions, selective input adaptation along each set of directions can be defined.

5.1.1 Directions of Invariance

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

$$\tilde{\mathbf{u}}(t;\eta) = \mathbf{u}^*(t) + \eta\,\boldsymbol{\xi}^{\mathbf{u}}(t), \quad \forall\, t \in [t_0, t_\mathrm{f}], \tag{5.1}$$

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 vector functions of size $n_\mathbf{u}$ on $[t_0, t_\mathrm{f}]$.[1] In the sequel, $\boldsymbol{\xi}^{\mathbf{u}}(t)$, as in (5.1), will be called an *input variation function*, or simply *input variation*, and the space $\hat{\mathcal{C}}[t_0, t_\mathrm{f}]^{n_\mathbf{u}}$ will be referred to as the *space of input variation functions*. Parameter η represents the *magnitude* of input variation.

The functions $\boldsymbol{\xi}^{\mathbf{u}}(t)$ can have a finite number of discontinuities over $[t_0, t_\mathrm{f}]$, but the points of discontinuities are not varied with η. In other words, the input variations chosen here act only on the magnitude of the nominal optimal inputs $\mathbf{u}^*(t)$ and not on the associated switching times. Note that parametric perturbations would typically cause variations in *both* the magnitude and the switching times of the optimal inputs [86]. Hence, since the class of input variations defined in (5.1) can only accommodate variations in the magnitude of $\mathbf{u}^*(t)$, the formulation proposed here cannot solve the parametric optimal control problem in full generality. However, this limitation on

[1] The wording 'size of a vector' is used to mean 'number of elements in a vector'.

the class of input variations allows keeping the ensuing analysis relatively simple and tractable.

Let the resulting perturbed states be denoted by $\tilde{\mathbf{x}}$, so that the pair $(\tilde{\mathbf{x}}(t), \tilde{\mathbf{u}}(t))$ satisfies (4.2) for the parameter values $\boldsymbol{\theta}_0$. From the continuous differentiability of $\mathbf{f}$ with respect to inputs and states at $(\mathbf{x}^*(t), \mathbf{u}^*(t))$, Taylor expansion of $\mathbf{f}$ around $(\mathbf{x}^*(t), \mathbf{u}^*(t))$ gives:[2]

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

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

$$\tilde{\mathbf{x}}(t;\eta) = \mathbf{x}^*(t) + \eta\,\boldsymbol{\xi}^{\mathbf{x}}(t) + O(\eta^2), \tag{5.2}$$

where $\boldsymbol{\xi}^{\mathbf{x}}(t)$ satisfies

$$\begin{aligned}\dot{\boldsymbol{\xi}}^{\mathbf{x}}(t) &= \mathbf{f}^*_{\mathbf{x}}[t]\boldsymbol{\xi}^{\mathbf{x}}(t) + \mathbf{f}^*_{\mathbf{u}}[t]\boldsymbol{\xi}^{\mathbf{u}}(t), \quad \forall\, t \in [t^*_{k-1}, t^*_k),\ k = 1, \ldots, N, \\ \boldsymbol{\xi}^{\mathbf{x}}(t_0) &= \mathbf{0}; \qquad \boldsymbol{\xi}^{\mathbf{x}}(t^{*+}_k) = \boldsymbol{\xi}^{\mathbf{x}}(t^{*-}_k), \quad k = 1, \ldots, N-1.\end{aligned} \tag{5.3}$$

The unique solution to the above linear system can be written in the form [94]

$$\boldsymbol{\xi}^{\mathbf{x}}(t) = \boldsymbol{\Phi}^{\mathbf{f}^*_{\mathbf{x}}}(t, t^*_{k-1})\boldsymbol{\xi}^{\mathbf{x}}(t^*_{k-1}) + \int_{t^*_{k-1}}^{t} \boldsymbol{\Phi}^{\mathbf{f}^*_{\mathbf{x}}}(t,s)\mathbf{f}^*_{\mathbf{u}}[s]\boldsymbol{\xi}^{\mathbf{u}}(s)\,ds \tag{5.4}$$

$$= \sum_{i=1}^{k-1} \int_{t^*_{i-1}}^{t^*_i} \boldsymbol{\Phi}^{\mathbf{f}^*_{\mathbf{x}}}(t,s)\mathbf{f}^*_{\mathbf{u}}[s]\boldsymbol{\xi}^{\mathbf{u}}(s)\,ds + \int_{t^*_{k-1}}^{t} \boldsymbol{\Phi}^{\mathbf{f}^*_{\mathbf{x}}}(t,s)\mathbf{f}^*_{\mathbf{u}}[s]\boldsymbol{\xi}^{\mathbf{u}}(s)\,ds, \tag{5.5}$$

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

$$\dot{\mathbf{z}}(t) = \mathbf{A}(t)\mathbf{z}(t),\ \forall\, t \geq t_0; \quad \mathbf{z}(t_0) = \mathbf{z}_0. \tag{5.6}$$

Next, consider a general function $\boldsymbol{\psi} \in \hat{\mathcal{C}}[t_0, t_{\mathrm{f}}]^{n_{\mathbf{u}}} \to \mathrm{I\!R}^{n_{\psi}}$ defined as:

[2] The following compact notations are used throughout the chapter: $y^*[t] := y(t, \mathbf{x}^*(t), \mathbf{u}^*(t), \boldsymbol{\theta}_0)$ and $z^*[t_{\mathrm{f}}] := z(\mathbf{x}^*(t_{\mathrm{f}}), \boldsymbol{\theta}_0)$.

$$\boldsymbol{\psi}(\mathbf{u}) := \boldsymbol{\Psi}(\underline{t}, \mathbf{x}(\underline{t}), \mathbf{u}(\underline{t}), \boldsymbol{\theta}),$$

with $\underline{t}$ a fixed time in $(t^*_{k-1}, t^*_k]$, for some $k \in \{1, \ldots, N\}$. The variation in the function $\boldsymbol{\psi}$ caused by the input variation (5.1) can be obtained as the Gâteaux derivative [15, 66, 112] of $\boldsymbol{\psi}$ in the direction $\boldsymbol{\xi}^{\mathbf{u}}$ at $\mathbf{u}^*$:

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

Using (5.4), this variation can be rewritten as

$$\delta\boldsymbol{\psi}(\mathbf{u}^*; \boldsymbol{\xi}^{\mathbf{u}}) = \mathcal{D}_{\boldsymbol{\Psi},\underline{t}}\boldsymbol{\xi}^{\mathbf{u}}, \tag{5.7}$$

where $\mathcal{D}_{\boldsymbol{\Psi},\underline{t}} : \hat{\mathcal{C}}[t_0, t_{\mathrm{f}}]^{n_{\mathbf{u}}} \to \mathrm{IR}^{n_{\boldsymbol{\psi}}}$ is the linear operator

$$\mathcal{D}_{\boldsymbol{\Psi},\underline{t}}\boldsymbol{\xi} := \boldsymbol{\Psi}^*_{\mathbf{x}}[\underline{t}]\left[\sum_{i=1}^{k-1}\int_{t^*_{i-1}}^{t^*_i}\boldsymbol{\Phi}^{\mathbf{f}^*_{\mathbf{x}}}(\underline{t}, s)\mathbf{f}^*_{\mathbf{u}}[s]\boldsymbol{\xi}(s)\,ds + \int_{t^*_{k-1}}^{\underline{t}}\boldsymbol{\Phi}^{\mathbf{f}^*_{\mathbf{x}}}(\underline{t}, s)\mathbf{f}^*_{\mathbf{u}}[s]\boldsymbol{\xi}(s)\,ds\right] + \boldsymbol{\Psi}^*_{\mathbf{u}}[\underline{t}]\boldsymbol{\xi}(\underline{t}).$$

If the value of $\boldsymbol{\psi}$ remains unaffected by a small variation in the direction $\boldsymbol{\xi}^{\mathbf{u}}$ around $\mathbf{u}^*$, then $\boldsymbol{\xi}^{\mathbf{u}}$ is called a *direction of invariance of* $\boldsymbol{\psi}$ *at* $\mathbf{u}$. This concept is formalized in the following definition.

Definition 5.1 (Direction of Invariance of $\boldsymbol{\psi}$ at $\mathbf{u}$)
A function $\boldsymbol{\xi}^{\mathbf{u}} \in \hat{\mathcal{C}}[t_0, t_{\mathrm{f}}]^{n_{\mathbf{u}}}$ *is called* a direction of invariance *for the function* $\boldsymbol{\psi}$ *at* $\mathbf{u}$ *and for* $\underline{t} \in [t_0, t_{\mathrm{f}}]$*, if*

$$\mathcal{D}_{\boldsymbol{\Psi},\underline{t}}\boldsymbol{\xi}^{\mathbf{u}} = \mathbf{0}.$$

Clearly, any linear combination of directions of invariance for the function $\boldsymbol{\psi}$ is itself a direction of invariance. Therefore, the set of all directions of invariance for $\boldsymbol{\psi}$, denoted by

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

is a subspace of $\hat{\mathcal{C}}[t_0, t_{\mathrm{f}}]^{n_{\mathbf{u}}}$.

5.1.2 Characterization of Sensitivity- and Constraint-Seeking Directions

A sensitivity-seeking direction at the nominal optimal solution $\mathbf{u}^*$ corresponds to a direction in the space of input variation functions along which an infinitesimal variation of $\mathbf{u}^*$ leaves the active constraints unchanged. A formal definition can now be provided based on the concept of direction of invariance introduced previously.

Definition 5.2 (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 OC($\boldsymbol{\theta}_0$) at* $\mathbf{u}^*$ *if* $\boldsymbol{\xi}^{\mathbf{u}}$ *is a direction of invariance for:*

1. *the active terminal constraints* $\mathbf{T}^a(\tilde{\mathbf{x}}(t_{\mathrm{f}};\eta), \boldsymbol{\theta}_0)$,

$$\mathbf{0} = \mathcal{D}_{\mathbf{T}^a,t_{\mathrm{f}}}\boldsymbol{\xi}^{\mathbf{u}} = \mathbf{T}^a_{\mathbf{x}}[t_{\mathrm{f}}] \sum_{k=1}^{N} \int_{t^*_{k-1}}^{t^*_k} \boldsymbol{\Phi}^{\mathbf{f}^*_{\mathbf{x}}}(t_{\mathrm{f}}, s)\mathbf{f}^*_{\mathbf{u}}[s]\boldsymbol{\xi}^{\mathbf{u}}(s)\, ds, \tag{5.8}$$

and

2. *the active path constraints* $\boldsymbol{\Omega}^a(t, \tilde{\mathbf{x}}(t;\eta), \tilde{\mathbf{u}}(t;\eta), \boldsymbol{\theta}_0)$,

$$\begin{aligned}\mathbf{0} = \mathcal{D}_{\boldsymbol{\Omega}^a,t}\boldsymbol{\xi}^{\mathbf{u}} = \boldsymbol{\Omega}^a_{\mathbf{x}}[t] &\left[\sum_{i=1}^{k-1} \int_{t^*_{i-1}}^{t^*_i} \boldsymbol{\Phi}^{\mathbf{f}^*_{\mathbf{x}}}(t, s)\mathbf{f}^*_{\mathbf{u}}[s]\boldsymbol{\xi}_{\mathbf{u}}(s)\, ds + \int_{t^*_{k-1}}^{t} \boldsymbol{\Phi}^{\mathbf{f}^*_{\mathbf{x}}}(t, s)\mathbf{f}^*_{\mathbf{u}}[s]\boldsymbol{\xi}_{\mathbf{u}}(s)\, ds\right] \\ &+ \boldsymbol{\Omega}^a_{\mathbf{u}}[t]\boldsymbol{\xi}^{\mathbf{u}}(t),\end{aligned} \tag{5.9}$$

at each $t \in (t^*_{k-1}, t^*_k]$, $k = 1, \ldots, N$.

Let the set of sensitivity-seeking (SS) directions for OC($\boldsymbol{\theta}_0$) at $\mathbf{u}^*$ be denoted by

$$\begin{aligned}\mathcal{V}^s &:= \{\boldsymbol{\xi}^{\mathbf{u}} \in \hat{\mathcal{C}}[t_0, t_{\mathrm{f}}]^{n_{\mathbf{u}}} : \mathcal{D}_{\mathbf{T}^a,t_{\mathrm{f}}}\boldsymbol{\xi}^{\mathbf{u}} = \mathbf{0} \text{ and } \mathcal{D}_{\boldsymbol{\Omega}^a,t}\boldsymbol{\xi}^{\mathbf{u}} = \mathbf{0}, \quad t_0 \le t \le t_{\mathrm{f}}\} \\ &= \mathcal{V}_{\mathbf{T}^a,t_{\mathrm{f}}} \bigcap \left(\bigcap_{t\in[t_0,t_{\mathrm{f}}]} \mathcal{V}_{\boldsymbol{\Omega}^a,t}\right).\end{aligned}$$

Clearly, $\mathcal{V}^s$ is a subspace of $\hat{\mathcal{C}}[t_0, t_{\mathrm{f}}]^{n_{\mathbf{u}}}$, by properties of the sets of invariance $\mathcal{V}_{\mathbf{T}^a,t_{\mathrm{f}}}$ and $\mathcal{V}_{\boldsymbol{\Omega}^a,t}$. It is referred to as the *sensitivity-seeking subspace* for OC($\boldsymbol{\theta}_0$) at $\mathbf{u}^*$ thereafter.

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

Definition 5.3 (Constraint-seeking Directions)
A function $\boldsymbol{\xi}^{\mathbf{u}} \in \hat{\mathcal{C}}[t_0, t_f]^{n_{\mathbf{u}}}$ *is called a* constraint-seeking direction *for the optimal control problem OC(*$\boldsymbol{\theta}_0$*) at* $\mathbf{u}^*$ *if* $\boldsymbol{\xi}^{\mathbf{u}}$ *is orthogonal to* $\mathcal{V}^s$*,*

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

in the sense of a given inner product $\langle \cdot, \cdot \rangle$ *on* $\hat{\mathcal{C}}[t_0, t_f]^{n_{\mathbf{u}}}$*.*

In the sequel, the following inner product on $\hat{\mathcal{C}}[t_0, t_f]^{n_{\mathbf{u}}}$ will be chosen to define the CS directions:

$$\langle \boldsymbol{\sigma}, \boldsymbol{\varphi} \rangle := \int_{t_0}^{t_f} \boldsymbol{\sigma}(t)^T \boldsymbol{\varphi}(t)\, dt, \quad \boldsymbol{\sigma}, \boldsymbol{\varphi} \in \hat{\mathcal{C}}[t_0, t_f]^{n_{\mathbf{u}}}. \tag{5.10}$$

Denote the set of all CS directions for OC($\boldsymbol{\theta}_0$) at $\mathbf{u}^*$ by $\mathcal{V}^c$. By the sesquilinearity property of an inner product, $\mathcal{V}^c$ is itself a subspace of $\hat{\mathcal{C}}[t_0, t_f]^{n_{\mathbf{u}}}$. It is referred to as the *constraint-seeking subspace* for OC($\boldsymbol{\theta}_0$) at $\mathbf{u}^*$ subsequently.

Thus, the SS and CS subspaces can be seen as a property of the nominal optimal solution $\mathbf{u}^*$ of OC($\boldsymbol{\theta}$).

Lemma 5.1
No non-zero $\mathbf{v}_c \in \mathcal{V}^c$ *satisfies* (5.8) *and* (5.9)*,*

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

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 $\boldsymbol{\xi} = \mathbf{0}$. □

The concept of *selective input adaptation* can now be defined formally.

Definition 5.4 (Selective Input Adaptation)
The process of adapting the nominal optimal inputs $\mathbf{u}^*$ *according to* (5.1) *in any nonzero direction* $\boldsymbol{\xi}^{\mathbf{u}} \in \mathcal{V}^s$ *is called* selective input adaptation along a SS direction. *Likewise, the process of adapting* $\mathbf{u}^*$ *in any nonzero direction* $\boldsymbol{\xi}^{\mathbf{u}} \in \mathcal{V}^c$ *is called* selective input adaptation along a CS direction.

Subscript s or c will henceforth be added to various notations to indicate a SS or a CS direction of input adaptation, respectively.

5.1.3 Numerical Procedure to Compute Sensitivity- and Constraint-Seeking Directions

This section proposes a numerical procedure to compute the SS and CS components of a given input variation.

Since the procedure is numerical, the direction of input variation under consideration will be a function that can be represented in terms of a finite number of basis functions $\chi_i \in \hat{\mathcal{C}}[t_0, t_\mathrm{f}]^{n_\mathbf{u}}$, $i = 1, \ldots, m$:

$$\boldsymbol{\xi}^\mathbf{u}(t) := \mathcal{U}(t, \boldsymbol{\xi}^{\boldsymbol{\omega}}) = \sum_{i=1}^{m} \boldsymbol{\xi}_i^{\omega} \chi_i(t), \quad t \in [t_0, t_\mathrm{f}], \tag{5.11}$$

where $\boldsymbol{\xi}^{\boldsymbol{\omega}} \in \mathrm{I\!R}^M$, $M = mn_\mathbf{u}$, denotes the vector obtained by *appending* the vectors $\boldsymbol{\xi}_i^{\omega} \in \mathrm{I\!R}^{n_\mathbf{u}}$, $i = 1, \ldots, m$, that is,

$$\boldsymbol{\xi}^{\boldsymbol{\omega}} := \begin{bmatrix} \boldsymbol{\xi}_1^{\omega} \\ \vdots \\ \boldsymbol{\xi}_m^{\omega} \end{bmatrix}. \tag{5.12}$$

Note that the vectors $\boldsymbol{\xi}_i^{\omega}$, $i = 1, \ldots, m$, do not depend on i; the index i only denotes their association with particular basis functions in (5.11).

In the sequel, we will consider a special case of (5.11), viz., when the *given* input variation $\mathcal{U}(t, \boldsymbol{\xi}^{\boldsymbol{\omega}})$ is a vector of $n_\mathbf{u}$ piecewise-constant functions on $[t_0, t_\mathrm{f}]$, such that the points of discontinuity of all elements of $\mathcal{U}(t, \boldsymbol{\xi}^{\boldsymbol{\omega}})$ are fixed at $t_i \in (t_0, t_\mathrm{f})$, $i = 1, \ldots, m-1$, and the times t_i divide $[t_0, t_\mathrm{f}]$ in m sub-intervals of equal length:

$$\mathcal{U}(t, \boldsymbol{\xi}^{\boldsymbol{\omega}}) = \boldsymbol{\xi}_i^{\omega}, \quad \forall\, t \in [t_{i-1}, t_i], \quad i = 1, \ldots, m, \tag{5.13}$$

$$\frac{t_\mathrm{f} - t_0}{m} = t_i - t_{i-1}, \quad i = 1, \ldots, m, \tag{5.14}$$

where the symbol t_m corresponds to the final time t_f.

5.1.3.1 Projection of a given Input Variation on the SS and CS Subspaces

Consider a specified direction $\boldsymbol{\xi}^{\mathbf{u}}(t) := \mathcal{U}(t, \boldsymbol{\xi}^{\boldsymbol{\omega}})$ of type (5.13), for which we would like to compute the SS and CS components $\boldsymbol{\xi}_s^{\mathbf{u}} \in \mathcal{V}_s$ and $\boldsymbol{\xi}_c^{\mathbf{u}} \in \mathcal{V}_c$.

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 parametric optimal control problem by a parametric nonlinear program (NLP):

1. Approximate the input profiles $\mathbf{u}(t)$ using the parametrization (5.13) as:

$$\mathbf{u}(t) \approx \mathcal{U}(t, \boldsymbol{\omega}), \quad \forall\, t \in [t_0, t_{\mathrm{f}}], \tag{5.15}$$

   where $\boldsymbol{\omega} \in \mathbb{R}^M$ denotes the vector obtained by appending the vectors $\boldsymbol{\omega}_i \in \mathbb{R}^{n_{\mathbf{u}}}$, $i = 1, \ldots, m$, that is,

$$\boldsymbol{\omega} := \begin{bmatrix} \boldsymbol{\omega}_1 \\ \vdots \\ \boldsymbol{\omega}_m \end{bmatrix}.$$

2. Use the *control parametrization* technique to transform the optimal control problem OC($\boldsymbol{\theta}$) into a parametric NLP in terms of the decision variables $\boldsymbol{\omega}$ [47]; note that:
   The path constraints $\boldsymbol{\Omega}$ in OC($\boldsymbol{\theta}$) will have to be transformed into a set of p discrete – typically nonlinear – constraints in the variables $\boldsymbol{\omega}$. The latter, together with the terminal constraints $\mathbf{T}$ in OC($\boldsymbol{\theta}$), will be denoted by $\mathbf{G}(\boldsymbol{\omega}, \boldsymbol{\theta})$. Note also that p may be chosen equal to m for simplicity. Let the resulting pNLP be denoted as follows:

$$\begin{aligned} \min_{\boldsymbol{\omega} \in \mathbb{R}^{n_{\boldsymbol{\omega}}}} \quad & J(\boldsymbol{\omega}, \boldsymbol{\theta}) \\ \text{s. t.} \quad & G_i(\boldsymbol{\omega}, \boldsymbol{\theta}) \leq 0, \quad i = 1, \ldots, n_{\mathbf{G}}. \end{aligned} \tag{5.16}$$

3. Solve the pNLP (5.16) 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. Compute the Jacobian matrix $\mathbf{G}^a_{\boldsymbol{\omega}}$ at $\boldsymbol{\omega}^*$, and use its singular value decomposition (SVD)[3]

$$\mathbf{G}^a_{\boldsymbol{\omega}} = \mathbf{U}\boldsymbol{\Sigma}\left[\mathbf{V}_c\ \mathbf{V}_s\right]^T,$$

to determine the orthogonal matrices $\mathbf{V}_s$ and $\mathbf{V}_c$ that define, respectively, the SS and CS directions for the NLP (5.16); see [16, 37] for details.

It is worth pointing out that the properties of the SVD ensure that the column space of $\mathbf{V}_s$, called SS subspace of the underlying NLP [16], is the null space of the Jacobian of active constraints. Hence, as remarked in Section 2.3.3, when *strict complementarity* condition holds for the NLP, the SS subspace coincides with the null space $\mathcal{N}^s$ of the Jacobian of strongly active constraints defined in (2.11).
5. Compute $\boldsymbol{\xi}^{\boldsymbol{\omega}}$, as in (5.12), from the given input variation $\boldsymbol{\xi}^{\mathbf{u}}(t)$ using (5.11).
6. Compute the orthogonal projections of the vector $\boldsymbol{\xi}^{\boldsymbol{\omega}}$ on the column space of $\mathbf{V}_s$ and $\mathbf{V}_c$:

$$\begin{aligned}\boldsymbol{\xi}^{\boldsymbol{\omega}}_s &= \mathbf{V}_s{\mathbf{V}_s}^T\boldsymbol{\xi}^{\boldsymbol{\omega}},\\ \boldsymbol{\xi}^{\boldsymbol{\omega}}_c &= \mathbf{V}_c{\mathbf{V}_c}^T\boldsymbol{\xi}^{\boldsymbol{\omega}}.\end{aligned} \tag{5.17}$$

7. Obtain the approximations of the desired SS and CS components $\boldsymbol{\xi}^{\mathbf{u}}_s(t)$ and $\boldsymbol{\xi}^{\mathbf{u}}_c(t)$ using the parameterization (5.13):

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

Steps 5 to 7 are depicted in Figure 5.1.

Next we show that, *as desired*, the computed functions $\mathcal{U}(t,\boldsymbol{\xi}^{\boldsymbol{\omega}}_s)$ and $\mathcal{U}(t,\boldsymbol{\xi}^{\boldsymbol{\omega}}_c)$ are orthogonal under the chosen inner product (5.10) on $\hat{\mathcal{C}}[t_0,t_\mathrm{f}]^{n_\mathbf{u}}$.

Lemma 5.2
$\langle\, \mathcal{U}(t,\boldsymbol{\xi}^{\boldsymbol{\omega}}_s), \mathcal{U}(t,\boldsymbol{\xi}^{\boldsymbol{\omega}}_c)\,\rangle = 0$, *where the inner product* $\langle .,. \rangle$ *is as defined in* (5.10).

Proof:

We first note that the vectors $\boldsymbol{\xi}^{\boldsymbol{\omega}}_s$ and $\boldsymbol{\xi}^{\boldsymbol{\omega}}_c$ are orthogonal under the standard inner product on the Euclidean space $\mathbb{R}^{n_\mathbf{u}}$ [16]:

$$(\boldsymbol{\xi}^{\boldsymbol{\omega}}_s)^T\boldsymbol{\xi}^{\boldsymbol{\omega}}_c = 0. \tag{5.18}$$

[3] It is assumed that $\mathbf{G}^a_{\boldsymbol{\omega}}$ of the resulting NLP (5.16) is full rank.

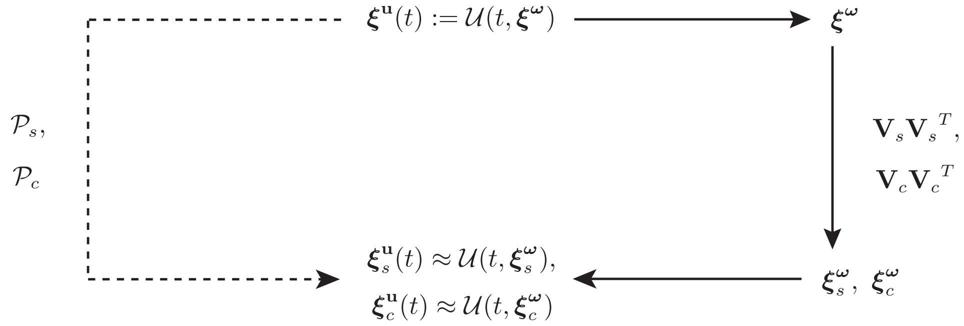

Figure 5.1 Computation of SS and CS directions. Exact computations (dotted arrow), approximate computations (solid arrows). $\mathcal{P}_s$ and $\mathcal{P}_c$ denote the projection operators from $\mathcal{V}$ on $\mathcal{V}_s$ and $\mathcal{V}_c$, respectively.

Next, consider the inner product of $\mathcal{U}(t, \boldsymbol{\xi}_s^{\boldsymbol{\omega}})$ and $\mathcal{U}(t, \boldsymbol{\xi}_c^{\boldsymbol{\omega}})$ as per (5.10):

$$\begin{aligned}
\langle \mathcal{U}(t, \boldsymbol{\xi}_s^{\boldsymbol{\omega}}), \mathcal{U}(t, \boldsymbol{\xi}_c^{\boldsymbol{\omega}}) \rangle &= \int_{t_0}^{t_\mathrm{f}} \mathcal{U}(t, \boldsymbol{\xi}_s^{\boldsymbol{\omega}})^T \mathcal{U}(t, \boldsymbol{\xi}_c^{\boldsymbol{\omega}})\, dt, \\
&= \sum_{i=1}^{m} \int_{t_{i-1}}^{t_i} (\boldsymbol{\xi}_s^{\boldsymbol{\omega}})_i^T\, (\boldsymbol{\xi}_c^{\boldsymbol{\omega}})_i\, dt, \quad \text{due to (5.13)}, \\
&= \sum_{i=1}^{m} (\boldsymbol{\xi}_s^{\boldsymbol{\omega}})_i^T\, (\boldsymbol{\xi}_c^{\boldsymbol{\omega}})_i \left(\frac{t_\mathrm{f} - t_0}{m} \right), \quad \text{due to (5.14)}, \\
&= \left(\frac{t_\mathrm{f} - t_0}{m} \right) (\boldsymbol{\xi}_s^{\boldsymbol{\omega}})^T \boldsymbol{\xi}_c^{\boldsymbol{\omega}}, \\
&= 0, \quad \text{due to (5.18)}.
\end{aligned}$$

Hence, the approximate directions $\mathcal{U}(t, \boldsymbol{\xi}_s^{\boldsymbol{\omega}})$ and $\mathcal{U}(t, \boldsymbol{\xi}_c^{\boldsymbol{\omega}})$ are orthogonal with respect to the inner product (5.10). □

It can further be shown that

$$\mathcal{U}(t, \boldsymbol{\xi}^{\boldsymbol{\omega}}) = \mathcal{U}(t, \boldsymbol{\xi}_c^{\boldsymbol{\omega}}) + \mathcal{U}(t, \boldsymbol{\xi}_s^{\boldsymbol{\omega}}), \quad \forall\, t \in [t_0, t_\mathrm{f}], \tag{5.19}$$

using the following property of the SVD [62] that was also mentioned in Section 1.2.2:

$$\mathbf{V}_s{\mathbf{V}_s}^T + \mathbf{V}_c{\mathbf{V}_c}^T = \mathbf{I}.$$

It should be noted that, it is also possible to subdivide each of the m sub-intervals of $[t_0, t_\mathrm{f}]$ in (5.15) in even smaller sub-intervals and to obtain another, and more refined, re-parameterization of type (5.13) in terms of m^+ variables such that $m^+ \gg m$.

5.2 Selective Input Adaptation under Parametric Uncertainty

Parametric perturbations of the following form are considered in this section:

$$\tilde{\boldsymbol{\theta}}(\eta) := \boldsymbol{\theta}_0 + \eta\, \boldsymbol{\xi}^{\boldsymbol{\theta}}, \quad \eta \in [-\eta^\circ, \eta^\circ], \quad \eta^\circ \ll 1, \tag{5.20}$$

where $\boldsymbol{\xi}^{\boldsymbol{\theta}}$ is a given direction in $\mathbb{R}^{n_{\boldsymbol{\theta}}}$.

For the purpose of this analysis, it is assumed that the magnitude η and direction $\boldsymbol{\xi}^{\boldsymbol{\theta}}$ of the parametric perturbations are known. The idea is to use an input adaptation of type (5.1) to compensate for the effect of the parametric perturbations (5.20). In particular, the aim is to assess the cost variation following input adaptation along either SS or CS directions in comparison to no adaptation.

5.2.1 Effect of Input Adaptation on Cost

If one wishes to avoid repeating the whole solution procedure to compute the optimal inputs $\tilde{\mathbf{u}}^*(t)$ for the perturbed system, two options are available:

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 (4.2) for $\tilde{\boldsymbol{\theta}}$. Since $\mathbf{f}$ is continuously differentiable with respect to $\mathbf{x}$ and $\boldsymbol{\theta}$, $\hat{\mathbf{x}}(t)$ has a first-order approximation around $\mathbf{x}^*(t)$ given by:

$$\hat{\mathbf{x}}(t;\eta) = \mathbf{x}^*(t) + \eta\boldsymbol{\xi}^{\hat{\mathbf{x}}}(t) + O(\eta^2), \tag{5.21}$$

   where

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

2. **Input Adaptation:**
The nominal optimal inputs are adapted according to (5.1) along a direction $\boldsymbol{\xi}^{\mathbf{u}} \in \hat{\mathcal{C}}[t_0, t_{\mathrm{f}}]^{n_{\mathbf{u}}}$, using the magnitude of parametric perturbation η as the magnitude of input variation. The resulting inputs $\tilde{\mathbf{u}}(t;\eta)$ are then applied to the perturbed system. Let the pair of perturbed states and resulting cost be denoted by $(\tilde{\mathbf{x}}(t), \tilde{J})$. Hence, $(\tilde{\mathbf{x}}(t), \tilde{\mathbf{u}}(t;\eta))$ satisfies (4.2) for $\tilde{\boldsymbol{\theta}}$. Since $\mathbf{f}$ is continuously differentiable with respect to $\mathbf{x}$, $\mathbf{u}$ and $\boldsymbol{\theta}$, the first-order approximation of $\tilde{\mathbf{x}}(t)$ around $\mathbf{x}^*(t)$ is given by:
$$\tilde{\mathbf{x}}(t;\eta) = \mathbf{x}^*(t) + \eta\boldsymbol{\xi}^{\tilde{\mathbf{x}}}(t) + O(\eta^2), \tag{5.22}$$
where
$$\dot{\boldsymbol{\xi}}^{\tilde{\mathbf{x}}}(t) = \mathbf{f}_{\mathbf{x}}[t]\boldsymbol{\xi}^{\tilde{\mathbf{x}}}(t) + \mathbf{f}_{\mathbf{u}}[t]\boldsymbol{\xi}^{\mathbf{u}}(t) + \mathbf{f}_{\boldsymbol{\theta}}[t]\boldsymbol{\xi}^{\boldsymbol{\theta}},$$
$$\boldsymbol{\xi}^{\tilde{\mathbf{x}}}(t_0) = \mathbf{h}_{\boldsymbol{\theta}}(\boldsymbol{\theta}_0)\boldsymbol{\xi}^{\boldsymbol{\theta}}.$$

Evidently, both of the above options will result in sub-optimal process operation, although Option 2 can be expected to perform better under judicious choice of the adaptation directions. The cost difference between input adaptation and no adaptation is
$$\delta J(\boldsymbol{\xi}^{\mathbf{u}}) := \tilde{J} - \hat{J}, \tag{5.23}$$
and is termed *cost variation* resulting from input adaptation. The objective in the next subsection will be to compare the cost variations $\delta J(\boldsymbol{\xi}^{\mathbf{u}}_s)$ and $\delta J(\boldsymbol{\xi}^{\mathbf{u}}_c)$.

5.2.2 Cost Variation Resulting from Selective Input Adaptation

A variational analysis will be conducted to assess the cost variation resulting from selective input adaptation. It should be noted that the directions $\boldsymbol{\xi}^{\mathbf{u}}_s$ and $\boldsymbol{\xi}^{\mathbf{u}}_c$ that will be used for the selective input adaptation are *general* directions in the infinite-dimensional spaces $\mathcal{V}_s$ and $\mathcal{V}_c$, respectively. Hence, the aim of the following analysis is to quantify the cost variations resulting from input adaptations along any general directions in $\mathcal{V}_s$ and $\mathcal{V}_c$. In particular, the subsequent analysis does not address the issue of how close the adapted costs are to the perturbed optimal cost.

For the purpose of the variational analysis, the cost functionals are augmented as follows [13]:

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

for some multiplier functions $\boldsymbol{\pi}(t) \in \mathcal{C}^1[t_0, t_\mathrm{f}]^{n_\mathbf{x}}$, where $\mathcal{C}^1[t_0, t_\mathrm{f}]^{n_\mathbf{x}}$ represents the linear space of continuously differentiable vector functions of size $n_\mathbf{x}$ on $[t_0, t_\mathrm{f}]$.

Using integration by parts, the expression for J^a can be rearranged as follows:

$$J^a = \varphi(\mathbf{x}(t_\mathrm{f}), \boldsymbol{\theta}) + \sum_{k=1}^{N} \left[\boldsymbol{\pi}(t_{k-1}^*)^T \mathbf{x}(t_{k-1}^*) - \boldsymbol{\pi}(t_k^*)^T \mathbf{x}(t_k^*)\right] + \sum_{k=1}^{N} \int_{t_{k-1}^*}^{t_k^*} \left[\phi(t, \mathbf{x}(t), \mathbf{u}(t), \boldsymbol{\theta}) + \boldsymbol{\pi}(t)^T \mathbf{f}(t, \mathbf{x}(t), \mathbf{u}(t), \boldsymbol{\theta}) + \dot{\boldsymbol{\pi}}(t)^T \mathbf{x}(t)\right] dt. \tag{5.24}$$

If the pair $(\mathbf{x}(t), \mathbf{u}(t))$ satisfies (4.2) for $\boldsymbol{\theta}$, then $J^a = J$ for *any* multiplier function $\boldsymbol{\pi}(t)$. It follows that, minimizing J with respect to $\mathbf{u}$ is equivalent to minimizing J^a with respect to $\mathbf{u}(t)$.

Since both pairs $(\tilde{\mathbf{x}}(t), \tilde{\mathbf{u}}(t))$ and $(\hat{\mathbf{x}}(t), \mathbf{u}^*(t))$ satisfy (4.2) for $\tilde{\boldsymbol{\theta}}$ and $\tilde{\mathbf{x}}(t_0) = \hat{\mathbf{x}}(t_0) = \mathbf{h}(\tilde{\boldsymbol{\theta}})$, the cost variation in (5.23) can be written as[4]

$$\delta J(\boldsymbol{\xi}^\mathbf{u}) = \tilde{\varphi}[t_\mathrm{f}] - \hat{\varphi}[t_\mathrm{f}] + \sum_{k=1}^{N} \left[\boldsymbol{\pi}(t_{k-1}^*)^T \left\{\tilde{\mathbf{x}}(t_{k-1}^*) - \hat{\mathbf{x}}(t_{k-1}^*)\right\} - \boldsymbol{\pi}(t_k^*)^T \left\{\tilde{\mathbf{x}}(t_k^*) - \hat{\mathbf{x}}(t_k^*)\right\}\right] + \sum_{k=1}^{N} \int_{t_{k-1}^*}^{t_k^*} \left[\tilde{\phi}[t] - \hat{\phi}[t] + \boldsymbol{\pi}(t)^T \left\{\tilde{\mathbf{f}}[t] - \hat{\mathbf{f}}[t]\right\} + \dot{\boldsymbol{\pi}}(t)^T \left\{\tilde{\mathbf{x}}(t) - \hat{\mathbf{x}}(t)\right\}\right] dt. \tag{5.25}$$

Taylor expanding $\tilde{\varphi}[t_\mathrm{f}]$, $\tilde{\phi}[t]$ and $\tilde{\mathbf{f}}[t]$ around $(\hat{\mathbf{x}}(t), \mathbf{u}^*(t))$ and rearranging the terms in (5.25) using (5.21) and (5.22) gives:

[4] The additional 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 chapter.

$$\delta J(\boldsymbol{\xi}^{\mathbf{u}}) = \eta \Bigg(\left[\hat{\varphi}_{\mathbf{x}}[t_{\mathrm{f}}]^T - \boldsymbol{\pi}(t_{\mathrm{f}})^T\right] \left[\boldsymbol{\xi}^{\tilde{\mathbf{x}}}(t_{\mathrm{f}}) - \boldsymbol{\xi}^{\hat{\mathbf{x}}}(t_{\mathrm{f}})\right]$$
$$+ \sum_{k=1}^{N} \int_{t_{k-1}^*}^{t_k^*} \left[\hat{\phi}_{\mathbf{x}}[t]^T + \boldsymbol{\pi}(t)^T \hat{\mathbf{f}}_{\mathbf{x}}[t] + \dot{\boldsymbol{\pi}}(t)^T\right] \left[\boldsymbol{\xi}^{\tilde{\mathbf{x}}}(t) - \boldsymbol{\xi}^{\hat{\mathbf{x}}}(t)\right] dt$$
$$+ \sum_{k=1}^{N} \int_{t_{k-1}^*}^{t_k^*} \left[\hat{\phi}_{\mathbf{u}}[t]^T + \boldsymbol{\pi}(t)^T \hat{\mathbf{f}}_{\mathbf{u}}[t]\right] \boldsymbol{\xi}^{\mathbf{u}}(t)\, dt \Bigg) + O(\eta^2). \tag{5.26}$$

Since the multiplier functions $\boldsymbol{\pi}(t)$ are arbitrary, they can be specialized as the (unique) solution $\hat{\boldsymbol{\pi}}$ to the following linear system:

$$\dot{\hat{\boldsymbol{\pi}}}(t) = -\hat{\mathbf{f}}_{\mathbf{x}}[t]^T \hat{\boldsymbol{\pi}}(t) - \hat{\phi}_{\mathbf{x}}[t], \tag{5.27}$$
$$\hat{\boldsymbol{\pi}}(t_{\mathrm{f}}) = \hat{\varphi}_{\mathbf{x}}[t_{\mathrm{f}}].$$

This way, and after 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 variation reduces to:

$$\delta J(\boldsymbol{\xi}^{\mathbf{u}}) = \eta \sum_{k=1}^{N} \int_{t_{k-1}^*}^{t_k^*} \left(\phi_{\mathbf{u}}^*[t]^T + \hat{\boldsymbol{\pi}}(t)^T \mathbf{f}_{\mathbf{u}}^*[t]\right) \boldsymbol{\xi}^{\mathbf{u}}(t)\, dt + O(\eta^2). \tag{5.28}$$

Since the optimality condition (4.5) holds along the nominal optimal trajectory $\mathbf{u}^*(t)$, (5.28) can be rewritten as

$$\delta J(\boldsymbol{\xi}^{\mathbf{u}}) = \eta \sum_{k=1}^{N} \int_{t_{k-1}^*}^{t_k^*} \left(\left[\hat{\boldsymbol{\pi}}(t) - \boldsymbol{\lambda}^*(t)\right]^T \mathbf{f}_{\mathbf{u}}^*[t] - \boldsymbol{\mu}^a(t)^T \boldsymbol{\Omega}_{\mathbf{u}}^a[t] \right) \boldsymbol{\xi}^{\mathbf{u}}(t)\, dt + O(\eta^2). \tag{5.29}$$

Let $\boldsymbol{\pi}^*(t)$ be the (unique) solution to the following linear system:

$$\dot{\boldsymbol{\pi}}^*(t) = -\mathbf{f}_{\mathbf{x}}^*[t]^T \boldsymbol{\pi}^*(t) - \phi_{\mathbf{x}}^*[t], \tag{5.30}$$
$$\boldsymbol{\pi}^*(t_{\mathrm{f}}) = \varphi_{\mathbf{x}}^*[t_{\mathrm{f}}].$$

Using (5.27) and (5.30), it can be verified that $\hat{\boldsymbol{\pi}}(t)$ has the following first-order approximation around $\boldsymbol{\pi}^*(t)$:

$$\hat{\boldsymbol{\pi}}(t) = \boldsymbol{\pi}^*(t) + \eta\, \boldsymbol{\xi}^{\boldsymbol{\pi}}(t) + O(\eta^2).$$

The term $\{\hat{\boldsymbol{\pi}}(t) - \boldsymbol{\lambda}^*(t)\}$ in (5.29) can thus be rearranged as

$$\hat{\boldsymbol{\pi}}(t) - \boldsymbol{\lambda}^*(t) = \boldsymbol{\beta}(t) + \eta\, \boldsymbol{\xi}^{\boldsymbol{\pi}}(t) + O(\eta^2), \tag{5.31}$$

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

$$\begin{aligned} \dot{\boldsymbol{\beta}}(t) &= -\mathbf{f}_{\mathbf{x}}^*[t]^T \boldsymbol{\beta}(t) + \boldsymbol{\Omega}_{\mathbf{x}}^a[t]^T \boldsymbol{\mu}^a(t), \quad \forall\, t \in (t_{k-1}^*, t_k^*],\ k = 1, \ldots, N, \\ \boldsymbol{\beta}(t_{\mathrm{f}}) &= -\mathbf{T}_{\mathbf{x}}^a[t_{\mathrm{f}}]^T \boldsymbol{\rho}^a, \qquad \boldsymbol{\beta}(t_k^{*-}) = \boldsymbol{\beta}(t_k^{*+}), \quad k = 1, \ldots, N-1, \end{aligned}$$

because $\boldsymbol{\lambda}^*(t)$ satisfies (4.6). The linear dynamic system for $\boldsymbol{\beta}(t)$ has the following unique solution on $[t_0, t_{\mathrm{f}}]$:

$$\begin{aligned} \boldsymbol{\beta}(t) = &- \boldsymbol{\Phi}^{\mathbf{f}_{\mathbf{x}}^*}(t_{\mathrm{f}}, t)^T \mathbf{T}_{\mathbf{x}}^a[t_{\mathrm{f}}]^T \boldsymbol{\rho}^a - \int_t^{t_k^*} \boldsymbol{\Phi}^{\mathbf{f}_{\mathbf{x}}^*}(s, t)^T \boldsymbol{\Omega}_{\mathbf{x}}^a[s]^T \boldsymbol{\mu}^a(s)\, ds \\ &- \sum_{i=k+1}^{N} \int_{t_{i-1}^*}^{t_i^*} \boldsymbol{\Phi}^{\mathbf{f}_{\mathbf{x}}^*}(s, t)^T \boldsymbol{\Omega}_{\mathbf{x}}^a[s]^T \boldsymbol{\mu}^a(s)\, ds, \quad t \in [t_{k-1}^*, t_k^*], \end{aligned} \tag{5.32}$$

for each $t \in [t_{k-1}^*, t_k^*)$, $k = 1, \ldots, N$. Combining (5.32) and (5.29) gives:

$$\begin{aligned} \delta J(\boldsymbol{\xi}^{\mathbf{u}}) = &- \eta \sum_{k=1}^{N} \int_{t_{k-1}^*}^{t_k^*} \Bigg[\boldsymbol{\mu}^a(t)^T \boldsymbol{\Omega}_{\mathbf{u}}^a[t] + \int_t^{t_k^*} \boldsymbol{\mu}^a(s)^T \boldsymbol{\Omega}_{\mathbf{x}}^a[s] \boldsymbol{\Phi}^{\mathbf{f}_{\mathbf{x}}^*}(s, t) \mathbf{f}_{\mathbf{u}}^*[t]\, ds \\ &\qquad + \sum_{i=k+1}^{N} \int_{t_{i-1}^*}^{t_i^*} \boldsymbol{\mu}^a(s)^T \boldsymbol{\Omega}_{\mathbf{x}}^a[s] \boldsymbol{\Phi}^{\mathbf{f}_{\mathbf{x}}^*}(s, t) \mathbf{f}_{\mathbf{u}}^*[t]\, ds \Bigg] \boldsymbol{\xi}^{\mathbf{u}}(t)\, dt \\ &- \eta\, \boldsymbol{\rho}^{aT} \mathbf{T}_{\mathbf{x}}^a[t_{\mathrm{f}}] \sum_{k=1}^{N} \int_{t_{k-1}^*}^{t_k^*} \boldsymbol{\Phi}^{\mathbf{f}_{\mathbf{x}}^*}(t_{\mathrm{f}}, t) \mathbf{f}_{\mathbf{u}}^*[t] \boldsymbol{\xi}^{\mathbf{u}}(t)\, dt + O(\eta^2). \end{aligned} \tag{5.33}$$

Using (5.8), the last term in (5.33) can be rewritten as

$$\eta \sum_{k=1}^{N} \boldsymbol{\rho}^{aT} \mathbf{T}_{\mathbf{x}}^a[t_{\mathrm{f}}] \int_{t_{k-1}^*}^{t_k^*} \boldsymbol{\Phi}^{\mathbf{f}_{\mathbf{x}}}(t_{\mathrm{f}}, t) \mathbf{f}_{\mathbf{u}}^*[t] \boldsymbol{\xi}^{\mathbf{u}}(t)\, dt \;=\; \eta \boldsymbol{\rho}^{aT} \mathcal{D}_{\mathbf{T}^a, t_{\mathrm{f}}} \boldsymbol{\xi}^{\mathbf{u}}. \tag{5.34}$$

Furthermore, the order of integration in all double integral terms in (5.33) can be changed as follows [25]:

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

Noting that $\sum_{k=1}^{N} \sum_{i=k+1}^{N} \alpha_{i,j} = \sum_{i=1}^{N} \sum_{k=1}^{i-1} \alpha_{i,j}$, the first summation term in (5.33) gives:

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

Using (5.9), it follows that the first term in (5.33) can be rewritten as

$$\begin{aligned}
&\sum_{k=1}^{N} \int_{t_{k-1}^*}^{t_k^*} \left[\boldsymbol{\mu}^a(t)^T \boldsymbol{\Omega}_{\mathbf{u}}^a[t] + \int_t^{t_k^*} \boldsymbol{\mu}^a(s)^T \boldsymbol{\Omega}_{\mathbf{x}}^a[s] \boldsymbol{\Phi}^{\mathbf{f}_{\mathbf{x}}^*}(s,t) \mathbf{f}_{\mathbf{u}}^*[t]\, ds \right. \\
&\qquad \left. + \sum_{i=k+1}^{N} \int_{t_{i-1}^*}^{t_i^*} \boldsymbol{\mu}^a(s)^T \boldsymbol{\Omega}_{\mathbf{x}}^a[s] \boldsymbol{\Phi}^{\mathbf{f}_{\mathbf{x}}^*}(s,t) \mathbf{f}_{\mathbf{u}}^*[t]\, ds \right] \boldsymbol{\xi}^{\mathbf{u}}(t)\, dt \\
= &\sum_{k=1}^{N} \int_{t_{k-1}^*}^{t_k^*} \boldsymbol{\mu}^a(t)^T \mathcal{D}_{\boldsymbol{\Omega}^a,t} \boldsymbol{\xi}^{\mathbf{u}}\, dt. \qquad (5.35)
\end{aligned}$$

Finally, using (5.34) and (5.35), the expression (5.33) for cost variation becomes:

$$\boxed{\delta J(\boldsymbol{\xi}^{\mathbf{u}}) = -\eta \left[\boldsymbol{\rho}^{aT} \left(\mathcal{D}_{\mathbf{T}^a, t_f} \boldsymbol{\xi}^{\mathbf{u}} \right) + \sum_{k=1}^{N} \int_{t_{k-1}^*}^{t_k^*} \boldsymbol{\mu}^a(t)^T \left(\mathcal{D}_{\boldsymbol{\Omega}^a, t} \boldsymbol{\xi}^{\mathbf{u}} \right) dt \right] + O(\eta^2)} \tag{5.36}$$

We are now ready to state the main result of the chapter.

Theorem 5.1 (Cost Variation resulting from Selective Input Adaptation) *Let* $\mathbf{u}^*$ *be an optimal solution for the optimal control problem OC(*$\boldsymbol{\theta}_0$*), and consider parametric perturbations of the form* (5.20)*. The cost variation resulting from selective input adaptation of type* (5.1) *along any (nonzero) SS direction* $\boldsymbol{\xi}_s^{\mathbf{u}} \in \mathcal{V}^s$ *is* $O(\eta^2)$*, whereas the cost variation resulting from adaptation along any (nonzero) CS direction* $\boldsymbol{\xi}_c^{\mathbf{u}} \in \mathcal{V}^c$ *is generally* $O(\eta)$*.*

Proof: By Definition 5.2, $\boldsymbol{\xi}_s^{\mathbf{u}}$ satisfies the system of linear integral equations (5.8) and (5.9). Therefore, from (5.36), $\delta J(\boldsymbol{\xi}_s^{\mathbf{u}}) = O(\eta^2)$. On the other hand, no nonzero direction in $\mathcal{V}^c$ satisfies (5.8) and (5.9) from Lemma 5.1. Since strict complementarity slackness holds for the terminal and path constraints at $\mathbf{u}^*$, it follows that the first-order term in (5.36) is nonzero in general, whence $\delta J(\boldsymbol{\xi}_c^{\mathbf{u}}) = O(\eta)$. □

5.2.3 Implications of Selective Input Adaptation

The main implication of Theorem 5.1 is that, for small parametric perturbations, adapting the inputs along CS directions has the largest impact on the performance of the perturbed system, while the effect of not adapting the inputs along SS directions is relatively smaller. Accordingly, when designing a practical input adaptation strategy for problem OC($\tilde{\boldsymbol{\theta}}$), priority should be given to meeting the active terminal constraints (4.3) and the active path constraints (4.4) over enforcing the Hamiltonian sensitivity condition (4.5).

As noted at the beginning of Section 5.2.2, the input variation $\boldsymbol{\xi}_c^{\mathbf{u}}$ chosen for the variational analysis is a general direction in $\mathcal{V}_c$. It turns out that a judicious choice of $\boldsymbol{\xi}_c^{\mathbf{u}}$ will lead to substantial *cost improvement*, while a poor choice of $\boldsymbol{\xi}_c^{\mathbf{u}}$ could potentially worsen the performance of the adapted system, even with respect to the no-adaptation scenario (Option 1). Special care must therefore be taken when selecting the input-adaptation directions.

5.2.3.1 Choice of input variation in the numerical procedure:

In the case of small parametric perturbations around $\boldsymbol{\theta}_0$, a possible choice of the input variation for the numerical procedure in Section 5.1.3 is

$$\mathcal{U}(t, \boldsymbol{\xi}^{\boldsymbol{\omega}^*}), \quad \forall\, t \in [t_0, t_{\mathrm{f}}], \tag{5.37}$$

where $\boldsymbol{\xi}^{\boldsymbol{\omega}^*}$ is the vector of (first-order) sensitivity of the nominal optimal solution $\boldsymbol{\omega}^*$ with respect to parameters $\boldsymbol{\theta}$ at $\boldsymbol{\theta}_0$. This sensitivity information can be computed, under certain conditions on the underlying NLP (5.16), via linearization of the corresponding KKT NCO. To be precise, the requisite conditions are *strict complementarity*, linear independence constraint qualification (LICQ) and weak second-order sufficient condition (WSOSC), which are explained in Section 2.3.3. Under these conditions, if $\tilde{\boldsymbol{\omega}}(\eta)$ and $\tilde{\boldsymbol{\rho}}(\eta)$ denote the optimal solution and associated Lagrange multipliers for (5.16) at $\tilde{\boldsymbol{\theta}}(\eta)$ given by (5.20), then

$$\begin{aligned} \tilde{\boldsymbol{\omega}}(\eta) &= \boldsymbol{\omega}^* + \eta\, \boldsymbol{\xi}^{\boldsymbol{\omega}^*} + O(\eta^2), \\ \tilde{\boldsymbol{\rho}}(\eta) &= \boldsymbol{\rho}^* + \eta\, \boldsymbol{\xi}^{\boldsymbol{\rho}^*} + O(\eta^2), \end{aligned} \tag{5.38}$$

where

$$\begin{bmatrix} \boldsymbol{\xi}^{\boldsymbol{\omega}^*} \\ \boldsymbol{\xi}^{\boldsymbol{\rho}^*} \end{bmatrix} := -\mathbf{M}(0)^{-1}\mathbf{N}(0)\boldsymbol{\xi}^{\boldsymbol{\theta}}, \tag{5.39}$$

where

$$\begin{aligned} \mathbf{M}(\eta) &:= \begin{bmatrix} \dfrac{\partial^2 \mathcal{L}}{\partial \boldsymbol{\omega}^2}(\tilde{\boldsymbol{\omega}}(\eta), \tilde{\boldsymbol{\rho}}(\eta), \tilde{\boldsymbol{\theta}}(\eta)) & \dfrac{\partial \mathbf{G}}{\partial \boldsymbol{\omega}}(\tilde{\boldsymbol{\omega}}(\eta), \tilde{\boldsymbol{\theta}}(\eta))^T \\ \mathrm{diag}\{\tilde{\boldsymbol{\rho}}(\eta)\}\dfrac{\partial \mathbf{G}}{\partial \boldsymbol{\omega}}(\tilde{\boldsymbol{\omega}}(\eta), \tilde{\boldsymbol{\theta}}(\eta)) & \mathrm{diag}\{\mathbf{G}(\tilde{\boldsymbol{\omega}}(\eta), \tilde{\boldsymbol{\theta}}(\eta))\} \end{bmatrix}, \\ \mathbf{N}(\eta) &:= \begin{bmatrix} \dfrac{\partial \mathcal{L}}{\partial \eta \partial \boldsymbol{\omega}}(\tilde{\boldsymbol{\omega}}(\eta), \tilde{\boldsymbol{\rho}}(\eta), \tilde{\boldsymbol{\theta}}(\eta)) \\ \mathrm{diag}\{\tilde{\boldsymbol{\rho}}(\eta)\}\dfrac{\partial \mathbf{G}}{\partial \eta}(\tilde{\boldsymbol{\omega}}(\eta), \tilde{\boldsymbol{\theta}}(\eta)) \end{bmatrix}, \end{aligned} \tag{5.40}$$

where $\mathcal{L}$ is the Lagrangian of the pNLP (5.16), i.e.,

$$\mathcal{L}(\boldsymbol{\omega}, \boldsymbol{\rho}, \boldsymbol{\theta}) := J(\mathbf{u}, \boldsymbol{\theta}) + \boldsymbol{\rho}^T \mathbf{G}(\mathbf{u}, \boldsymbol{\theta}),$$

and diag$\{\mathbf{y}\}$ denotes the diagonal matrix whose diagonal is formed by vector $\mathbf{y}$.

The strict complimentarity condition on (5.16) is needed to ensure the invertibility of $\mathbf{M}(0)$ in (5.40); for more details see, Theorem 3.2.2 and Corollary 3.2.3 of [29].

5.3 Illustrative Examples

This section computes SS and CS directions for the optimization of two dynamic systems, namely, a batch chemical reactor and a space shuttle reentry problem. The first system is simple as it comprises of only 2 states, 1 input and 1 terminal constraint. The second system is more complex as it is highly nonlinear and comprises of 5 states, 2 bounded inputs, 1 mixed path constraint and 3 terminal constraints.

5.3.1 Optimization of a Batch Chemical Reactor

This parametric optimal control problem is concerned with the performance optimization of a batch chemical reactor, in which the reactions $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ take place non-isothermally [90]. The problem comprises a single input variable, the reactor temperature $u(t)$, and a single (terminal) constraint, the reactant concentration at final time $x_A(t_\mathrm{f})$. The objective is to determine the temperature profile that maximizes the amount of product B for a given batch time. In addition, there is uncertainty in the kinetic parameter k_1. The optimization problem can be formulated mathematically as

$$
\begin{aligned}
&\max_{u(t)} \quad x_B(t_\mathrm{f}), && (5.41)\\
\text{s.t.} \quad &\dot{x}_A(t) = -k_1(u(t))\, x_A(t), && x_A(0) = 0.53 \ \ \text{kmol m}^{-3},\\
&\dot{x}_B(t) = k_1(u(t))\, x_A(t) - k_2(u(t))\, x_B(t), && x_B(0) = 0.43 \ \ \text{kmol m}^{-3},\\
&k_1(u(t)) = \ \theta\, k_1^\circ \exp\left(-\frac{E_1}{u(t)}\right),\\
&k_2(u(t)) = \ k_2^\circ \exp\left(-\frac{E_2}{u(t)}\right),\\
&x_A(t_\mathrm{f}) - 0.1 \le 0,
\end{aligned}
$$

where the parameter θ denotes the uncertainty in modeling the kinetic parameter k_1, with the nominal value $\theta_0 = 1$. The numerical values of the other parameters are given in Table 5.1. The relative values of E_1 and E_2 indicate that low temperatures will slow down the second reaction more than the first one, and thus favor the production of B, which is desired.

Table 5.1 Parameter values

Parameter	Value	
k_1°	0.535×10^{11}	h^{-1}
k_2°	0.461×10^{18}	h^{-1}
E_1	9×10^3	K
E_2	15×10^3	K
t_f	8	h

Following the procedure outlined in Section 5.1.3, a piecewise-constant input parameterization involving $m = 100$ equal-length stages over $[0, t_\mathrm{f}]$ is considered. Figures 5.2 and 5.3 show the nominal optimal solution of Problem (5.41) reconstructed from the solution $\boldsymbol{\omega}^*$ of the associated NLP.

The relative production of B is favored by low temperatures. However, at low temperatures, the reactions proceed slowly and the desired conversion of A will not be achieved in the given batch time. Hence, there exists a compromise, with the temperature being high initially – to favor both reactions – and reducing with time to limit the second reaction as more B is produced.

Based on the nominal solution $\boldsymbol{\omega}^*$ and on the associated Jacobian $\mathbf{G}^a_{\boldsymbol{\omega}}$, the projection matrices $\mathbf{V}_c{\mathbf{V}_c}^T$ and $\mathbf{V}_s{\mathbf{V}_s}^T$ are computed according to Step 4 of the numerical procedure in Section 5.1.3. The chosen input variation is $\mathcal{U}(t, \boldsymbol{\xi}^{\boldsymbol{\omega}^*})$, as in (5.37). The

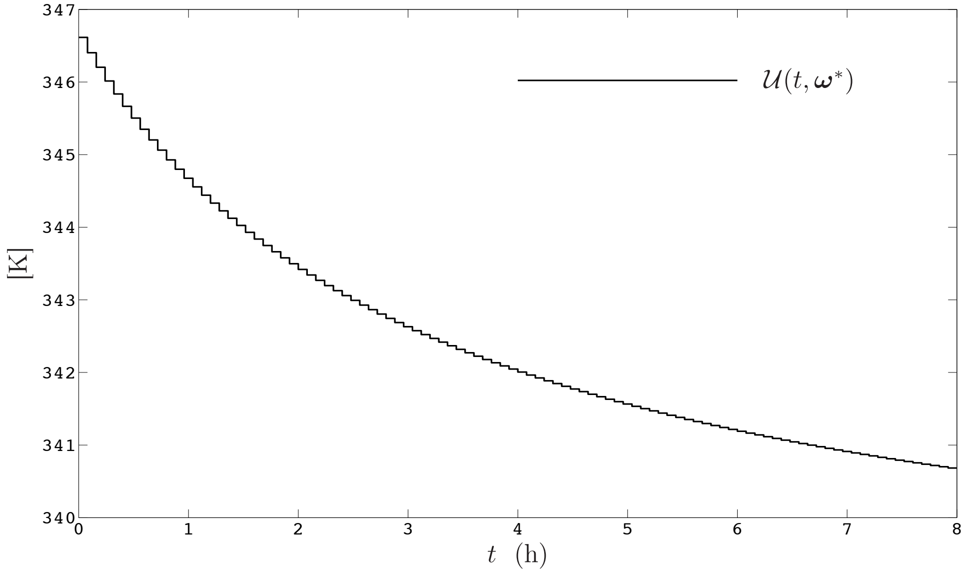

Figure 5.2 Nominal optimal temperature profile approximated as a piecewise-constant signal.

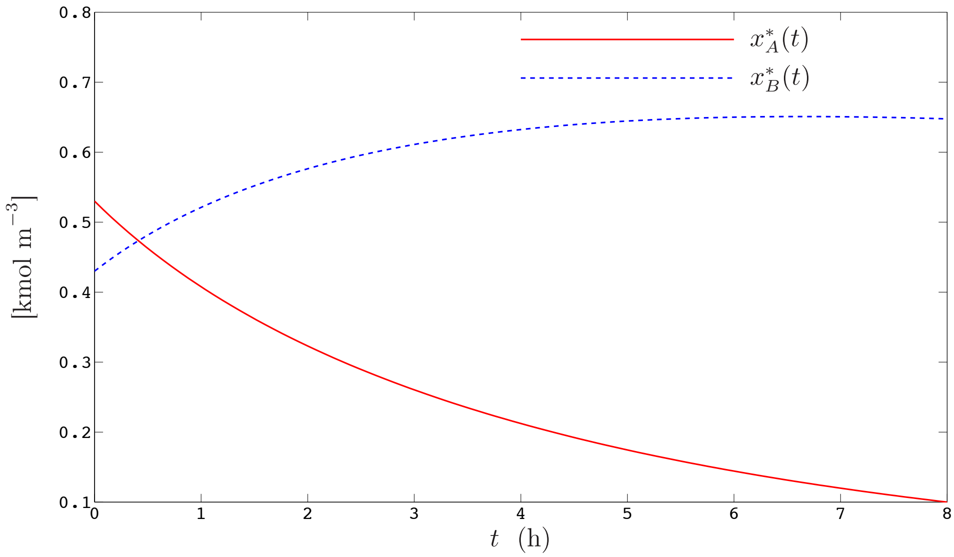

Figure 5.3 Nominal optimal concentration trajectories.

approximations of its SS and CS components are then computed according to Steps 6 and 7. The input variation profiles are shown in Figure 5.4.

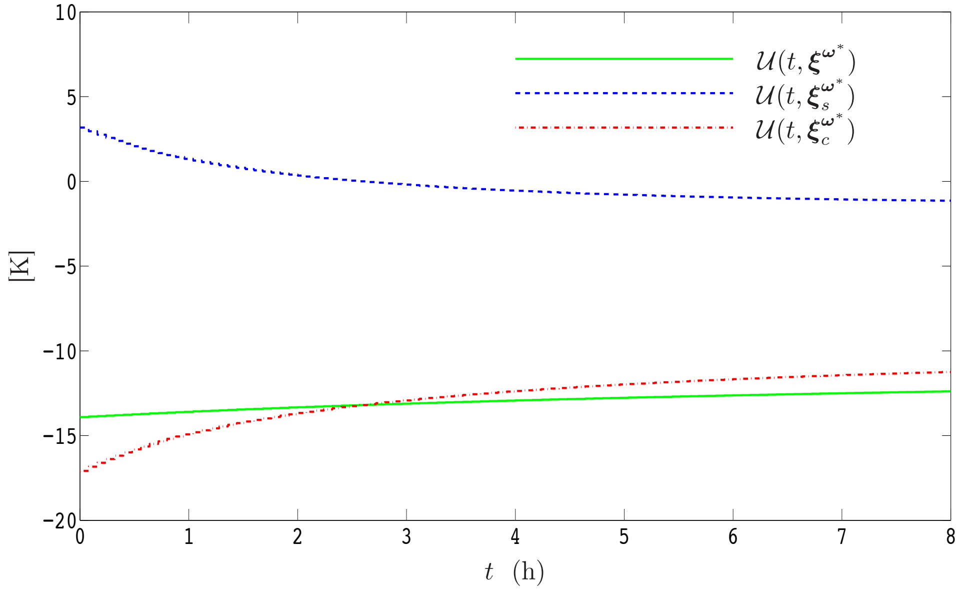

Figure 5.4 Input variation $\mathcal{U}(t, \boldsymbol{\xi}^{\boldsymbol{\omega}^*})$ and its approximated SS and CS components.

As was noted in (5.19), it can be observed that the input variation $\mathcal{U}(t, \boldsymbol{\xi}^{\boldsymbol{\omega}^*})$ is the pointwise sum of its SS and CS components.

Note that, for the considered uncertainty direction $\xi^\theta = 1$, the forward reaction is faster than in the nominal system, which produces more B. This allows the optimal temperature to be lower (thus more favorable from an equilibrium viewpoint) than the nominal optimal solution and still meet the terminal constraint. Figure 5.4 shows that the input variation $\mathcal{U}(t, \boldsymbol{\xi}^{\boldsymbol{\omega}^*})$ is negative for all t, thus consistent with the need of a lower temperature. The CS component $\mathcal{U}(t, \boldsymbol{\xi}_c^{\boldsymbol{\omega}^*})$ is also negative, which says that, to be able to meet the terminal constraint regarding $x_A(t_\mathrm{f})$ in the presence of a faster forward reaction, the temperature has to be reduced, and in fact a bit more initially than towards the end. In comparison, the SS component is much smaller, initially positive and then negative, indicating that, for the perturbed reactor, an initially slightly higher temperature followed by a slightly lower temperature would improve productivity *without affecting the terminal constraint*. Based on the relative magnitudes of the CS and SS components, one might conclude that the input variation in this case is mostly constraint-seeking.

Next, parametric perturbations of type (5.20) are considered for $\eta^\circ = 0.05$. The cost variation resulting from input adaptation along the SS direction, $\delta J_s :=$

$\delta J(\mathcal{U}(t, \boldsymbol{\xi}_s^{\boldsymbol{\omega}^*}))$, is plotted versus η in Figure 5.5. The plot can be seen to have a $O(\eta^2)$ fit, which is consistent with the derivations in Section 5.2. In contrast, the cost variation $\delta J_c := \delta J(\mathcal{U}(t, \boldsymbol{\xi}_c^{\boldsymbol{\omega}^*}))$ shown in Figure 5.6 is seen to have a O(η) fit, as predicted by the theory.

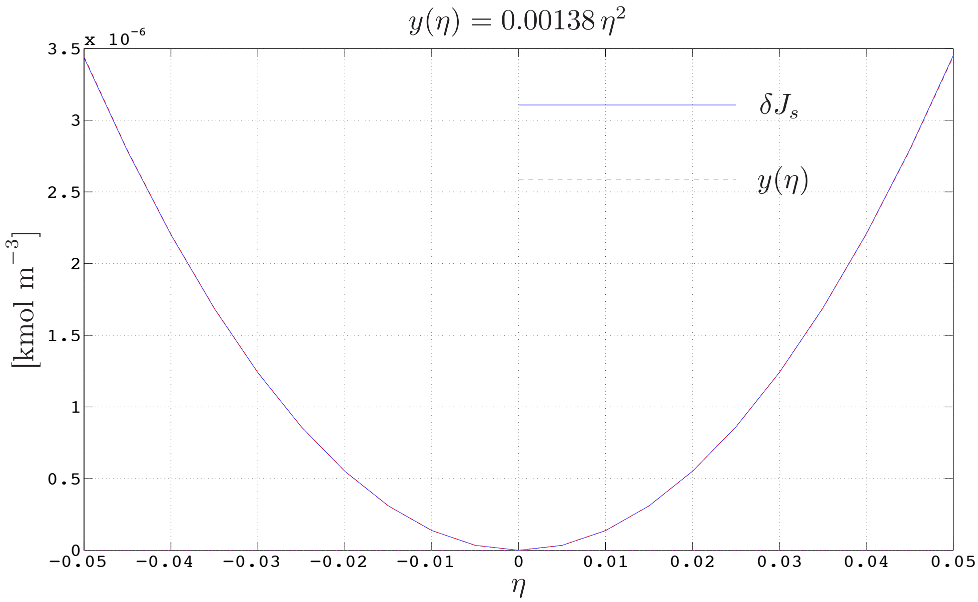

Figure 5.5 Cost variation resulting from input adaptation along $\mathcal{U}(t, \boldsymbol{\xi}_s^{\boldsymbol{\omega}^*})$ versus η.

Note that CS adaptation can lead to cost worsening (negative cost variation). This is, for example, the case for positive values of η, that is, when the forward reaction is faster than in the nominal case. Indeed, the adaptation forces the terminal constraint to become active by lowering the temperature, whereas the constraint is violated when the nominal solution is applied to the perturbed system. Note also the relative size of the cost variations resulting from adaptations along the SS and CS directions, the latter being three orders of magnitude larger than the former.

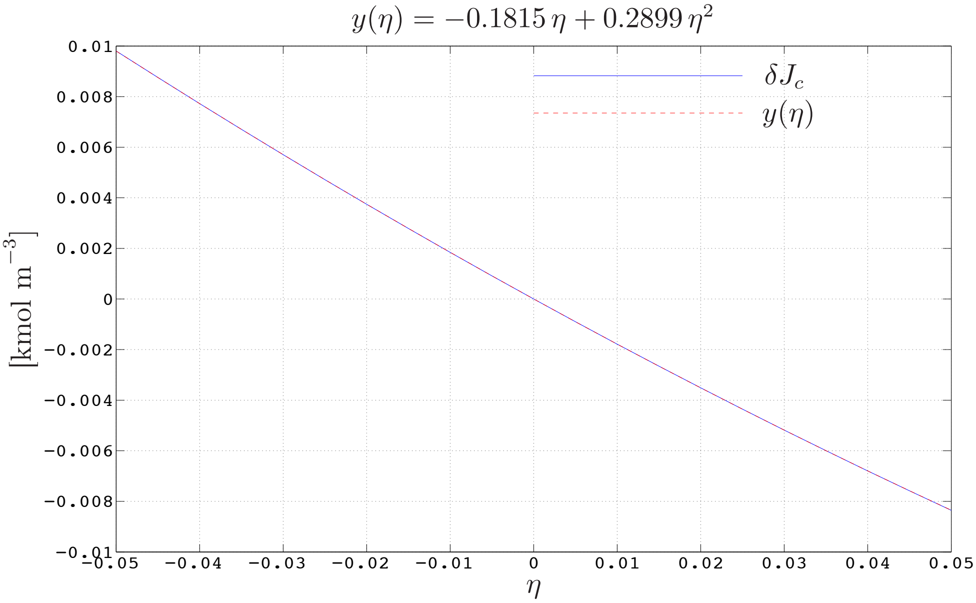

Figure 5.6 Cost variation resulting from input adaptation along $\mathcal{U}(t, \boldsymbol{\xi}_c^{\boldsymbol{\omega}^*})$ versus η.

5.3.2 Space Shuttle Reentry Trajectory Optimization

This subsection investigates directional input adaptation for the optimization of the reentry trajectory of a space shuttle. The parametric optimal control problem is a slight modification of the space shuttle reentry problem in [8] and [49].

The system comprises 5 states and 2 inputs, the details of which are given in Table 5.2.

Table 5.2 The five states and two inputs in the space shuttle reentry problem.

h	altitude (ft)	a	angle of attack (radians)
ϑ	latitude (radians)	b	bank angle (radians)
v	velocity (ft / sec)		
γ	flight path angle (radians)		
ψ	azimuth (radians)		

The optimization problem is subject to lower and upper bounds on both inputs (5.43), an upper limit on the aerodynamic heating of the vehicle wing leading edge (5.44), which results in a mixed control-state path constraint. Furthermore, there are 3 terminal constraints, namely, an upper limit on the final altitude of the space shuttle and lower limits on its final velocity and final flight path angle (5.45).

The objective is to maximize the cross-range of the space shuttle, that is, the final value of its latitude:

$$
\begin{aligned}
\max_{a(t),\, b(t)} \quad & \vartheta(t_{\mathrm{f}}), \\
\text{s.t.} \quad & \dot{h} = v \sin\gamma, \\
& \dot{\vartheta} = \frac{v}{r} \cos\gamma \cos\psi, \\
& \dot{v} = -\frac{D(h,v,a,\theta)}{m} - g(h) \sin\gamma, \\
& \dot{\gamma} = \frac{L(h,v,a)}{mv} \cos b + \cos\gamma \left(\frac{v}{r(h)} - \frac{g(h)}{v} \right), \\
& \dot{\psi} = \frac{1}{mv\cos\gamma} L(h,v,a) \sin b + \frac{v}{r\cos\vartheta} \cos\gamma \sin\psi \sin\vartheta, && (5.42) \\
& 0 \le a(t) \le \frac{\pi}{2}, \\
& -\frac{\pi}{2} \le b(t) \le -\frac{\pi}{6}, && (5.43) \\
& \Omega(a,h,v) = \frac{q_a(a) q_r(h,v)}{q_U} - 1.0 \le 0, && (5.44) \\
& h(t_{\mathrm{f}}) \le 8.0 \times 10^4, \\
& v(t_{\mathrm{f}}) \ge 2.5 \times 10^3, \\
& \gamma(t_{\mathrm{f}}) \ge -\frac{5\pi}{180}, && (5.45)
\end{aligned}
$$

where the functions r, g, ρ, D, L, q_a and q_r are as follows:

$$
\begin{aligned}
r(h) &= R_e + h, \\
g(h) &= \frac{\mu}{r^2}, \\
\rho(h) &= \rho_0 \exp\left(-\frac{h}{h_r} \right), \\
D(h,v,a,\theta) &= \frac{1}{2} \theta c_D S \rho(h) v^2, \quad c_D := d_0 + d_1 \hat{a}, \quad \hat{a} := \frac{180a}{\pi}, \qquad (5.46) \\
L(h,v,a) &= \frac{1}{2} c_L S \rho(h) v^2, \quad c_L := l_0 + l_1 \hat{a} + l_2 \hat{a}^2, \\
q_a(a) &= c_0 + c_1 \hat{a} + c_2 \hat{a}^2 + c_3 \hat{a}^3, \\
q_r(h,v) &= k_1 \sqrt{\rho} (k_2 v)^{3.07}.
\end{aligned}
$$

The parameter θ, with the nominal value $\theta_0 = 1$, is uncertain in the modeling of the aerodynamic drag D. The final time t_f is 2000 sec. The initial values of the states are given in Table 5.3. All other parameters are specified in Table 5.4.

Table 5.3 Initial conditions for the space shuttle reentry problem.

$h(0)$	$\vartheta(0)$	$v(0)$	$\gamma(0)$	$\psi(0)$
2.6×10^5	0.0	2.56×10^4	$-\pi/180$	$\pi/2$

Table 5.4 Parameter values for the space shuttle reentry problem.

Parameter	Value	Parameter	Value
m	6.30944×10^3	d_0	-0.20704
R_e	2.09029×10^7	d_1	2.9244×10^{-2}
μ	1.4076539×10^{16}	l_0	7.854×10^{-2}
ρ_0	2.378×10^{-3}	l_1	-6.1592×10^{-3}
h_r	2.38×10^4	l_2	6.21408×10^{-4}
q_U	70.0	c_0	1.0672181
S	2.69×10^3	c_1	$-1.9213774 \times 10^{-2}$
k_1	1.77×10^4	c_2	2.1286289×10^{-4}
k_2	1.0×10^{-4}	c_3	$-1.0117249 \times 10^{-6}$

The solution of the above problem is obtained by using a piecewise-constant control vector parameterization involving $m = 150$ equidistant stages and discretizing the path constraint at the end of each stage. The two nominal optimal inputs and the value of the path constraint are shown in Figures 5.7, which also depicts the nature of the optimal solution in terms of four arcs. The input $\mathcal{U}(t, \boldsymbol{\alpha}^*)$ consists of the interior arc $\boldsymbol{\alpha}_1$, followed by the boundary arc $\boldsymbol{\alpha}_2$, and finally the interior arcs $\boldsymbol{\alpha}_3$ and $\boldsymbol{\alpha}_4$. The input $\mathcal{U}(t, \boldsymbol{\beta}^*)$ consists of the interior arcs $\boldsymbol{\beta}_1, \boldsymbol{\beta}_2$ and $\boldsymbol{\beta}_3$, followed by the boundary arc $\boldsymbol{\beta}_4$.

The nominal state trajectories are depicted in Figure 5.8. The terminal constraints on the states v and γ are seen to be active.

Using the knowledge of the nominal optimal solution, the projection matrices $\mathbf{V}_c{\mathbf{V}_c}^T$ and $\mathbf{V}_s{\mathbf{V}_s}^T$ are computed as described in Step 4 of the numerical procedure in Section 5.1.3.

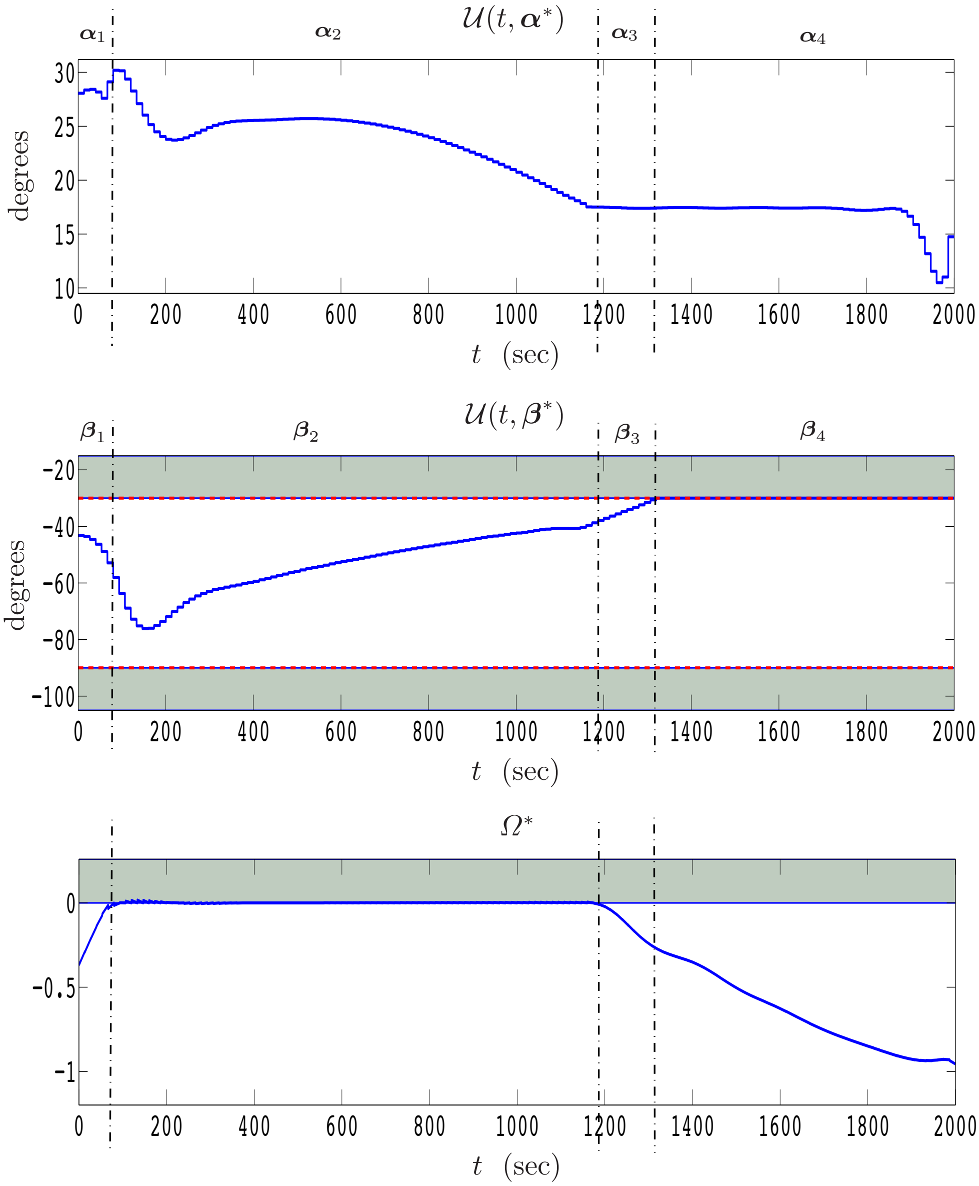

Figure 5.7 Two nominal optimal inputs and one path constraint. Dashed lines show the corresponding bounds. Shaded regions depict the regions of infeasible operation.

The input variations are chosen according to (5.37), and their SS and CS components computed by following Steps 6 and 7 are shown in Figure 5.9. Again, as noted in (5.19), the two input variations $\mathcal{U}(t, \boldsymbol{\xi}^{\boldsymbol{\alpha}^*})$ and $\mathcal{U}(t, \boldsymbol{\xi}^{\boldsymbol{\beta}^*})$ are equal to the pointwise sum of their respective SS and CS components.

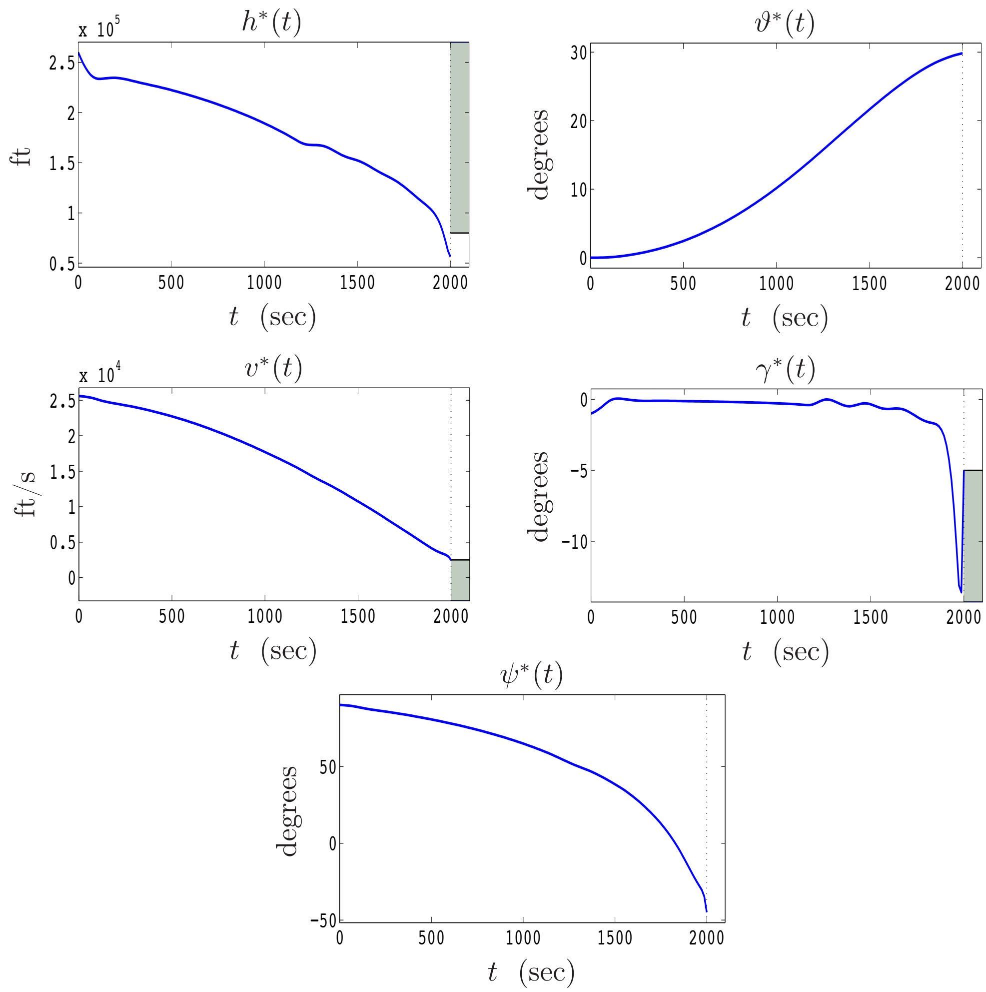

Figure 5.8 Five nominal optimal state trajectories. Shaded bands depict the infeasible regions of the respective terminal constraints. Vertical dotted line is the $t = 2000$ sec line.

Note that the SS component $\mathcal{U}(t, \boldsymbol{\xi}_s^{\boldsymbol{\alpha}^*})$ becomes small after about 500 sec, an indication that the variation in the input $a(t)$ is mostly constraint-seeking. The first contribution of $\mathcal{U}(t, \boldsymbol{\xi}_c^{\boldsymbol{\alpha}^*})$ between 500 sec and 1150 sec is needed to enforce the path constraint, the second contribution, towards the end, is to meet a terminal constraint. For the input $b(t)$, since it is on its upper bound after about 1300 sec, and since the upper bound does not depend on the parameter θ, the input variation $\mathcal{U}(t, \boldsymbol{\xi}^{\boldsymbol{\beta}^*})$ is 0 on this interval. Since, except for the initial part, $\mathcal{U}(t, \boldsymbol{\xi}_c^{\boldsymbol{\beta}^*})$ is small, the variation in the input $b(t)$ is mostly sensitivity-seeking.

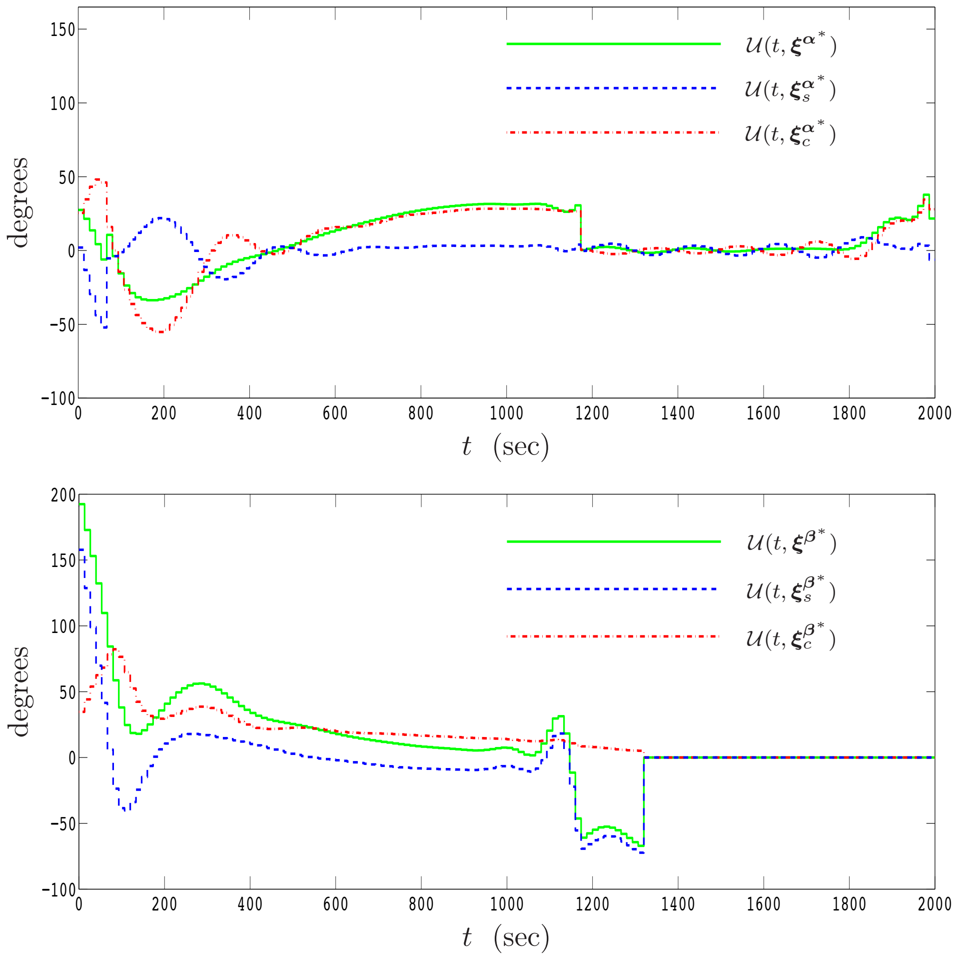

Figure 5.9 SS and CS components of the input variations $\mathcal{U}(t, \boldsymbol{\xi}^{\boldsymbol{\alpha}^*})$ and $\mathcal{U}(t, \boldsymbol{\xi}^{\boldsymbol{\beta}^*})$.

Finally, parametric perturbations of type (5.20) were considered for $\eta^\circ = 0.05$ and $\xi^\theta = 1$. The cost variation δJ_s resulting from input adaptation along the SS directions $\mathcal{U}(t, \boldsymbol{\xi}_s^{\boldsymbol{\alpha}^*})$ and $\mathcal{U}(t, \boldsymbol{\xi}_s^{\boldsymbol{\beta}^*})$ is plotted versus η in Figure 5.10. The $O(\eta^2)$ fit of the plot is in agreement with the theory presented in Section 5.2. Furthermore, the $O(\eta)$ fit for the cost variation δJ_c resulting from input adaptation along the CS directions $\mathcal{U}(t, \boldsymbol{\xi}_c^{\boldsymbol{\alpha}^*})$ and $\mathcal{U}(t, \boldsymbol{\xi}_c^{\boldsymbol{\beta}^*})$ can be seen in Figure 5.11. δJ_c is one order of magnitude larger than δJ_s.

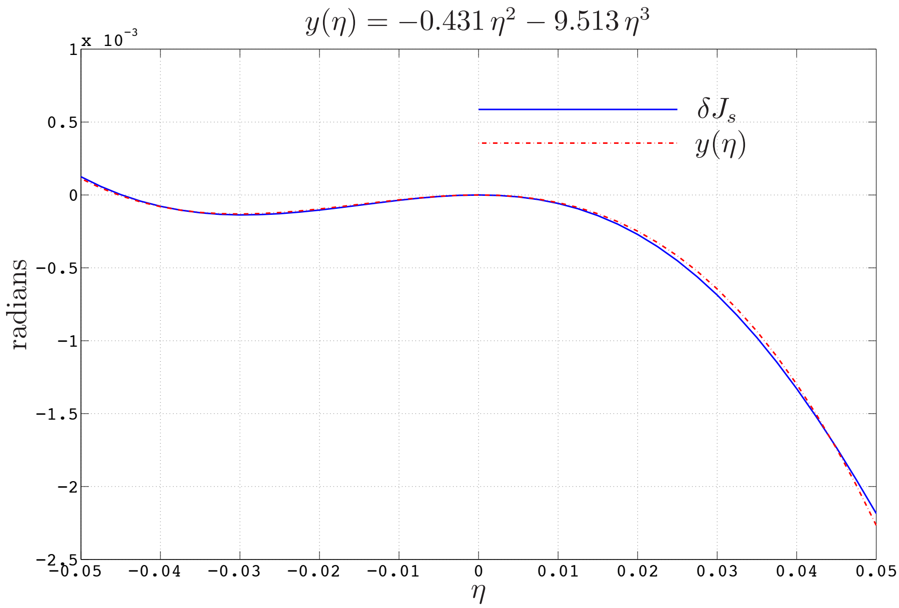

Figure 5.10 Cost variation resulting from input adaptation along the SS directions versus η.

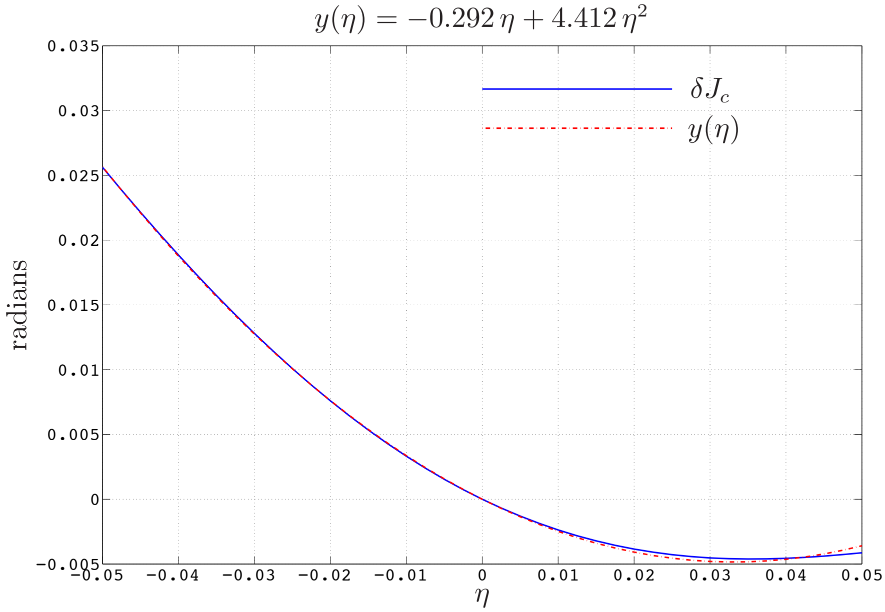

Figure 5.11 Cost variation resulting from input adaptation along the CS directions versus η.

5.4 Extension to more Complex Problems

The results of Section 5.1 and Subsection 5.2.2 were obtained for continuous signals, in particular continuous nominal optimal inputs $\mathbf{u}^*(t)$. This is, however, not the case for many practical applications. Fortunately, careful inspection of the derivations reveals that the procedure is not limited by the requirement of continuity of $\mathbf{u}^*(t)$, though it is much simplified by the latter assumption. Indeed, if we include the points of discontinuity of $\mathbf{u}^*$ in the set $\mathcal{T}$, the derivation holds as is, provided the number of continuous arcs in $\mathbf{u}^*$ is finite. Furthermore, since the results are valid for piecewise-continuous $\mathbf{u}^*(t)$, we can forgo the assumption of *regularity* of the Hamiltonian. This allows the results to be extended to more complex problems like singular optimal control problems.

Finally, in the case of problems having pure state constraints, additional care must be taken in the derivation since there might be jumps in the adjoint functions $\boldsymbol{\lambda}^*(t)$ at some interior points [54]. Since the nominal solution is known, these interior points are known and need to be added to $\mathcal{T}$. Definition 5.2 of the SS directions will include an additional condition - in the form of suitable integral equations - representing the zero change in the values of the pure state constraints due to small local variation in the nominal inputs of type (5.1). In the cost variational analysis, the expression of $\boldsymbol{\beta}(t)$ in (5.32), and thus also that of $\delta J(\boldsymbol{\xi}^{\mathbf{u}})$ in (5.33) and (5.36), will be modified to accommodate the appropriate terms involving the pure state constraints. The rest of the procedure, and thus also the results, remain the same.

5.5 Summary

The complexity of solving optimal control problems plays a decisive role in controller design considerations for practical applications. Various practical limitations dictate that real-time optimization methods should not require recomputing the exact solution. Hence, methods that involve only adaptation of the nominal optimal inputs, which can be computed off-line, at the cost of acceptable optimality loss are appealing.

Clearly, a theoretical framework is essential for identifying useful input adaptation schemes and analyzing the effect on the cost of such adaptations. For a fairly general class of parametric OC problems, two input adaptation schemes are envisaged by focusing on the role of constraints in OC problems and the cost variation that results from each adaptation scheme are studied.

For problems involving terminal and mixed control-state constraints, it is possible to identify directions in the space of input variation functions, along which small variations in the nominal optimal inputs *do not* cause any change in the nominal active path constraints for all $t \in [t_0, t_\mathrm{f}]$ as well as the nominal active terminal constraints. These directions are defined as the SS directions and 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.

The main result of the analysis of constrained parametric optimal control problems is that, in the case of parametric perturbations of type (5.20), the cost variation due to selective input adaptation along SS directions – with respect to no adaptation – is $O(\eta^2)$, whereas it is $O(\eta)$ with selective input adaptation along CS directions. Hence, the main implication of this result for DRTO problems is that, for small parametric perturbations, 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.

Thus, the aim set at the end of Chapter 4, viz., to extend the directional variational analysis to DRTO problems under conditions as general as possible, is accomplished. The contributions of this chapter can be shown in a schematic diagram as in Figure 5.12:

These results might prove valuable in the design of adaptive methodologies for constrained DRTO problems, e.g. the NCO tracking methodology mentioned earlier [101, 103]. Recall from Introduction that in NCO tracking various parts of the input profiles are adapted selectively by tracking separately the NCO related to constraints and to sensitivities. Hence, prioritization of selective adaptation strategies is crucial for the implementation of practical NCO-tracking controllers. More specifically, the tracking of NCO related to sensitivities necessitates neighboring-extremal (NE) control [51, 101]. As the study [51] of NE control techniques for NCO tracking reveals, the said techniques are valid only under restrictive assumptions and moreover, the computation of NE control can be difficult and time consuming. Under these circumstances, given the trade-off between

- computational complexity of NE control, assuming it is possible in the first place, for tracking NCO related to sensitivities, and
- the practically negligible gains obtained by enforcing sensitivities as indicated by the results presented above,

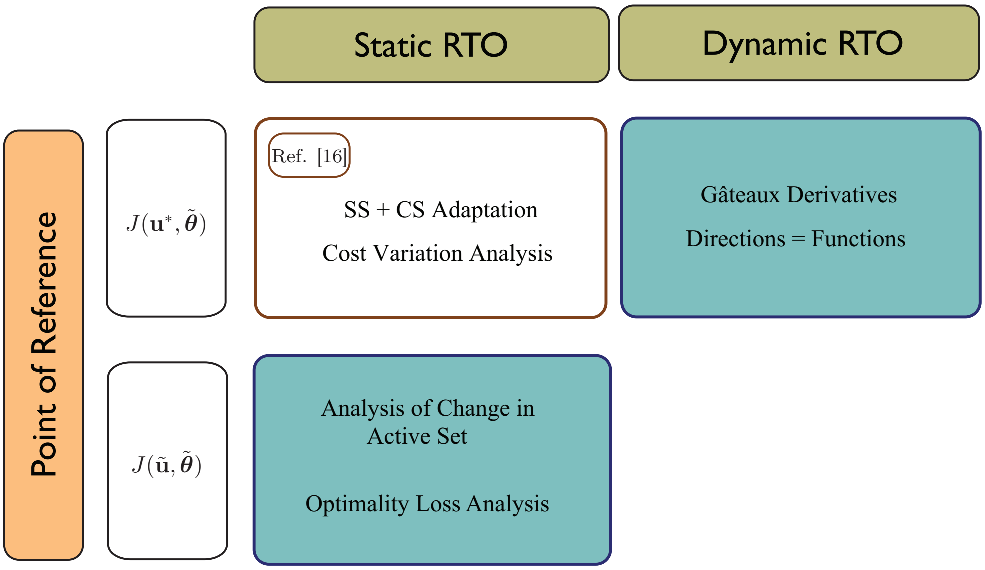

Figure 5.12 Contributions of the thesis to the analytical study of DRTO.

it may be possible in practice to dispense altogether with the efforts of building an NE control unit to enforce sensitivities and still suffer only a negligible loss of optimality. Needless to say, the design of NCO-tracking controller for enforcing the remaining component, viz., NCO for constraints, is already simpler than enforcing both. Moreover, it is well-documented [36, 101, 110], that the implementation of NCO-tracking controllers for enforcing constraints using standard tools from control theory, especially when the active set is unchanged after parametric perturbations, is fairly easy.

As mentioned in Section 5.1.1, a limitation of the present work is that the class of adapted inputs (5.1) does not consider switching times that depend on η.

Chapter 6

Conclusions

This chapter summarizes the main contributions of the thesis and provide some perspectives for future research.

6.1 Summary of Main Contributions

This thesis has addressed some key analytical aspects of the real-time process optimization in the presence of uncertainty.

It is well known that, since a process model is typically used to compute the optimal operating conditions, both plant-model mismatch and process disturbances can result in suboptimal or, worse, infeasible operation. Hence, methodologies for practical applications that try to avoid re-optimization during process operation, at the cost of an acceptable optimality loss, become important. A careful analysis of the components of the necessary conditions of optimality (NCO) is essential for the design and analysis of such approximate solution strategies in real-time optimization (RTO). This thesis has attempted to analyze, under fairly general conditions, the role of constraints in process optimality in the presence of uncertainty.

6.1.1 Contributions to the Analytical Studies of Static RTO

A careful study of numerous RTO methods for static RTO problems reveals that it is possible to abstract important common features of some of the most promising methods. It is seen that these features are mainly *selectivity* in either adapting or enforcing the various components of the NCO. Hence, it is possible that two different RTO methods generate the same solutions by two different means (e.g., the way they are implemented).

Based on this insight, we proposed to consider a general class of feasible adapted inputs, which are designed using the *model* of the plant but in fact attempt to optimize the *plant*. In this approach, the inputs are not limited to being local adaptation of the model optimal inputs but, instead, they can change significantly to optimize the plant. It is then proposed to develop a *joint* analysis of the model optimal, plant optimal and adapted inputs under conditions as general as possible. The conceptual importance of this formulation is that

- the possibility of change in optimal active set can be naturally incorporated in this formulation,
- since the plant optimum is incorporated in the analysis, it is possible to quantify the *optimality loss* due to adaptation.

Note that the main drawback of the existing analytical study of static RTO problems is that it is based on local variational analysis around the model optimal solution [16, 70] and so cannot address either of the important possibilities above. Of course, incorporation of the two possibilities in the present analysis makes it much more complicated than the local variational analysis, but with the added advantage of being more *constructive* in its approach.

The most important contribution of the thesis for static RTO problems has been to prove that, for a wide class of systems, the detection of a change in the active set contributes only negligibly to optimality, as long as the adapted solution remains feasible. More precisely, if η denotes the magnitude of the parametric variations, and if the LICQ (2.5) and SSOSC (2.11) conditions are satisfied for the underlying pNLP, then the optimality loss due to any feasible input that maintains the strict active set of the model inputs is of magnitude $O(\eta^2)$, irrespective of whether or not there is a change in the set of active constraints. The implication of this result for a static RTO algorithm is to satisfy only a core set of constraints with priority, as long as it is possible to meet the feasibility requirements.

6.1.2 Contributions to the Analytical Studies of Dynamic RTO

The second part of the thesis has presented an analytical study of the effect of local adaptation of the *model* optimal inputs of dynamic RTO problems. This adaptation is made along two sets of directions such that one type of adaptation does not affect the active constraints, while the other does. These directions are termed the sensitivity-seeking (SS) and the constraint-seeking (CS) directions, respectively.

Although the basic concept of SS and CS directions is taken from the similar analytical study of static RTO problems [16, 37], none of the technical results for static problems can be extended in a straightforward manner to the dynamic problems since the latter are infinite-dimensional optimization problems.

The first main contribution of the thesis for this problem has been to identify that the most crucial feature of dynamic RTO problems, especially in contrast with static problems, is that *temporal* effect of input adaptations on both path and terminal constraints of the problem needs to be taken into account. In particular, input variations at all the past instants and the present instant need to be taken into account to compute the current change in path and terminal constraints.

The next important contribution has been to define the SS and CS directions as elements of a fairly general function space of input variations and to derive a mathematical criterion to define SS directions for a general class of optimal control problems involving both path and terminal constraints. According to this criterion, the SS directions turn out to be solutions of certain linear integral equations that are completely defined by the model optimal solution. The CS directions are then chosen orthogonal to the subspace of SS directions, where orthogonality is defined with respect to a chosen inner product on the space of input variations. It follows that the corresponding subspaces are infinite-dimensional subspaces of the function space of input variations.

The most important contribution of the thesis in the analytical study of the dynamic RTO problem has been to prove that, when uncertainty is modeled in terms of small parametric variations, the aforementioned classification of input adaptation leads to clearly distinguishable cost variations. More precisely, if η denotes the magnitude of the parametric variations, adaptation of the model optimal inputs along SS directions causes a cost variation of magnitude $O(\eta^2)$. On the other hand, the cost variation due to input adaptation along CS directions is of magnitude $O(\eta)$.

Thus, for small parametric variations (η in a small neighborhood of 0), the cost variation due to input adaptation along SS directions is negligible compared to that due to adaptation along CS directions. In other words, satisfaction of active constraints typically has more influence on cost than satisfaction of sensitivities.

Another contribution of the thesis has been to develop a numerical procedure for computing the SS and CS components of a given input variation. These components are projections of the input variation on the infinite-dimensional subspaces of SS and CS directions. The numerical procedure consists of the following three steps: approximation of the optimal control problem by a nonlinear programming (NLP) problem, projection of the optimal direction on the finite-dimensional SS and CS subspaces of the NLP and, finally, reconstruction of the SS and CS components of the original problem from those of the NLP.

6.2 Future Perspectives

We propose to close the thesis by offering a couple of perspectives for future research.

- The two research objectives imagined at the start of the thesis (Section 1.3) have been accomplished in the thesis, viz., developing a fairly general joint analysis of the model optimal, plant optimal and adapted inputs for static RTO problems and developing a local variational analysis for dynamic RTO problems.

  It is most natural to think of combining the insights developed in these two analyses to develop a fairly general joint analysis of the model optimal, plant optimal and adapted inputs for *dynamic* RTO problems. We represent this direction of research by the two long arrows in Figure 6.1.
- The analysis of static RTO problems is made under the assumption that the magnitude of parametric perturbations η is in a small neighborhood of 0. Hence, the results are not applicable for processes that experience large uncertainty, i.e., significant disturbances and/or large plant-model mismatch. Of course, such scenarios are common in practical applications.

  Analytical results on change in optimal inputs of parametric NLP problems for finite parametric perturbations are not as prolific as that of the (local) sensitivity analysis. In a general parametric NLP, finite parametric perturbations can result in a variety of (undesirable) behaviors of optimal solutions [53]. In such a scenario, it seems difficult to develop a fairly general analysis of the kind developed in this thesis (under the assumption of small perturbations). Probably, a case-based approach can be developed by restricting attention to a few classes of NLP problems that are of practical interest and have various special features. An example of an RTO method for quadratic programming problems based on this type of analysis can be seen in [28].

We represent this direction of research by the small arrow in the Static RTO block in Figure 6.1.

- As remarked at the end of Chapter 5, one limitation of the local variational analysis developed for dynamic RTO problems is that the class of input variations is not generic enough to allow for a dependence of the switching times on the magnitude of parameters η. Hence, a possible direction of future research is to extend the results of Chapter 5 for the said class of input variations.

  We represent this direction of research by the small arrow in the Dynamic RTO block in Figure 6.1.

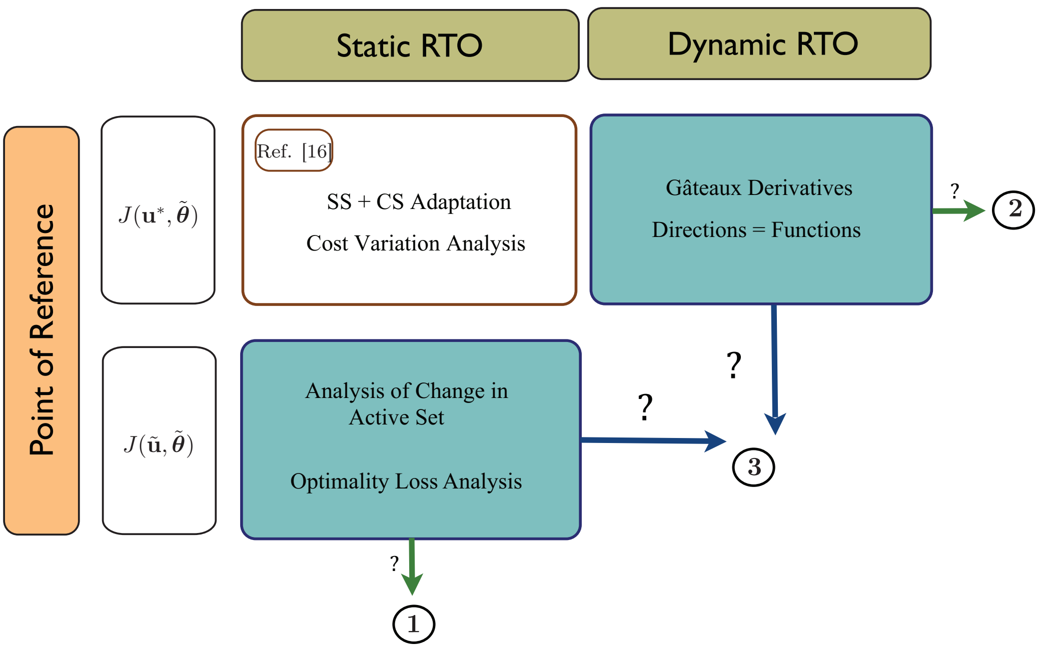

Figure 6.1 Small arrows denote possible generalizations of the existing results. Long arrows denote extension of the existing results to the DRTO case.

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