Optimizing Process Economics in Model Predictive Control

by

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To Papa, Mummy, my better self Mannu and the love of my life Sayani.

Optimizing Process Economics in Model Predictive Control

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The overall objective of any process is to convert certain raw material into desired products using available resources. During its operation, the plant must satisfy several requirements imposed by its designers and the general technical, economic and social conditions in the presence of ever-changing external influences. Among such requirements are product specifications, operational constraints and safety and environmental regulations. But the most significant incentive for using automated feedback control is the fact, that under the effect of external disturbances, the system must be operated in such a fashion, that it makes the maximum profit. In current practice, this incentive is answered by means of the setpoint/target terminology, which is essentially the process control objective translation of the main economic objective. Translation of objectives in this fashion, results in a loss of economic information and the dynamic regulation layer has no information about the original plant economics except for a fixed steady state target.

This thesis aims to address the primary aim of any feedback control strategy, to optimize plant economics. This thesis presents a plantwide model predictive control strategy that optimizes plant economics directly in the dynamic regulation problem. A class of systems is identified for which optimizing economic objective would lead to stable plant operation, and consequently the asymptotic stability is established for these systems. Not all of the existing tools of stability analysis for feedback control systems work for generic nonlinear problems, hence new tools have been developed and used to establish stability properties.

This thesis also addresses the applications for which nonsteady operation may be desired and proposes MPC strategies for nonsteady operation. These strategies are demonstrated by means of suitable examples from the literature. The economic superiority of economic optimizing controllers is also established.

The benefit of optimizing economics is demonstrated using various chemical engineering process examples from literature. The economic performance is compared to the standard tracking type controllers and the benefit is calculated as a fraction of the steady state profit. To demonstrate the feasibility of online solution to economics optimizing dynamic regulation problem, a software tool is developed using open source nonlinear solvers and automatic differentiation packages. The utility of this tool is demonstrated by using it to perform all the simulation studies in this thesis.

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Chapter 1

Introduction

Process control is an integral part of chemical engineering. Chemical plants convert large quantities of raw material into value-added products. Each process within a plant must function efficiently, requiring process units to respond to internal disturbances, e.g., temperature or flow fluctuations, and to external disturbances, e.g., raw material or product price. Efficient operation of processes requires efficient control. The drive toward greater productivity led to the development of PID control. PID controllers reject local disturbances but require complicated ad-hoc methods to stabilize constrained processes (Pannocchia, Laachi, and Rawlings, 2005). The need to consider system constraints in a natural way and the need for better Multi-Input-Multi-Output (MIMO) control led to optimization based controllers such as Model Predictive Control (MPC) (Mayne, Rawlings, Rao, and Scokaert, 2000). MPC satisfies these needs efficiently and, consequently, has had a significant impact in industry (Qin and Badgwell, 2003; Young, Bartusiak, and Fontaine, 2001; Morari and Lee, 1997).

1.1 Model Predictive Control

Model Predictive Control (MPC) is one of the most widely used multi-variable control techniques in the chemical industry. Among its strengths are the ability to handle constraints directly in its framework and satisfaction of some optimal performance criteria by solving online optimization problems. The most vital component of MPC regulator is the process model, which is used not only to forecast the effects of future inputs, but also to estimate the current state of the plant given the history of past measurements and controls.

In the MPC dynamic optimization problem, the future behavior of the system is predicted using the process model, and based on this prediction, a cumulative cost is minimized. This optimization is usually solved online accounting for the current process conditions and process operation and safety constraints. Then the first move of this optimal input sequence is injected into the system, and based on the measurements and information about the process model and the disturbances, the next state of the system is estimated. This estimate is used to call the dynamic optimizer again and the feedback loop repeats.

1.2 Optimizing process economics in MPC

The primary goal of any control system is to operate the plant such that the net return is maximized in the presence of disturbances and uncertainties, exploiting the available

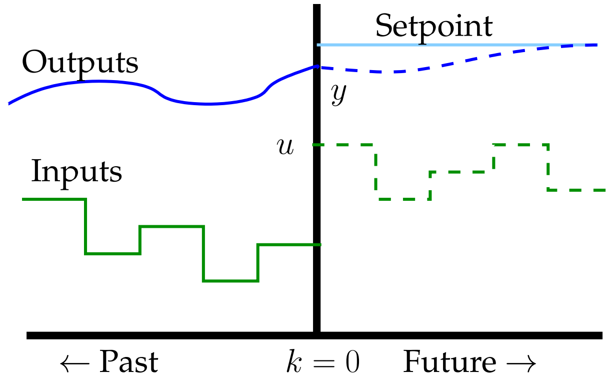

Figure 1.1: MPC strategy

measurements. In current practice, this this done in a two step process, where the process economics are solved to obtain the economically best steady operating state called the setpoint. Hence the economic objective is converted into control objective by means of a steady-state optimization and the controller is designed such that these control objectives are tracked. Hence the controller generates a solution that will drive the system to the economically best steady state. However in the process of converting the process economic measure into steady-state setpoints, a lot of economic information is lost.

For example, Figure 1.2 shows an economic cost surface where the steady-state optimum is different from the global economic optimum. When the economic objective is converted into control objective in terms of the setpoint, information about these potential high profit regions is lost as the controller is unaware of these high profit states. The control objective becomes centered around the setpoint instead. Hence, this motivates the use of economic objective in the dynamic regulations layer directly, so that the controller optimizes over cumulative economic profit allowing it to possible make the system

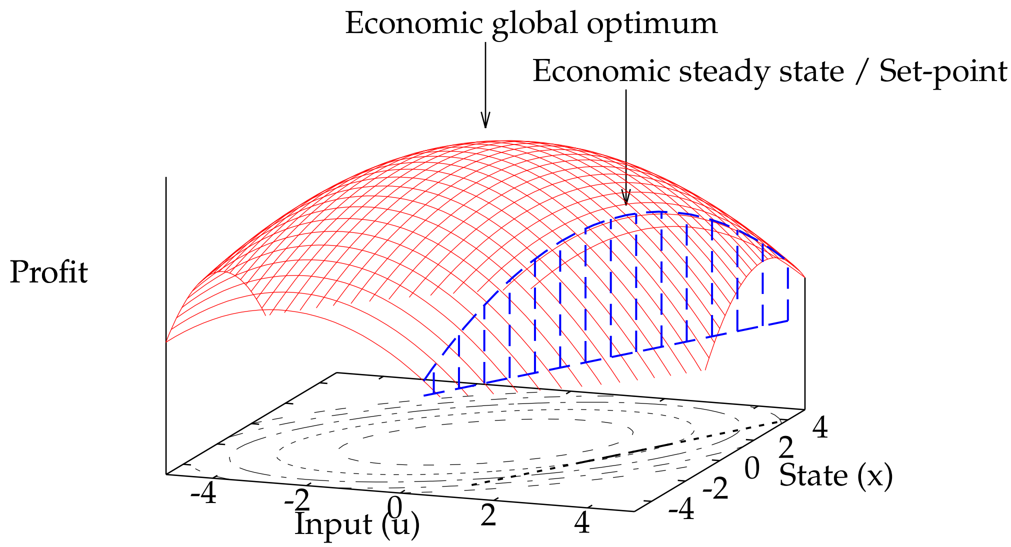

Figure 1.2: Economic cost surface and the steady-state plane showing the difference between the economic steady optimum and the economic global optimum

transient through the high profit areas.

1.3 Academic impact

Trying to optimize process economics in the dynamic optimization problem poses a big challenge for nonlinear MPC researchers. The standard approach of tracking setpoints involves convex quadratic objectives, which are easier to optimize. Proposing to optimize nonlinear and possibly nonconvex objectives subject to nonlinear process models opens up the vast horizon of problems related to nonlinear model predictive control. Stability properties have been well established for linear controllers but there is relatively less literature on the theory of nonlinear MPC. In this thesis we throw light on some outstanding issues in the stability theory of nonlinear MPC by identifying the class of systems for which closed loop stability is expected. New tools for constructing a Lyapunov function are introduced and asymptotic stability is established. A performance comparison is established for nonsteady operation establishing the superiority of the economic optimizing controllers.

1.4 Industrial impact

Process industries today thrive on the performance of advanced control systems. In a competition based economy, most of the developments in advanced control applications aim at better economic performance of the control system. In the present day two layer approach, a lot of focus is on the real time optimization layer, which optimizes the process economics under steady state assumption. A small gain in profit from a subsystem in a plant translates into substantial profits for the whole plant. Hence improving economic performance of the controller is highly attractive for process industries. In this thesis we demonstrate the benefit of optimizing economics directly over tracking steady-state setpoints by means of various examples from the literature.

Proposing to optimize process economics instead of tracking setpoints also opens up the possibility of nonsteady operation, which even though might be unfavorable from the operator's perspective, but a possible significant economic advantage may motivate to rethink the operational strategy of that process. In this thesis, we discuss some applications where nonsteady operation may be desirable and discuss possible ways to control such operation.

1.5 Overview of the thesis

Chapter 2: Literature review

We review the literature used in this thesis and summarize all the previous research on and related to optimizing process economics in dynamic regulation problems.

Chapter 3: Formulations and nominal stability theory

This chapter formulates present the fundamental nominal stability theory for nonlinear systems subject to nonlinear costs. A class of systems is identified for which nominal closed-loop stability is expected for the MPC feedback-control system. The tools for determining Lyapunov functions are extended to this new class of systems and nominal stability is established.

Chapter 4: Suboptimal control

Global optimality is hard to guarantee for nonlinear optimization problems. The nominal stability theory is formulated in Chapter 3 based on the assumption that the global optimum is determined for the dynamic regulation problem. This assumption is relaxed in this chapter to establish the stability properties for suboptimal MPC algorithms.

Chapter 5: Nonsteady operation

This chapter discusses scenarios in which asymptotic stability is not expected and a nonsteady operation is economically better. A performance comparison is established for such scenarios and two MPC algorithms are discussed for controlling such operations.

Chapter 6: Computational methods

Methods to numerically solve dynamic optimization problems are discussed in this chapter. The direct methods for dynamic optimization are discussed in detail and the use of these methods for the development of a software tool to solve dynamic regulation problems is presented. A brief manual of the new tool is presented in Appendix B.

Chapter 7: Case studies

Three case studies are presented to demonstrate the economic benefit of optimizing process economics in the dynamic regulation layer. The performance is compared with the tracking type controllers as a fraction of the steady state profit.

Chapter 8: Conclusions

The thesis concludes with a summary of contributions of this thesis and recommend some research issues for future work.

Chapter 2

Literature Review

2.1 Introduction

The controllers proposed in this thesis are model predictive controllers. The theory of model predictive control (MPC) has evolved a lot over the past three decades. Several texts on MPC are available (Maciejowski, 2002; Camacho and Bordons, 2004; Rossiter, 2004; Wang, 2009). In particular, this thesis makes use of the monograph by Rawlings and Mayne (2009) as a standard baseline reference. Rawlings and Mayne (2009, Ch. 2) investigate the MPC regulation problem in detail. Two types of dynamic regulation formulations are presented and the corresponding stability theory is developed for standard convex costs. The monograph provides key control principles, such as dynamic regulation stability theory and suboptimal MPC, used in this thesis.

2.2 Economics literature

The high level objective for any plant operation is to optimize an economic measure of the plant, usually the net profit. Optimizing economics in control problems is not a new concept. Even before extensive research on advanced process control systems, optimal control problems have been common in economics literature. The earliest work on optimal economic control problems dates back to 1920s (Ramsey, 1928), in which the objective was to determine optimal savings rates to maximize capital accumulation. An array of works followed in the 1950s focussing on various economic considerations like scarce resources, expanding populations, multiple products and technologies. All the economic optimal control problems in these works were infinite time horizon problems since they tried to optimize based on long term predictions. Among these works was the popular concept of "turnpikes" (Dorfman, Samuelson, and Solow, 1958), which was used to characterize the optimal trajectories for these economic control problems. Dorfman et al. (1958, Ch. 12) were the first ones to introduce this concept, and proposed that in an economy, if planning a long-run growth, i.e. the planning horizon is sufficiently long, it is always optimal to reach the optimial steady rate of growth and stay there for most of the time, even if towards the end of the planning period, the growth needs to drop from the steady value. This bevaiour, seen in econimics optimal control problems, was called the "tunrpike" behavior since it was exactly like a turnpike paralleled by a network of minor roads. Hence the asymptotic properties of efficient paths of capital accumulation were known as "turnpike theorems." (McKenzie, 1976). This literature provided the seed for research on optimizing economic performance in the control literature. For infinite horizon optimal control of continuous time systems, Brock and Haurie (1976) established the existence of overtaking optimal trajectories. Convergence of these trajectories to an optimal steady state is also demonstrated. Leizarowitz (1985) extended the results of (Brock and Haurie, 1976) to infinite horizon control of discrete time systems. Reduction of the unbounded cost, infinite horizon optimal control problem to an equivalent optimization problem with finite costs is established. Carlson, Haurie, and Leizarowitz (1991) provide a comprehensive overview of these infinite horizon results.

2.3 Real time optimization

In most industrial advanced control systems, the goal of optimizing dynamic plant economic performance is addressed by a control structure that splits the problem into a number of levels (Marlin and Hrymak, 1997). The overall plant hierarchical planning and operations structure is summarized in numerous books, for example Findeisen, Bailey, Bryds, Malinowski, Tatjewski, and Wozniak (1980); Marlin (1995); Luyben, Tyreus, and Luyben (1999). Planning focuses on economic forecasts and provides production goals. It answers questions like what feed-stocks to purchase, which products to make and how much of each product to make. Scheduling addresses the timing of actions and events necessary to execute the chosen plan, with the key consideration being feasibility. The planning and scheduling unit also provides parameters of the cost functions (e.g. prices of products, raw materials, energy costs) and constraints (e.g. availability of raw materials). The RTO is concerned with implementing business decisions in real time based on a fundamental steady-state model of the plant. It is based on a profit function of the plant and it seeks additional profit based on real-time analysis using a calibrated non-linear model of the process. The data are first analyzed for stationarity of the process and, if a stationary situation is confirmed, reconciled using material and energy balances to compensate for systematic measurement errors. The reconciled plant data are used to compute a new set of model parameters (including unmeasured external inputs) such that the plant model represents the plant as accurately as possible at the current (stationary) operating point. Then new values for critical state variables of the plant are computed that optimize an economic cost function while meeting the constraints imposed by the equipment, the product specifications, and safety and environmental regulations as well as the economic constraints imposed by the plant management system. These values are filtered by a supervisory system that usually includes the plant operators (e.g. checked for plausibility, mapped to ramp changes and clipped to avoid large changes (Miletic and Marlin, 1996)) and forwarded to the process control layer as set points. When viewed from the dynamic layer, these setpoints are often inconsistent and unreachable because of the discrepancies between the models used for steady-state optimization and dynamic regulation. Rao and Rawlings (1999) discuss methods for resolving these inconsistencies and finding reachable steady-state targets that are as close as possible to the unreachable setpoints provided by the RTO.

The two main disadvantages of the current two layer approach are:

- Models in the optimization layer and in the control layer are not fully consistent (Backx, Bosgra, and Marquardt, 2000; Sequeira, Graells, and Puigjaner, 2002). It is pointed out that, in particular, their steady-state gains may be different.

- The two layers have different time scales. The delay in optimization is inevitable because of the steady-state assumption (Cutler and Perry, 1983).

Because of the disadvantages of long sampling times, several authors have proposed reducing the sampling time in the RTO layer (Sequeira et al., 2002). In an attempt to narrow the gap between the sampling rates of the nonlinear steady-state optimization performed in the RTO layer and the linear MPC layer, the so called LP-MPC and QP-MPC two-stage MPC structures have been suggested (Morshedi, Cutler, and Skrovanek, 1985; Yousfi and Tournier, 1991; Muske, 1997; Brosilow and Zhao, 1988).

Engell (2007) reviews the developments in the field of feedback control for optimal plant operations, in which the various disadvantages of the two layer strategy are pointed out. Jing and Joseph (1999) perform a detailed analysis of this approach and analyze its properties. The task of the upper MPC layer is to compute the setpoints both for the controlled variables and for the manipulated inputs for the lower MPC layer by solving a constrained linear or quadratic optimization problem, using information from the RTO layer and from the MPC layer. The optimization is performed with the same sampling period as the lower-level MPC controller.

Forbes and Marlin (1996); Zhang and Forbes (2000) introduce a performance measure for RTO systems to compare the actual profit with theoretic profit. Three losses were considered as a part of the cost function: the loss in the transient period before the system reaches a steady state, the loss due to model errors, and the loss due to propagation of stochastic measurement errors. The issue of model fidelity is discussed by Yip and Marlin (2004). Yip and Marlin (2003) proposed the inclusion of effect of setpoint changes on the accuracy of the parameter estimates into the RTO optimization. Duvall and Riggs (2000) evaluate the performance of RTO for Tennessee Eastman Challenge Problem and point out "RTO profit should be compared to optimal, knowledgeable operator control of the process to determine the true benefits of RTO. Plant operators, through daily control of the process, understand how process setpoint selection affects the production rate and/or operating costs."

Kadam, Marquardt, Schlegel, Backx, Bosgra, Brouwer, Dunnebier, van Hessem, Tiagounov, and de Wolf (2003) point out that the RTO techniques are limited with respect to the achievable flexibility and economic benefit, especially when considering intentionally dynamic processes such as continuous processes with grade transitions and batch processes. They also describe dynamics as the core of plant operation, motivating economically profitable dynamic operation of processes.

2.4 Dynamic optimization of process economics

Morari, Arkun, and Stephanopoulos (1980) state that the objective in the synthesis of a control structure is to *translate the economic objectives into process control objectives*. Backx et al. (2000) describe the need for dynamic operations in the process industries in an increasingly market-driven economy where plant operations are embedded in flexible supply chains striving for just-in-time production in order to maintain competitiveness. They point out that minimizing operation cost while maintaining the desired product quality in such an environment is considerably harder than in an environment with infrequent changes and disturbances, and this minimization cannot be achieved by relying solely on experienced operators and plant managers using their accumulated knowledge about the performance of the plant. Profitable agile operations call for a new look at the integration of process control with process operations.

Huesman, Bosgra, and Van den Hof (2007) point out that doing economic optimization in the dynamic sense leaves some degrees of freedom of the system unused. With the help of examples, it is shown that economic optimization problems can result in multiple solutions suggesting unused degrees of freedom. It is proposed to utilize these additional degrees of freedom for further optimization based on non-economic objectives to get a unique solution.

2.4.1 Controller designs

Helbig, Abel, and Marquardt (2000) introduce the concept of a dynamic real time optimization (D-RTO) strategy, in which, instead of doing a steady-state economic optimization to compute setpoints, a dynamic optimization over a fixed horizon is done to compute a reference trajectory. To avoid dynamic re-optimization, the regulator tracks the reference trajectory using a simpler linear model (or PID controller) with the standard tracking cost function, hence enabling the regulator to act at a faster sampling rate. When using a simplified linear model for tracking a dynamic reference trajectory, an inconsistency remains between the model used in the two layers. Often an additional disturbance model would be required in the linear dynamic model to resolve this inconsistency. These disturbance states would have to be estimated from the output measurements. Kadam and Marquardt (2007) review the D-RTO strategy and improvements to it, and discuss the practical considerations behind splitting the dynamic real-time optimization into two parts. A trigger strategy is also introduced, in which D-RTO reoptimization is only invoked if predicted benefits are significant, otherwise linear updates to the reference trajectory are provided using parametric sensitivity techniques.

Skogestad (2000) describes one approach to implement optimal plant operation by a conventional feedback control structure, termed "self-optimizing" control. In this approach, the feedback control structure is chosen so that maintaining some function of the measured variables constant automatically maintains the process near an economically optimal steady state in the presence of disturbances. The problem is posed from the plantwide perspective, since the economics are determined by overall plant behavior. Aske, Strand, and Skogestad (2008) also point out the lack of capability in steady-state RTO, in the cases when there are frequent changes in active constraints of large economic importance. The important special case is addressed in which prices and market conditions are such that economic optimal operation of the plant is the same as maximizing plant throughput. A coordinator model predictive control strategy is proposed in which a coordinator controller regulates local capacities in all the units.

Sakizlis, Perkins, and Pistikopoulos (2004) describe an approach of integrating optimal process design with process control. They discuss integration of process design, process control and process operability together, and hence deal with the economics of the process. The incorporation of advanced optimizing controllers in simultaneous process and control design is the goal of the optimization strategy. It deals with an offline control approach where an explicit optimizing control law is derived for the process. The approach is reported to yield a better economic performance.

Extremum-seeking control is another approach in which the controller drives the system states to steady values that optimize a chosen performance objective. Krstic and Wang (2000) address closed-loop stability of the general extremum-seeking approach when the performance objective is directly measured online. Guay and Zhang (2003) address the case in which the performance objective is not measurable and available for feedback. This approach has been evaluated for temperature control in chemical reactors subject to state constraints (Guay, Dochain, and Perrier, 2003; DeHaan and Guay, 2004).

awrynczuk, Marusak, and Tatjewski (2007) propose two versions of the integrated MPC and set-point calculation algorithms. In the first one, the nonlinear steady-state model is used. This leads to a nonlinear optimization problem. In the second version, the model is linearized on-line. It leads to a quadratic programming problem, which can be effectively solved using standard routines. In both these problems, the economic objective used in the steady-state optimization as well as the dynamic optimization is either linear or quadratic in the outputs and inputs.

Heidarinejad, Liu, and Christofides (2011b,a) propose an economic MPC scheme based on explicit Lyapunov-based nonlinear controller design techniques that allows for an explicit characterization of the stability region of the closed-loop system. The underlying assumption for this design is the existence of a Lyapunov-based controller which renders the origin of the nominal closed-loop system asymptotically stable. Hence the methodology assumes that a control law is known such that some corresponding Lyapunov function has a negative gradient in time. The authors point out that there are currently no general methods for constructing Lyapunov functions for generic nonlinear systems, and bases on previous results, use a quadratic controller and a quadratic Lyapunov function. A two-tier controller approach is proposed in this paper. In the first mode, the controller drives the system optimizing the economic performance measure subject to the states of the system remaining inside a defined stability region. The stability region is defined as a level set of the chosen Lyapunov function such that it is the largest subset of the neighborhood of the equilibrium point in which a Lyapunov based controller can be defined. A terminal time is chosen for this first mode and after this time, an additional constraint is turned on, which is the second mode. In this second mode, an additional constraint ensures that the chosen Lyapunov function decreases at least at the rate given by the Lyapunov based controller. The paper is a direct extension on the authors' previous work (Mhaskar, El-Farra, and Christofides, 2006). Heidarinejad et al. (2011b) extended the approach to account for bounded disturbances and asynchronous delayed measurements.

Huang, Harinath, and Biegler (2011b) point out applications like simulated moving bed (SMB) and pressure swing adsorption (PSA) in which non-steady operation is desirable due to economic benefit and the design of the process. They provide a nonlinear MPC scheme for cyclic processes for which the period of the process is known. They present two different formulations. In the first formulation, a finite horizon problem is formulated with the horizon chosen as a multiple of the process period. A terminal periodic constraint is implemented which forces the state at the end of the horizon to be the same as one period before the end of the horizon. The second formulation is an infinite horizon formulation. To deal with the infinite sum of an economically oriented cost, a discount factor is used to project the future profit. There is no terminal periodic constraint since the problem is infinite dimensional. Both the formulations are assumed to satisfy optimality conditions to assume local uniqueness of the solution, and regularization tracking terms are added to the economic stage cost to satisfy these assumptions. Hence the objective is not purely economic. Asymptotic stability is proved for both the controllers by proposing the optimal value of the shifted cost as the Lyapunov function for the system. Huang, Biegler, and Harinath (2011a) extend the concept of concept of rotated cost, introduced in this thesis and Diehl, Amrit, and Rawlings (2011), and extend it to the framework of cyclic systems. The authors propose a requirement of convexity on the rotated cost to ensure closed loop stability. The nominal stability results are then extended to robust stability using the standard Input-to-State stability framework.

2.4.2 Implementation and applications

Zanin, Tvrzska de Gouvea, and Odloak (2000, 2002); Rotava and Zanin (2005) report the formulation, solution and industrial implementation of a combined MPC/optimizing control scheme for a fluidized bed catalytic cracker. The economic criterion is the amount of liquified petroleum gas produced. The optimization problem that is solved in each controller sampling period is formulated in a mixed manner: range control MPC with a fixed linear plant model (imposing soft constraints on the controlled variables by a quadratic penalty term that only becomes active when the constraints are violated) plus a quadratic control move penalty plus an economic objective that depends on the values of the manipulated inputs at the end of the control horizon.

Ma, Qin, Salsbury, and Xu (2011) demonstrate the effectiveness of model predictive control (MPC) technique in reducing energy and demand costs, which form the objective of the controller, for building heating, ventilating, and air conditioning (HVAC) systems. A simulated multi-zone commercial building equipped with a set of variable air volume (VAV) cooling system is studied. System identification is performed to obtain zone temperature and power models, which are used in the MPC framework. The economic objective function in MPC accounts for the daily electricity costs, which include time of use energy cost and demand cost. In each time step, a min-max optimization is formulated, converted into a linear programming problem and solved. Cost savings by MPC are estimated by comparing with the baseline and other open-loop control strategies.

Chapter 3

Formulations and nominal stability theory

Note: The text of this chapter appears in Angeli, Amrit, and Rawlings (2011a); Amrit et al. (2011).

3.1 Introduction

The dynamic optimization problem in model predictive control can be formulated in two different ways, depending on the choice of objective function and the stabilizing constraints, as discussed in detail by Rawlings and Mayne (2009, Ch. 2). In the standard MPC problem, in which the stage cost is defined as the deviation from the best steady state, the stability of the closed-loop system is established by observing that the optimal cost along the closed-loop trajectory is a Lyapunov function. In the economic MPC problem the optimal cost is not a Lyapunov function. In this chapter we present the model predictive control formulations using a generic nonlinear economic objective. In Section 3.2, we first introduce our basic notation and definitions that will be used in developing the theory in this chapter and the rest of the thesis. We present the terminal constraint and the terminal penalty MPC formulations in Section 3.3 and Section 3.4 respectively, and state and prove the respective stability properties of these formulations. In Section 3.5 we propose a third formulation in which the stabilizing constraint is removed. The performance of the three formulations is then compared with each other and with the steady state performance.

3.2 Preliminaries and Definitions

We first establish the notation that defines the dynamic nonlinear system and the economic cost function. Consider the following nonlinear discrete time system

$$x^+ = f(x,u) \tag{3.1}$$

with state $x \in \mathbb{X} \subseteq \mathbb{R}^n$, control $u \in \mathbb{U} \subset \mathbb{R}^m$, and state transition map $f : \mathbb{Z} \to \mathbb{R}^n$, where the system is subject to the mixed constraint

$$(x(k), u(k)) \in \mathbb{Z} \qquad k \in \mathbb{I}_{\geq 0}$$

for some compact set $\mathbb{Z} \subseteq \mathbb{X} \times \mathbb{U}$. We consider a cost function $\ell(x,u) : \mathbb{Z} \to \mathbb{R}$, which is based on the process economics. Consider the following steady-state problem

$$\min_{(x,u)\in\mathbb{Z}} \ell(x,u) \quad \text{subject to} \quad x = f(x,u) \tag{3.2}$$

The solution of the steady-state problem is denoted by (x_s, u_s), and is assumed to be unique. We now review some important definitions that will be used in the theory developed in the chapter and rest of the thesis.

Definition 3.1 (Positive definite function). *A function $\rho(\cdot)$ is positive definite with respect to $x = a$ if it is continuous, $\rho(a) = 0$, and $\rho(x) > 0$ for all $x \neq a$.*

Definition 3.2 (Class $\mathcal{K}$ function). *A function $\gamma(\cdot) : \mathbb{R} \to \mathbb{R}_{\geq 0}$ is a class $\mathcal{K}$ if it is continuous, zero at zero and strictly increasing.*

Lemma 3.3. *Given a positive definite function $\rho(x)$ defined on a compact set $\mathbb{C}$ containing the origin, there exists a class $\mathcal{K}$ function $\gamma(\cdot)$ such that*

$$\rho(x) \geq \gamma(|x|), \quad \forall x \in \mathbb{C}$$

Definition 3.4 (Positive invariant set). *A set $\mathcal{A}$ is positive invariant for the nonlinear system $x^+ = f(x)$, if $x \in \mathcal{A}$ implies $x^+ \in \mathcal{A}$.*

Definition 3.5 (Asymptotic stability). *The steady state x_s of a nonlinear system $x^+ = f(x)$ is* asymptotically stable *on $\mathcal{X}$, $x_s \in \mathcal{X}$, if there exist a class $\mathcal{K}$ function $\gamma(\cdot)$ such that for any $x \in \mathcal{X}$,* all *solutions $\phi(k; x)$ satisfy:*

$$\phi(k;x) \in \mathcal{X}, \quad |\phi(k;x) - x_s| \leq \gamma(|x - x_s|, k) \quad \textit{for all } k \in \mathbb{I}_{\geq 0}.$$

Definition 3.6 (Lyapunov function). *A function $V : \mathbb{R}^n \to \mathbb{R}_{\geq 0}$ is said to be a Lyapunov function for the nonlinear system $x^+ = f(x)$ in the set $\mathcal{X}$ if there exist class $\mathcal{K}$ functions γ_i,*

$i \in \{1, 2, 3\}$ *such that for any* $x \in \mathcal{X}$

$$\gamma_1(|x|) \leq V(x) \leq \gamma_2(|x|) \quad V(f(x)) - V(x) \leq -\gamma_3(|x|)$$

Lemma 3.7 (Lyapunov function and asymptotic stability)**.** *Consider a set $\mathcal{X}$, that is positive invariant for the nonlinear system $x^+ = f(x)$; $f(x_s) = x_s$. The steady state x_s is an asymptotically stable equilibrium point for the system $x^+ = f(x)$ on $\mathcal{X}$, if and only if there exists a Lyapunov function V on $\mathcal{X}$ such that $V(x - x_s)$ satisfies the properties in Definition 3.6.*

Definition 3.8 (Strictly dissipative system)**.** *The system $x^+ = f(x, u)$ is strictly dissipative with respect to the supply rate $s : \mathbb{Z} \to \mathbb{R}$ if there exists a storage function $\lambda : \mathbb{X} \to \mathbb{R}$ and a positive definite function $\rho : \mathbb{Z} \to \mathbb{R}_{\geq 0}$, such that for all $(x, u) \in \mathbb{Z} \subseteq X \times \mathbb{U}$*

$$\lambda(f(x, u)) - \lambda(x) \leq -\rho(x - x_s, u - u_s) + s(x, u) \tag{3.3}$$

Next we introduce the concept of *rotated cost* which forms the backbone of the stability theory of economic nonlinear MPC.

3.2.1 Rotated cost

Unlike the standard MPC problem, the optimal cost along the closed loop, may not be a Lyapunov function for the nonlinear system. Hence we introduce a modified stage cost, which we call the '*rotated cost*'. To define the rotated cost, we first make the following assumptions:

Assumption 3.9 (Dissipative system)**.** *The nonlinear system* $x^+ = f(x,u)$ *is dissipative with respect to the supply rate* $s(x,u) = \ell(x,u) - \ell(x_s,u_s)$.

Assumption 3.10 (Continuity of cost, system and storage)**.** *The cost* $\ell(\cdot)$*, the system dynamics function* $f(\cdot)$*, and the storage function* $\lambda(\cdot)$ *are continuous on* $\mathbb{Z}$.

We define the *rotated stage cost* $L(x,u) : \mathbb{Z} \to \mathbb{R}_{\geq 0}$ as a function of the economic stage cost $\ell(\cdot)$, and the corresponding storage function $\lambda(\cdot)$:

$$L(x,u) := \ell(x,u) + \lambda(x) - \lambda(f(x,u)) - \ell(x_s,u_s) \tag{3.4}$$

Let Assumptions 3.9–3.10 hold. Then the rotated cost has the following properties

1. **Steady-state solution**: Consider the following steady-state problem

$$\min_{(x,u)\in\mathbb{Z}} L(x,u) \quad \text{subject to} \quad x = f(x,u) \tag{3.5}$$

   Problems (3.2) and (3.5) have the same solution (x_s,u_s).

2. **Lower bound**: The dissipation inequality (3.3) implies that the rotated stage cost $L(x,u) \geq \rho(x - x_s, u - u_s)$ for all $(x,u) \in \mathbb{Z}$ and hence can be underbounded by a class $\mathcal{K}$ function (Lemma 3.3).

$$L(x,u) \geq \gamma(|(x - x_s, u - u_s)|) \geq \gamma(|x - x_s|) \geq 0, \quad \forall (x,u) \in \mathbb{Z} \tag{3.6}$$

3.3 Terminal constraint formulation

We now formulate the terminal constraint MPC formulation in which the nonlinear system is stabilized by means of an equality constraint on the terminal state.

3.3.1 Objective function

In this formulation, we define the economic objective function for the dynamic regulation problem as the sum of N stage costs, i.e.

$$V_{N,c}(x, \mathbf{u}) = \sum_{k=0}^{N-1} \ell(x(k), u(k)) \tag{3.7}$$

in which x is the initial state, $\ell(\cdot) : \mathbb{Z} \to \mathbb{R}$ is the economic stage cost, N is the control horizon, and the control sequence is denoted as $\mathbf{u} := \{u(0), u(1), \ldots, u(N-1)\}$.

3.3.2 Constraints

One method to stabilize nonlinear systems using MPC is to add the requirement that the system terminates at the optimal steady state. Hence we include an equality terminal state constraint of the form

$$x(N) = x_s$$

The control constraint set $\mathcal{U}_{N,c}(x)$ is then the set of control sequences $\mathbf{u}$ satisfying the control constraints and terminal state constraint. It is defined by

$$\mathcal{U}_{N,c}(x) := \{\mathbf{u} \mid (x, \mathbf{u}) \in \mathbb{Z}_{N,c}\} \tag{3.8}$$

in which the set $\mathbb{Z}_{N,c} \subset \mathbb{X} \times \mathbb{U}^N$ is defined by

$$\mathbb{Z}_{N,c} := \left\{(x, \mathbf{u}) \mid (\phi(k; x, \mathbf{u}), u(k)) \in \mathbb{Z}, \forall k \in \mathbb{I}_{0:N-1}, \phi(N; x, \mathbf{u}) = x_s\right\} \tag{3.9}$$

where $\phi(k; x, \mathbf{u})$ is the solution to (3.1) at time $k \in \mathbb{I}_{0:N}$ for initial state x and control sequence $\mathbf{u}$. The set of admissible states $\mathcal{X}_{N,c}$ is defined as the projection of $\mathbb{Z}_{N,c}$ onto $\mathbb{X}$.

$$\mathcal{X}_{N,c} = \{x \in \mathbb{X} \mid \exists\, \mathbf{u} \text{ such that } (x, \mathbf{u}) \in \mathbb{Z}_{N,c}\}$$

3.3.3 Stability

We now propose a candidate Lyapunov function and establish asymptotic stability of the nonlinear system driven by the terminal constraint MPC. We first make the following assumptions

Assumption 3.11 (Weak controllability)**.** *There exists γ of class $\mathcal{K}_\infty$ such that for each $x \in \mathcal{X}_{N,c}$ there exists a feasible $\mathbf{u}$, with*

$$|\mathbf{u} - [u_s, \dots, u_s]'| \leq \gamma(|x - x_s|)$$

Candidate Lyapunov function

With the rotated stage cost as defined in (3.4), we define the rotated regulator cost function as follows

$$\overline{V}_{N,c}(x, \mathbf{u}) := \sum_{k=0}^{N-1} L(x(k), u(k)) \tag{3.10}$$

The standard and auxiliary nonlinear optimal control problems $\mathbb{P}_{N,c}(x)$ and $\overline{\mathbb{P}}_{N,c}(x)$ are

$$\mathbb{P}_{N,c}(x): \qquad V^0_{N,c}(x) := \min_{\mathbf{u}}\{V_{N,c}(x, \mathbf{u}) \mid \mathbf{u} \in \mathcal{U}_{N,c}(x)\}$$

$$\overline{\mathbb{P}}_{N,c}(x): \qquad \overline{V}^0_{N,c}(x) := \min_{\mathbf{u}}\{\overline{V}_{N,c}(x, \mathbf{u}) \mid \mathbf{u} \in \mathcal{U}_{N,c}(x)\}$$

Due to Assumptions 3.10, both $V_{N,c}(\cdot)$ and $\overline{V}_{N,c}(\cdot)$ are defined and continuous on the set $\mathcal{U}_{N,c}$. Since the set $\mathbb{Z}$ is compact, the set $\mathcal{U}_{N,c}(x)$ is compact for all $x \in \mathcal{X}_{N,c}$. Hence solutions exist for both problems $\mathbb{P}_{N,c}(x)$ and $\overline{\mathbb{P}}_{N,c}(x)$ for $x \in \mathcal{X}_{N,c}$. As we shall establish later, the two problems have identical solution sets. Denote the optimal solution of these problems as

$$\mathbf{u}^0(x) = \{u^0(0;x), u^0(1;x), \cdots, u^0(N-1,x)\} \tag{3.11}$$

In MPC, the control applied to the plant is the first element of the optimal control sequence, yielding the implicit MPC control law $\kappa_{N,c}(\cdot)$ defined as

$$\kappa_{N,c}(x) = u^0(0;x)$$

Then the close loop system evolves according to

$$x^+ = f(x, \kappa_{N,c}(x)) \tag{3.12}$$

We propose $\overline{V}^0_{N,c}(x)$ as the candidate Lyapunov function for the system under the control law $\kappa_{N,c}(x)$.

Proposition 3.12 (Equivalence of solutions). *The solution sets for $\overline{\mathbb{P}}_{N,c}(x)$ and $\mathbb{P}_{N,c}(x)$ are identical.*

Proof. Expanding the rotated regulator cost function gives

$$\begin{aligned}
\overline{V}_{N,c}(x,\mathbf{u}) &= \sum_{k=0}^{N-1} L(x(k),u(k)) \\
&= \sum_{k=0}^{N-1} \left(\ell(x(k),u(k)) - \ell(x_s,u_s)\right) + \sum_{k=0}^{N-1} \left(\lambda(x(k)) - \lambda(f(x(k),u(k)))\right) \\
&= V_{N,c}(x,\mathbf{u}) + \lambda(x) - \lambda(x_s) - N\ell(x_s,u_s)
\end{aligned}$$

Since $\lambda(x)$, $\lambda(x_s)$ and $N\ell(x_s, u_s)$ are independent of the decision variable vector $\mathbf{u}$, the two objective functions $\overline{V}_{N,c}$ and $V_{N,c}$ differ by terms which are constant for a given initial state x, and hence the two optimization problems $\overline{\mathbb{P}}_{N,c}(x)$ and $\mathbb{P}_{N,c}(x)$ have the same solution sets. □

Theorem 3.13 (Asymptotic stability)**.** *If Assumptions 3.9, 3.10 and 3.11 hold, then the steady-state solution x_s is an asymptotically stable equilibrium point of the nonlinear system* (3.12) *with a region of attraction $\mathcal{X}_{N,c}$.*

Proof. Consider the rotated cost function (3.10)

$$\overline{V}_{N,c}(x, \mathbf{u}) = \sum_{k=0}^{N-1} L(x(k), u(k)), \quad x \in \mathcal{X}_{N,c}$$

The candidate Lyapunov function for the problem is $\overline{V}^0_{N,c}(x) = \overline{V}_{N,c}(x, \mathbf{u}^0(x))$, where $\mathbf{u}^0(x)$ is the optimal control sequence as defined in (3.22). The resulting optimal state sequence is $\mathbf{x}^0(x) = \{x^0(0; x), x^0(1; x), \ldots, x^0(N; x)\}$. We choose a candidate input sequence and a corresponding state sequence as follows

$$\mathbf{u}(x) = \{u^0(1; x), u^0(2; x), \ldots, u^0(N-1; x),\ u_s)\}$$

$$\mathbf{x}(x) = \left\{x^0(1; x), x^0(2; x), \ldots, x^0(N; x), x_s)\right\}$$

Due to the terminal state constraint, $x^0(N; x) = x_s$, and hence $x^0(N+1; x) = x_s$. For all $x \in \mathcal{X}_{N,c}$, the definition of $\overline{V}_{N,c}(\cdot)$ gives

$$\begin{aligned}\overline{V}_{N,c}(x^+, \mathbf{u}) &= \sum_{k=1}^{N-1} L(x^0(k; x), u^0(k; x)) + L(x_s, u_s) \\ &= \overline{V}^0_{N,c}(x) - L(x, u^0(0; x))\end{aligned}$$

Since $\overline{V}^0_{N,c}(x^+) \leq \overline{V}_{N,c}(x^+, \mathbf{u})$, it follows that

$$\begin{aligned}\overline{V}^0_{N,c}(x^+) - \overline{V}^0_{N,c}(x) &\leq -\, L(x, u^0(0; x)) \\ &\leq -\, \gamma(|x - x_s|) \qquad \text{using (3.6)}\end{aligned}$$

We also observe that due to (3.6):

$$\overline{V}^0_{N,c}(x) \geq L(x, u(0)) \geq \gamma(|x - x_s|), \qquad x \in \mathcal{X}_{N,c}$$

Also using Assumption 3.11, it can be shown that $\overline{V}^0_{N,c}(x) \leq \overline{\gamma}(|x - x_s|)$ for all $x \in \mathcal{X}_{N,c}$, where $\overline{\gamma}(|x - x_s|)$ is a class $\mathcal{K}$ function. Hence $\overline{V}^0_{N,c}$ is a Lyapunov function and x_s is an asymptotically stable equilibrium point of (3.12) with a region of attraction $\mathcal{X}_{N,c}$.

□

Hence we have established nominal asymptotic stability for the nonlinear system under the terminal constraint MPC.

3.4 Terminal penalty/control formulation

Having a terminal equality constraint in the problem can be a demanding constraint, especially if the control horizon is short. Equality constraints, in general, makes the nonlinear optimization problem, hard to solve for the NLP solver In this section we propose the terminal control MPC formulation, which attempts to relax the terminal equality constraint as used in the previous formulation, and replace it with a terminal state penalty and a terminal region pair.

3.4.1 Objective function

The economic objective function for the dynamic regulation problem in the terminal penalty formulation is defined as the sum of N stage costs and a penalty cost on the terminal state

$$V_{N,p}(x, \mathbf{u}) = \sum_{k=0}^{N-1} \ell(x(k), u(k)) + V_f(x(N)) \tag{3.13}$$

in which x is the initial state, $\ell(\cdot) : \mathbb{Z} \to \mathbb{R}$ is the economic stage cost, $V_f(\cdot) : \mathbb{X}_f \to \mathbb{R}$ is the terminal penalty, where $\mathbb{X}_f \subseteq \mathbb{X}$ is a compact terminal region containing the steady-state operating point in its interior, N is the control horizon, and the control sequence is denoted as $\mathbf{u} := \{u(0), u(1), \ldots, u(N-1)\}$.

3.4.2 Constraints

For nonlinear models, one often can define $\mathbb{X}_f$ in which a control Lyapunov function is available (Rawlings and Mayne, 2009, Ch. 2). The second method to stabilize nonlinear systems using MPC is to add the requirement that the terminal state lie in this terminal region, instead of at the best steady state x_s. Hence we include a terminal state constraint of the form

$$x(N) \in \mathbb{X}_f$$

The standard control constraint set $\mathcal{U}_{N,p}(x)$ is then the set of control sequences $\mathbf{u}$ satisfying the control constraints and terminal state constraint. It is defined by

$$\mathcal{U}_{N,p}(x) := \{\mathbf{u} \mid (x, \mathbf{u}) \in \mathbb{Z}_{N,p}\} \tag{3.14}$$

in which the set $\mathbb{Z}_{N,p} \subset \mathbb{X} \times \mathbb{U}^N$ is defined by

$$\mathbb{Z}_{N,p} := \left\{ (x, \mathbf{u}) \mid (\phi(k; x, \mathbf{u}), u(k)) \in \mathbb{Z}, \forall k \in \mathbb{I}_{0:N-1}, \phi(N; x, \mathbf{u}) \in \mathbb{X}_f \right\} \tag{3.15}$$

where $\phi(k; x, \mathbf{u})$ is the solution to (3.1) at time $k \in \mathbb{I}_{0:N}$ for initial state x and control sequence $\mathbf{u}$. The set of admissible states $\mathcal{X}_{N,p}$ is defined as the projection of $\mathbb{Z}_{N,p}$ onto $\mathbb{X}$.

$$\mathcal{X}_{N,p} = \{x \in \mathbb{X} \mid \exists\, \mathbf{u} \text{ such that } (x, \mathbf{u}) \in \mathbb{Z}_{N,p}\}$$

3.4.3 Stability

Similar to the terminal constraint formulation presented in Section 3.3, we propose a Lyapunov function for the closed loop system to establish closed-loop stability. We make the following assumptions.

Assumption 3.14 (Stability assumption)**.** *There exists a compact terminal region $\mathbb{X}_f \subseteq \mathbb{X}$, containing the point x_s in its interior, and control law $\kappa_f : \mathbb{X}_f \to \mathbb{U}$, such that the following holds*

$$V_f(f(x, \kappa_f(x))) \leq V_f(x) - \ell(x, \kappa_f(x)) + \ell(x_s, u_s), \quad \forall x \in \mathbb{X}_f \tag{3.16}$$

This assumption requires that for each $x \in \mathbb{X}_f$, $f(x, \kappa_f(x)) \in \mathbb{X}_f$, i.e. the set $\mathbb{X}_f$ is control invariant under control law $u = \kappa_f(x)$.

Remark 3.15. *Since Assumption 3.14 is the only requirement on V_f, we can assume $V_f(x_s) = 0$ without loss of generality. It should be noted that unlike the standard MPC problem, $V_f(x)$ is not necessarily positive definite with respect to x_s.*

Candidate Lyapunov function

For ease of notation, we first define the *shifted* stage cost as following

$$\overline{\ell}(x,u) = \ell(x,u) - \ell(x_s,u_s) \tag{3.17}$$

Next we define the *rotated* terminal cost in the region $(x,u) \in \mathbb{Z}$. Correspondingly we define the rotated regulator cost function.

$$\overline{V}_f(x) := V_f(x) + \lambda(x) - V_f(x_s) - \lambda(x_s) \tag{3.18}$$

$$\overline{V}_{N,p}(x,\mathbf{u}) := \sum_{k=0}^{N-1} L(x(k),u(k)) + \overline{V}_f(x(N)) \tag{3.19}$$

The standard and auxiliary nonlinear optimal control problems $\mathbb{P}_{N,p}(x)$ and $\overline{\mathbb{P}}_{N,p}(x)$ are

$$\mathbb{P}_{N,p}(x): \qquad V^0_{N,p}(x) := \min_{\mathbf{u}}\{V_{N,p}(x,\mathbf{u}) \mid \mathbf{u} \in \mathcal{U}_{N,p}(x)\} \tag{3.20}$$

$$\overline{\mathbb{P}}_{N,p}(x): \qquad \overline{V}^0_{N,p}(x) := \min_{\mathbf{u}}\{\overline{V}_{N,p}(x,\mathbf{u}) \mid \mathbf{u} \in \mathcal{U}_{N,p}(x)\} \tag{3.21}$$

Due to Assumption 3.10, both $V_{N,p}(\cdot)$ and $\overline{V}_{N,p}(\cdot)$ are defined and continuous on the set $\mathcal{U}_{N,p}$. Since the set $\mathbb{Z}$ is compact, the set $\mathcal{U}_{N,p}(x)$ is compact for all $x \in \mathcal{X}_N$. Hence solutions exist for both problems $\mathbb{P}_{N,p}(x)$ and $\overline{\mathbb{P}}_{N,p}(x)$ for $x \in \mathcal{X}_N$. As we shall establish later, the two problems have identical solution sets. Denote the optimal solution of these problems as

$$\mathbf{u}^0(x) = \{u^0(0;x), u^0(1;x), \cdots, u^0(N-1,x)\} \tag{3.22}$$

In MPC, the control applied to the plant is the first element of the optimal control sequence, yielding the implicit MPC control law $\kappa_{N,p}(\cdot)$ defined as

$$\kappa_{N,p}(x) = u^0(0;x)$$

Then the close loop system evolves according to

$$x^+ = f(x, \kappa_{N,p}(x)) \tag{3.23}$$

We propose $\overline{V}^0_{N,p}(x)$ as the candidate Lyapunov function for the system under the control law $\kappa_{N,p}(x)$.

Properties of the rotated costs

We now present some interesting properties of the rotated stage and terminal costs defined above and use them later in the stability analysis of the terminal penalty controller.

Lemma 3.16 (Modified terminal cost)**.** *The pair* $(\overline{V}_f(\cdot), L(\cdot))$ *satisfies the following property if and only if* $(V_f(\cdot), \ell(\cdot))$ *satisfies Assumption 3.14.*

$$\overline{V}_f(f(x, \kappa_f(x))) \leq \overline{V}_f(x) - L(x, \kappa_f(x)) \qquad \forall x \in \mathbb{X}_f \tag{3.24}$$

Proof. Adding $\lambda(f(x, \kappa_f(x))) + \lambda(x)$ to both sides of (3.16) and rearranging gives the desired inequality

$$\begin{aligned} \overline{V}_f(f(x, \kappa_f(x))) - \overline{V}_f(x) \leq & - \big(\ell(x, \kappa_f(x)) + \lambda(x) - \\ & \lambda(f(x, \kappa_f(x))) - \ell(x_s, u_s)\big) \\ = & - L(x, \kappa_f(x)) \end{aligned}$$

□

Lemma 3.17. *If Assumptions 3.9, 3.10 and 3.14 hold, then the rotated terminal cost $\overline{V}_f(x)$ defined by* (3.18) *is positive definite on $\mathbb{X}_f$ with respect to $x = x_s$.*

Proof. From Assumption 3.10, $\overline{V}_f(\cdot)$ is continuous on $\mathbb{X}_f$ and from (3.18), $\overline{V}_f(x_s) = 0$. Next we show $\overline{V}_f(x) > 0$ for $x \in \mathbb{X}_f, x \neq x_s$. Let $\mathbf{x}(x;\kappa_f)$ and $\mathbf{u}(x;\kappa_f)$ denote the state and control sequences starting from $x \in \mathbb{X}_f$ and using the control law $u = \kappa_f(x)$, defined in Assumption 3.14, in the closed-loop system $x^+ = f(x, \kappa_f(x))$. Consider the sequence $\{\overline{V}_f(x(k;x,\kappa_f))\}, k \in \mathbb{I}_{\geq 0}$, which satisfies for all $k \in \mathbb{I}_{\geq 0}$ by (3.24)

$$\overline{V}_f(x(k+1;x,\kappa_f)) - \overline{V}_f(x(k;x,\kappa_f)) \leq -L(x(k;x,\kappa_f), u(k;x,\kappa_f)) \tag{3.25}$$

From (3.6) we have that the sequence $\{\overline{V}_f(x(k;x,\kappa_f))\}$ is nonincreasing with k. It is bounded below since $\overline{V}_f(\cdot)$ is continuous and $\mathbb{X}_f$ is compact. Therefore, the sequence converges and $L(x(k;x,\kappa_f), u(k;x,\kappa_f)) \to 0$ as $k \to \infty$, and, from (3.6), $x(k;x,\kappa_f) \to x_s$ as $k \to \infty$. Since $\overline{V}_f(\cdot)$ is continuous and $\overline{V}_f(x_s) = 0$, we also have that $V_f(x(k;x,\kappa_f)) \to 0$ as $k \to \infty$. Summing (3.25) for $k \in \mathbb{I}_{0:M-1}$ gives

$$\overline{V}_f(x) \geq \sum_{k=0}^{M-1} L(x(k;x,\kappa_f), u(k;x,\kappa_f)) + \overline{V}_f(x(M;x,\kappa_f))$$

Taking the limit as $M \to \infty$ gives

$$\overline{V}_f(x) \geq \sum_{k=0}^{\infty} L(x(k;x,\kappa_f), u(k;x,\kappa_f))$$

By (3.6), $L(x, \kappa_f(x) > 0$ for $x \neq x_s$, so we have established that $\overline{V}_f(x) > 0$ for $x \in \mathbb{X}_f, x \neq x_s$ and the proof is complete. $\square$

Lemma 3.18 (Rawlings and Mayne (2011))**.** *Let a function $V(x)$ be defined on a set X, which is a closed susbset of $\mathbb{R}^n$. If $V(\cdot)$ is continuous at the origin and $V(0) = 0$, then there exists a class $\mathcal{K}$ function $\alpha(\cdot)$ such that*

$$V(x) \leq \alpha(|x|), \quad \forall x \in X$$

Lemma 3.19 (Bounds on the rotated terminal cost)**.** *If Assumptions 3.9, 3.10 and 3.14 hold, the rotated terminal cost $\overline{V}_f(x)$ satisfies*

$$\gamma(|x - x_s|) \leq \overline{V}_f(x) \leq \gamma(|x - x_s|), \quad \forall x \in \mathbb{X}_f$$

in which functions $\gamma(\cdot), \gamma(\cdot)$ are class $\mathcal{K}$.

Proof. The lower bound follows from (3.24) and (3.6) and Lemma 3.17. For the upper bound, from Assumption 3.10 and Lemma 3.18 it follows that

$$\overline{V}_f(x) \leq \gamma(|x - x_s|), \quad \forall x \in \mathbb{X}_f$$

which completes the proof. $\square$

Lemma 3.20 (Equivalence of solutions)**.** *Let Assumptions 3.10 and 3.14 hold. The solution sets for $\overline{\mathbb{P}}_{N,p}(x)$ and $\mathbb{P}_{N,p}(x)$ are identical.*

Proof. Expanding the rotated regulator cost function gives

$$\begin{aligned}
\overline{V}_{N,p}(x,\mathbf{u}) &= \sum_{k=0}^{N-1} L(x(k),u(k)) + \overline{V}_f(x(N)) \\
&= \sum_{k=0}^{N-1} \ell(x(k),u(k)) + V_f(x(N)) - V_f(x_s) - \lambda(x_s) + \\
&\quad \sum_{k=0}^{N-1} \left(\lambda(x(k)) - \lambda(f(x(k),u(k))) - \ell(x_s,u_s)\right) + \lambda(x(N)) \\
&= V_{N,p}(x,\mathbf{u}) + \lambda(x) - \lambda(x(N)) + \lambda(x(N)) - \\
&\quad V_f(x_s) - \lambda(x_s) - N\ell(x_s,u_s) \\
&= V_{N,p}(x,\mathbf{u}) - N\ell(x_s,u_s) + \lambda(x) - \lambda(x_s) - V_f(x_s)
\end{aligned}$$

Since $\lambda(x)$, $\lambda(x_s)$, $V_f(x_s)$ and $N\ell(x_s,u_s)$ are independent of the decision variable vector $\mathbf{u}$, the two objective functions $\overline{V}_{N,p}$ and $V_{N,p}$ differ by terms that are constant for a given initial state x, and hence the two optimization problems $\overline{\mathbb{P}}_{N,p}(x)$ and $\mathbb{P}_{N,p}(x)$ have the same solution sets. □

Theorem 3.21. *Let Assumptions 3.9, 3.10 and 3.14 hold. Then the steady-state solution x_s is an asymptotically stable equilibrium point of the nonlinear system* (3.23) *with a region of attraction $\mathcal{X}_{N,p}$.*

Proof. Consider the rotated cost function (3.19)

$$\overline{V}_{N,p}(x,\mathbf{u}) = \sum_{k=0}^{N-1} L(x(k),u(k)) + \overline{V}_f(x(N)), \quad x \in \mathcal{X}_N$$

The candidate Lyapunov function for the problem is $\overline{V}^0_{N,p}(x) = \overline{V}_{N,p}(x,\mathbf{u}^0_p(x))$, where $\mathbf{u}^0_p(x)$ is the optimal control sequence as defined in (3.22). The resulting optimal state sequence is $\mathbf{x}^0_p(x) = \left\{x^0_p(0;x), x^0_p(1;x), \ldots, x^0_p(N;x)\right\}$. We choose a candidate input sequence and a corresponding state sequence as follows

$$\mathbf{u}(x) = \{u_p^0(1;x), u_p^0(2;x), \ldots, u_p^0(N-1;x),\ \kappa_f(x^0(N;x)))\} \tag{3.26}$$

$$\mathbf{x}(x) = \left\{x_p^0(1;x), x_p^0(2;x), \ldots, x_p^0(N;x), x_p^0(N+1;x))\right\} \tag{3.27}$$

where $x_p^0(N+1;x) = f(x_p^0(N;x), \kappa_f(x_p^0(N;x))$. Due to the terminal state constraint, $x_p^0(N;x) \in \mathbb{X}_f$, and hence $x_p^0(N+1;x) \in \mathbb{X}_f$ due to the invariance property of $\mathbb{X}_f$ (Assumption 3.14). For all $x \in \mathcal{X}_N$, the definition of $\overline{V}_{N,p}(\cdot)$ gives

$$\begin{aligned}
\overline{V}_{N,p}(x^+, \mathbf{u}) = &\sum_{k=1}^{N-1} L(x_p^0(k;x), u_p^0(k;x)) + \\
&L(x_p^0(N,x), \kappa_f(x_p^0(N;x))) + \overline{V}_f(x_p^0(N+1;x)) \\
=&\overline{V}_N^0(x) - L(x, u_p^0(0;x)) + L(x_p^0(N,x), \kappa_f(x_p^0(N;x))) - \\
&\overline{V}_f(x_p^0(N;x)) + \overline{V}_f(x_p^0(N+1;x)) \\
\leq&\overline{V}_N^0(x) - L(x, u_p^0(0;x)), \quad \text{(from Lemma 3.16)}
\end{aligned}$$

Since $\overline{V}_{N,p}^0(x^+) \leq \overline{V}_{N,p}(x^+, \mathbf{u})$, it follows that

$$\begin{aligned}
\overline{V}_{N,p}^0(x^+) - \overline{V}_{N,p}^0(x) \leq& -L(x, u_p^0(0;x)) \\
\leq& -\gamma(|x - x_s|) \qquad \text{using (3.6)}
\end{aligned} \tag{3.28}$$

Due to Lemmas 3.16 and 3.19, $\gamma(|x - x_s|) \leq \overline{V}_{N,p}^0(x) \leq \overline{\gamma}(|x - x_s|)$ for all $x \in \mathcal{X}_N$ (Rawlings and Mayne, 2009, Propositions 2.17 and 2.18), where $\overline{\gamma}(|x - x_s|$ is a class $\mathcal{K}$ function. Hence $\overline{V}_{N,p}^0$ is a Lyapunov function and x_s is an asymptotically stable equilibrium point of (3.23) with a region of attraction $\mathcal{X}_N$. □

Hence we have established nominal asymptotic stability of the nonlinear system under terminal penalty/control formulation.

3.4.4 Terminal cost prescription

Finding terminal cost function $V_f(\cdot)$ and region $\mathbb{X}_f$ that satisfy the stability assumption (Assumption 3.14) is not obvious for generic costs and nonlinear systems. The most common case of positive, quadratic cost is addressed in Rawlings and Mayne (2009, Sec. 2.5). In this section we propose candidate terminal cost functions $V_f(\cdot)$ that satisfy (3.16) inside well-defined terminal region $\mathbb{X}_f$.

For notational simplicity, in the following discussion we shift the origin to (x_s, u_s), i.e., the optimal steady state of the system. Similarly, we shift the origin of the sets $\mathbb{X}$, $\mathbb{U}$, $\mathbb{Z}$, and $\mathbb{X}_f$. We make the following assumption.

Assumption 3.22. *The functions $f(\cdot)$ and $\ell(\cdot)$ are twice continuously differentiable on $\mathbb{R}^n \times \mathbb{R}^m$, and the linearized system $x^+ = Ax + Bu$, where $A := f_x(0,0)$ and $B := f_u(0,0)$, is stabilizable.*

We choose any controller $u = Kx$ such that the origin is exponentially stable for the system $x^+ = A_K x, A_K := A + BK$. Such a K exists since (A, B) is stabilizable. The following establishes the existence of the invariant set required for Assumption 3.14.

In the standard case, where $\ell(\cdot)$ is positive definite, one chooses $\mathbb{X}_f$ to be a level set of $V_f(\cdot)$ to inherit control invariance from (3.16). In economic case, $\ell(\cdot)$ is not positive definite and hence we use the control invariant set defined in the following way:

Lemma 3.23 (Control invariant set for $f(\cdot)$ (Rawlings and Mayne, 2009))**.** *Let Assumption 3.22 hold and consider K such that $A + BK$ is stable. Then there exist matrices $P > 0$, $Q > 0$, and scalar $b > 0$, such that the following holds for all $b' \leq b$*

$$V(f(x, Kx)) - V(x) \leq -(1/2)x'Qx, \quad \forall x \in \operatorname{lev}_{b'} V$$

in which $V(x) := (1/2)x'Px$.

Proof. This result is established in (Rawlings and Mayne, 2009, pp.136–137). □

Remark 3.24. *From Lemma 3.23 we have the existence of a family of nested ellipsoidal neighborhoods of the origin, $\operatorname{lev}_{b'} V$, with $b' \leq b$, and each member of the family (corresponding to a b' value) is control invariant for the nonlinear system $x^+ = f(x, u)$ under the linear control law $u = Kx$.*

We next classify the function $V_f(\cdot)$ based on whether or not a storage function $\lambda(\cdot)$ is known for the system (Assumption 3.9.)

Prescription 1: Storage function $\lambda(\cdot)$ unknown

The ideal choice for $V_f(x)$ satisfying (3.16), is the infinite horizon shifted cost to go for the optimal nonlinear control law $\kappa_f(x)$. Since there are no generic ways to know the nature of this nonlinear control law, we chose the linear control law $u = Kx$ defined above, and compute the cost to go based on this choice.

$$V_f(x) = \sum_{k=0}^{\infty} \bar{\ell}(x, Kx), \qquad x^+ = A_K x, \qquad x(0) = 0$$

One can immediately see this choice of V_f satisfies (3.16). In general the summability of the above infinite sum is not guaranteed. For special cases like quadratic costs, the infinite sum can be analytically computed. But for most cases, in which the above sum cannot be explicitly determined, we propose ways to compute a terminal penalty satisfying (3.16) in the following sections. If the above infinite sum can be determined, one can use the invariant region $\mathbb{X}_f = \text{lev}_{b'} V$ as the desired terminal region.

Prescription 2: Storage function $\lambda(\cdot)$ unknown

Note: The results of this section are taken from Amrit et al. (2011).

We now construct a $V_f(\cdot)$ without knowledge of $\lambda(\cdot)$.

Lemma 3.25. *Let Assumption 3.22 hold and let $\overline{\ell}(x) := \ell(x, Kx) - \ell(0, 0)$. Then there exists matrix $Q^\star$ such that for any compact set $\mathcal{C} \subset \mathbb{R}^n$*

$$x' \left(Q^\star - \overline{\ell}_{xx}(x)\right) x \geq 0, \quad \forall x \in \mathcal{C}$$

Proof. Let $\lambda_i(\overline{\ell}_{xx}(x)), i \in \mathbb{I}_{1:n}$ denote the real-valued eigenvalues of symmetric matrix $\overline{\ell}_{xx}(x)$, which depends on x. The eigenvalues are continuous functions of the elements of the matrix (Horn and Johnson, 1985, p.540), and the elements of the matrix $\overline{\ell}_{xx}(x)$ are continuous functions of x on $\mathcal{C}$ by Assumption 3.22, so the following optimization problem has a solution

$$\lambda^\star = \max_{x,i} \left\{ \lambda_i(\overline{\ell}_{xx}(x)) \mid x \in \mathcal{C}, \quad i \in \mathbb{I}_{1:n} \right\}$$

for an arbitrary Hermitian matrix H, $x'Hx \leq \lambda_m x'x$ for all $x \in \mathbb{R}^n$, where $\lambda_m = \max_i(\lambda_i(H))$ (Horn and Johnson, 1985, p.176). Hence we conclude that $\lambda^\star x'x \geq x'\overline{\ell}_{xx}(x)x$ for all $x \in \mathcal{C}$. Define $Q^\star$ as the diagonal matrix $Q^\star := \lambda^\star I_n$. We have

$$x'Q^\star x = \lambda^\star x'x \geq x'\overline{\ell}_{xx}(x)x, \quad \forall x \in \mathcal{C}$$

□

Next we define the quadratic cost function $\ell_q(x) := (1/2)x'Qx + q'x$.

Lemma 3.26. *Let Assumption 3.22 hold. Choose matrices (Q, q) such that $q := \overline{\ell}_x(0,0)$ and $Q := Q^\star + \alpha I$, with $Q^\star$ defined in Lemma 3.25 and $\alpha \in \mathbb{R}$. Then $\ell_q(x) \geq \overline{\ell}(x) + (\alpha/2)x'x$ for all $x \in \mathbb{X}$ and $\alpha \in \mathbb{R}$.*

Proof. Choose compact set $\mathcal{C}$ in Lemma 3.25 to be convex and contain $\mathbb{X}$, which is possible since $\mathbb{X}$ is bounded. Then we have that if $x \in \mathcal{C}, sx \in \mathcal{C}$ for $s \in [0,1]$. From Proposition A.11 (b) (Rawlings and Mayne, 2009), we have that for all $x \in \mathcal{C}$

$$\begin{aligned}
\ell_q(x) - \overline{\ell}(x) &= (q - \overline{\ell}_x(0,0))'x + \\
&\qquad \int_0^1 (1-s)x' \left(Q - \overline{\ell}_{xx}(sx)\right) x ds \\
&= \int_0^1 (1-s)x' \left(Q^\star - \overline{\ell}_{xx}(sx) + \alpha I\right) x ds \\
&\geq (\alpha/2)x'x
\end{aligned}$$

Since $\mathbb{X} \subseteq \mathcal{C}$, the inequality holds on $\mathbb{X}$ and the result is established. □

We define the candidate $V_f(x)$ as follows

$$V_f(x) := \sum_{k=0}^{\infty} \ell_q(x(k)), \quad x^+ = A_K x, \quad x(0) = x$$
$$= (1/2)x'Px + p'x \tag{3.29}$$

where Q and q are selected as in Lemma 3.26 with $\alpha > -\lambda^\star$ so that $Q > 0$. Hence P is the solution to the Lyapunov equation $A_K' P A_K - P = -Q$ and $p = (I - A_K)^{-T} q$. Note that P depends on the parameter α. In fact,

$$P = P^* + \alpha P_I$$

in which P^* and P_I satisfy the Lyapunov equations $A_K' P^* A_K - P^* = -Q^*$ and $A_K' P^* A_K - P^* = -I$, respectively.

Next we establish that there exists a nonzero neighborhood of the origin in which (3.16) is satisfied. Define the set $\mathbb{X}_u \subseteq \mathbb{X}$ as follows

$$\mathbb{X}_u := \left\{ x \in \mathbb{X} \mid Kx \in \mathbb{U} \right\}$$

and note that $\mathbb{X}_u$ contains the origin in its interior because $\mathbb{U}$ contains the origin in its interior and Kx goes to zero with x. The next lemma characterizes a set on which we can meet the stability assumption inequality.

Lemma 3.27 (Amrit et al. (2011))**.** *Let Assumption 3.22 hold. There exists $\delta_1 > 0$ such that $\delta_1 \mathcal{B} \subseteq \mathbb{X}_u$ and the following holds for all $x \in \delta_1 \mathcal{B}$*

$$V_f(f(x, Kx)) - V_f(x) \leq -\overline{\ell}(x)$$

Proof. The proof of the lemma is provided in Amrit et al. (2011), and is omitted from this thesis.

□

Theorem 3.28 (Amrit et al. (2011)). *Let Assumption 3.22 hold. There exists a compact set $\mathbb{X}_f$ containing the origin in its interior such that the quadratic function $V_f(x)$ defined in* (3.29) *and the linear control law $\kappa_f(x) = Kx$ satisfy Assumption 3.14.*

Proof. With $\delta_1 > 0$ chosen to satisfy Lemma 3.27, choose $b' > 0$ with $b' \leq b$ of Lemma 3.23 such that $\mathrm{lev}_{b'} V \subseteq \delta_1 \mathcal{B}$. Since the set $\delta_1 \mathcal{B}$ contains the origin in its interior, such a $b' > 0$ exists. Then choose $\mathbb{X}_f = \mathrm{lev}_{b'} V$. We have that the control law $\kappa_f(\cdot)$ is feasible on $\mathbb{X}_f$ since $\mathbb{X}_f \subseteq \delta_1 \mathcal{B} \subseteq \mathbb{X}_u$. The set $\mathbb{X}_f$ is forward invariant from Lemma 3.23 since $b' < b$, and we know that

$$V_f(f(x, Kx)) - V_f(x) \leq -\bar{\ell}(x) \quad \forall x \in \mathbb{X}_f$$

by Lemma 3.27 because $\mathbb{X}_f \subseteq \delta_1 \mathcal{B}$. □

Remark 3.29. *Unlike the standard MPC tracking problem, $\bar{\ell}(\cdot)$ is not necessarily positive, and hence sublevel sets of $V_f(\cdot)$ are not forward invariant under the terminal control law. See Figure 3.1 for the depiction of sublevel sets of $V_f(\cdot)$ and V. Notice that the center of sublevel sets of $V_f(\cdot)$ is located at $x = -P^{-1}p$ rather than at $x = 0$. That is why we choose a sublevel set of $V(\cdot)$ rather than $V_f(\cdot)$ for the terminal region $\mathbb{X}_f$ in economic MPC problems.*

Prescription 3: Storage function $\lambda(\cdot)$ known

Let Assumption 3.9 hold, and it is assumed that the storage function $\lambda(\cdot)$ is known.

Assumption 3.30 (Lipschitz continuity)**.** *There exists a $r > 0$ such that the functions $\ell(\cdot)$ and $\lambda(\cdot)$, and hence the rotated cost $L(\cdot)$, as defined in* (3.4)*, are Lipschitz continuous for all $(x, u) \in r\mathcal{B}$. Denote the corresponding Lipschitz constants as L_ℓ, L_λ and L_L.*

We assume the following error bound.

Assumption 3.31. *There exists a $\delta_2 > 0$ and $c_\delta > 0$, such that*

$$|e(x)| \leq c_\delta \gamma(|x|), \quad \forall x \in \delta_2 \mathcal{B}$$

where $\gamma(|x|)$ is the class $\mathcal{K}$ function that underbounds the rotated cost satisfying (3.6).

Remark 3.32. *Since we assume $f(\cdot)$ to be twice continuously differentiable, for any $\delta > 0$, there exists a $c_{l\delta} > 0$ such that $|e(x)| \leq (1/2)c_{l\delta} |x|^2$ for all $x \in \delta\mathcal{B}$ (Rawlings and Mayne, 2009, p. 137). Hence it follows that if $\lim_{x\to 0} \frac{|x|^2}{\gamma(|x|)}$ is bounded, then there exists a $\delta > 0$ and $c_\delta > 0$ such that $|e(x)| \leq (1/2)c_{l\delta} |x|^2 \leq c_\delta \gamma(|x|)$ for all $x \in \delta\mathcal{B} \subseteq \mathbb{X}_u$ (Figure 3.1), and hence Assumption 3.31 is satisfied. For example, if $\ell(\cdot)$ and $\lambda(\cdot)$ are at most second order [1] functions, then $L(\cdot)$ is at most a second order function, and hence $\gamma(|x|)$ is at most second order, making the above limit bounded.*

Now consider the function

$$\overline{V}_f(x) = \alpha \sum_{k=0}^{\infty} L(x(k), u(k)), \quad x^+ = Ax + Bu, \quad u = Kx, \quad \alpha > 0 \tag{3.30}$$

[1] A function is said to be of finite order if there exists numbers $a, r > 0$ such that $|f(z)| \leq \exp(|z|^a), \quad \forall |z| > r$. The infimum of all such numbers a, is called the order of the function f (Krantz, 1999, p. 121)

Lemma 3.33. *If a continuous function $V(x)$ is Lipschitz continuous in $r\mathcal{B}$, $r > 0$, with a Lipschitz constant L_V and $V(0) = 0$, then there exists a $c > 0$ such that the following holds true in a compact set $\mathcal{C}$ containing the origin.*

$$V(x) \leq c\,|x|\,, \quad \forall x \in \mathcal{C}$$

Proof. The proof is analogous to the proof of Proposition 2.18 in Rawlings and Mayne (2009). □

Note that because of Assumption 3.30 and Lemma 3.33, there exists a $c_L > 0$ such that

$$L(x,u) \leq c_L\,|(x,u)|\,, \quad \forall (x,u) \in \mathbb{X}_u \tag{3.31}$$

Since $x(k)$ converges to the origin exponentially as $k \to \infty$ and $L(x,u)$ is defined and satisfies (3.31) on all trajectories starting from $x \in \mathbb{X}_u$, the above infinite sum converges for all $x \in \mathbb{X}_u$. We claim that $\overline{V}_f(x)$ is a local control Lyapunov function for the system $x^+ = f(x, Kx)$ in the region $\mathbb{X}_f$ and hence $\mathbb{X}_f$ is control invariant for the nonlinear system $x^+ = f(x, Kx)$.

Lemma 3.34. *Let Assumptions 3.9, 3.22, 3.30 and 3.31 hold. There exists an $\overline{\alpha} > 0$ such that for all $\alpha \geq \overline{\alpha}$, $\overline{V}_f(\cdot)$ defined in (3.30) is a local control Lyapunov function for the system $x^+ = f(x,u)$ in some neighborhood of the origin.*

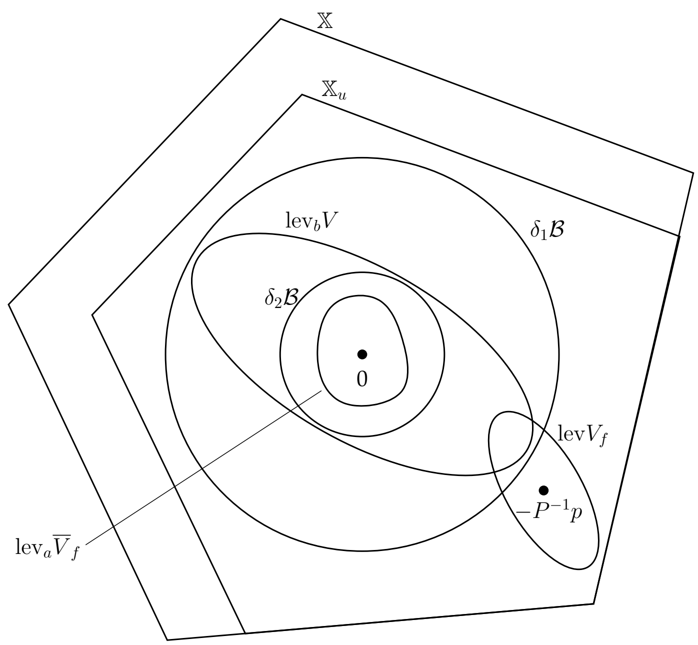

Figure 3.1: (Amrit et al., 2011); Relationships among the sets $\text{lev}_a \overline{V}_f$, $\delta_2\mathcal{B}$, $\text{lev}_b V$, $\text{lev} V_f$, $\delta_1\mathcal{B}$, $\mathbb{X}_u$, and $\mathbb{X}$. Lemma 3.27 holds in $\delta_1\mathcal{B}$; Theorem 3.28 holds in $\text{lev}_b V$; Theorem 3.35 holds in $\delta_2\mathcal{B}$; Theorem 3.38 holds with $\mathbb{X}_f$ in $\text{lev}_a \overline{V}_f$. Recall that the origin is shifted to the optimal steady state x_s.

Proof. From the definition of $\overline{V}_f(x)$, we know

$$\overline{V}_f(A_K x) - \overline{V}_f(x) = -\alpha L(x, Kx), \quad \forall x \in \mathbb{X}_u \tag{3.32}$$

From (3.30) and (3.31) we have

$$\begin{aligned}
\overline{V}_f(x) &= \alpha \sum_{k=0}^{\infty} L(x(k), Kx(k)) \\
&\leq c_L \left(|x| + A_K |x| + \cdots\right) \\
&= c_{\overline{V}_f} |x|, \quad \forall x \in \mathbb{X}
\end{aligned}$$

where $c_{\overline{V}_f} = c_L(I - A_K)^{-1}$. Hence using Assumption 3.31 we can write

$$\begin{aligned}
\overline{V}_f(f(x, Kx)) - \overline{V}_f(A_K x) &\leq c_{\overline{V}_f} \left(|f(x, Kx)| - |A_K x|\right) \\
&\leq c_{\overline{V}_f} |f(x, Kx) - A_k x| \\
&= c_{\overline{V}_f} |e(x)| \\
&\leq (1/2) c_{\overline{V}_f} c_\delta \gamma(|x|), \quad \forall x \in \delta_2 \mathcal{B} \qquad (3.33)
\end{aligned}$$

From (3.32) and (3.33) we have

$$\begin{aligned}
\overline{V}_f(f(x, Kx)) - \overline{V}(x) &\leq (1/2) c_{\overline{V}_f} c_\delta \gamma(|x|) - \alpha L(x, Kx) \\
&\leq c_{\overline{V}_f} c_\delta L(x, Kx) - \alpha L(x, Kx) \quad \text{(using (3.6))} \\
&= (c_{\overline{V}_f} c_\delta - \alpha) L(x, Kx), \quad \forall x \in \delta_2 \mathcal{B}
\end{aligned}$$

Defining $\overline{\alpha} := 1 + c_{\overline{V}_f} c_\delta$ and choosing $\alpha \geq \overline{\alpha}$ gives $\overline{V}_f(f(x, Kx)) - \overline{V}(x) \leq -L(x, Kx)$, for all $x \in \delta_2 \mathcal{B}$. $\square$

Theorem 3.35. *Let Assumptions 3.9, 3.22, 3.30 and 3.31 hold. There exists a compact set $\mathbb{X}_f$ containing the origin in its interior such that the function $V_f(x) = \overline{V}_f(x) - \lambda(x) + \lambda(x_s)$, where $\overline{V}_f(x)$ is defined in* (3.30)*, and the linear control law $\kappa_f(x) = Kx$ satisfy Assumption 3.14.*

Proof. With $\delta_2 > 0$ chosen to satisfy Lemma 3.34, choose $b' > 0$ with $b' \leq b$ of Lemma 3.23 such that $\text{lev}_{b'}V \subseteq \delta_2\mathcal{B}$. Since the set $\delta_2\mathcal{B}$ contains the origin in its interior, such a $b' > 0$ exists. Then choose $\mathbb{X}_f = \text{lev}_{b'}V$. We have that the control law $\kappa_f(\cdot)$ is feasible on $\mathbb{X}_f$ since $\mathbb{X}_f \subseteq \delta_2\mathcal{B} \subseteq \mathbb{X}_u$. The set $\mathbb{X}_f$ is forward invariant from Lemma 3.23 since $b' < b$, and from Lemma 3.34 we know that $\overline{V}_f(f(x, Kx)) - \overline{V}_f(x) \leq -L(x, Kx)$ for all $x \in \mathbb{X}_f$ because $\mathbb{X}_f \subseteq \delta_2\mathcal{B}$. Hence due to Lemma 3.16 we have

$$V_f(f(x, Kx)) - V_f(x) \leq -\overline{\ell}(x, Kx) \quad \forall x \in \mathbb{X}_f$$

where $V_f(x) = \overline{V}_f(x) - \lambda(x) + \lambda(x_s)$. □

3.5 Replacing the terminal constraint

As mentioned in the previous section, the more the number of constraints in the nonlinear optimization problem, the harder it is to solve. We new extend the idea of relaxing equality constraints by adding penalty to the terminal state, to completely remove any terminal constraint from the system. We achieve this by modifying our terminal penalty. To do so, we first assume that the system is dissipative (Assumption 3.9) and the storage function $\lambda(\cdot)$ is known. We assume that the terminal region is a sublevel set of $\overline{V}_f(x)$. To show that we can find an $a > 0$ such that $\text{lev}_a\overline{V}_f \subseteq \text{lev}_bV$ (Figure 3.1), we observe from

(3.6) and Lemma 3.16 that $\overline{V}_f(x) \geq L(x, Kx) \geq \gamma(|x - x_s|)$ for all $x \in \mathbb{X}_u$. It follows that $x \in \text{lev}_a\overline{V}_f$ implies $|x - x_s| \leq \gamma^{-1}(a)$. We also know that there exists a $c > 0$ such that $V(x - x_s) \leq c\,|x - x_s|^2$ for all $x \in \mathbb{R}^n$. Choose a as follows

$$a = \gamma(\sqrt{b/c})$$

With this choice $|x - x_s| \leq \gamma^{-1}(a)$ implies $V(x - x_s) \leq c\,|x - x_s|^2 \leq b$. Hence $x \in \text{lev}_a\overline{V}_f$ implies $x \in \text{lev}_b V$ for this choice of a. Hence we use the set $\text{lev}_a\overline{V}_f$ as the terminal region. Consider the following modified cost function and the corresponding rotated cost function

$$\begin{aligned} V_N^\beta(x, \mathbf{u}) &= \sum_{k=0}^{N-1} \ell(x(k), u(k)) + \beta V_f(x(N)) + (\beta - 1)\lambda(x(N) \\ \overline{V}_N^\beta(x, \mathbf{u}) &= \sum_{k=0}^{N-1} L(x(k), u(k)) + \beta \overline{V}_f(x(N)), \quad \beta \geq 1 \end{aligned} \tag{3.34}$$

For $\beta \geq 1$, define the standard and auxiliary nonlinear optimal control problems as following:

$$\begin{aligned} \mathbb{P}_N^\beta(x) : &\qquad V_N^{0,\beta}(x) := \min_{\mathbf{u}}\{V_N^\beta(x, \mathbf{u}) \mid \mathbf{u} \in \mathcal{U}_{N,p}(x)\} \\ \overline{\mathbb{P}}_N^\beta(x) : &\qquad \overline{V}_N^{0,\beta}(x) := \min_{\mathbf{u}}\{\overline{V}_N^\beta(x, \mathbf{u}) \mid \mathbf{u} \in \mathcal{U}_{N,p}(x)\} \end{aligned} \tag{3.35}$$

in which the control constraint set $\mathcal{U}_N(x)$ does not include a terminal state constraint

$$\mathcal{U}_N(x) := \{\mathbf{u} \in \mathbb{U}_N \mid (\phi(k; x, \mathbf{u}), u(k)) \in \mathbb{Z}, \forall k \in \mathbb{I}_{0,N-1}\}$$

Define the set of admissible states as follows

$$\mathcal{X}_N^\beta := \left\{x \mid \overline{V}_N^{0,\beta}(x) \leq \overline{V}\right\} \tag{3.36}$$

where $\overline{V} > 0$ is an arbitrary constant. Denote the optimal solution and the corresponding implicit MPC control law as

$$\mathbf{u}^{\beta}(x) = \{u^{\beta}(0;x), \cdots, u^{\beta}(N-1,x)\} \quad \kappa_N^{\beta}(x) = u^{\beta}(0;x)$$

The corresponding closed-loop system evolves according to

$$x^+ = f(x, \kappa_N^{\beta}(x)) \tag{3.37}$$

3.5.1 Properties of the modified cost function

We now establish some useful properties of the modified cost function $\overline{V}_N^{\beta}$, that we shall later use to establish stability properties of the new controller.

Lemma 3.36 (Equivalence of solutions)**.** *Let Assumptions 3.10 and 3.14 hold. The solution sets for $\overline{\mathbb{P}}_N^{\beta}(x)$ and $\mathbb{P}_N^{\beta}(x)$ are identical.*

Proof. Similar to the proof of Lemma 3.20, expanding the rotated regulator cost function gives

$$\overline{V}_N^{\beta}(x,\mathbf{u}) = V_N^{\beta}(x,\mathbf{u}) - N\ell(x_s,u_s) + \lambda(x) - \beta\lambda(x_s) - \beta V_f(x_s)$$

Since $\lambda(x)$, $\lambda(x_s)$, $V_f(x_s)$ and $\ell(x_s,u_s)$ are constants for a given initial state, the two objective functions $\overline{V}_N^{\beta}$ and V_N^{β} differ by a constant, and hence the two optimization problems $\overline{\mathbb{P}}_N^{\beta}(x)$ and $\mathbb{P}_N^{\beta}(x)$ have the same solution sets. $\square$

Lemma 3.37. *If $(\overline{V}_f(\cdot), \mathbb{X}_f)$ satisfies* (3.24) *of Lemma 3.16 and $L(x,u)$ satisfies Assumption 3.9, then $(\beta\overline{V}_f(\cdot), \mathbb{X}_f)$ also satisfies* (3.24) *for $\beta \geq 1$.*

Proof. Assumption 3.9 implies that $-L(x, u) \leq -\rho(x)$, where $\rho : \mathbb{X} \to \mathbb{R}_{\geq 0}$. Since $\rho(x)$ is positive definite, $-L(x, u) \leq -\frac{1}{\beta} L(x, u)$ for $\beta \geq 1$. Using (3.24)

$$\begin{aligned} \overline{V}_f(f(x, \kappa_f(x))) - \overline{V}_f(x) &\leq -L(x, \kappa_f(x)) \qquad \forall x \in \mathbb{X}_f \\ &\leq -\frac{1}{\beta} L(x, \kappa_f(x)) \end{aligned}$$

Hence $\beta \left(\overline{V}_f(f(x, \kappa_f(x))) - \overline{V}_f(x) \right) \leq -L(x, \kappa_f(x)), \quad \forall x \in \mathbb{X}_f, \beta \geq 1$, which completes the proof. $\square$

3.5.2 Stability

We now show that by removing the terminal state constraint and modifying the terminal penalty appropriately, nominal stability of the closed-loop system is preserved under the strict dissipativity assumption.

Theorem 3.38. *Let Assumptions 3.10 and 3.14 hold. Suppose $\mathbf{u}^\beta(x)$ is optimal for the terminally unconstrained problem $\mathbb{P}_N^\beta(x)$, and $\mathbf{x}^\beta(x)$ is the associated optimal state trajectory. There exists a $\overline{\beta} > 1$ such that for all $\beta \geq \overline{\beta}$ and $x \in \mathcal{X}_N^\beta$, $x^\beta(N; x) \in \mathbb{X}_f$.*

Proof. From (3.36), for any $x \in \mathcal{X}_N^\beta$, we have

$$\sum_{k=0}^{N-1} L(x^\beta(k; x), u^\beta(k; x)) + \beta \overline{V}_f(x^\beta(N; x)) \leq \overline{V}$$

$$\beta \overline{V}_f(x^\beta(N; x)) \leq \overline{V} \quad \text{(due to (3.6))}$$

Choosing $\beta \geq \overline{\beta} = \max\{1, \overline{V}/a\}$, gives $\overline{V}_f(x^\beta(N;x)) \leq a$. Hence $x^\beta(N;x) \in \mathbb{X}_f$, which completes the proof. □

Theorem 3.39. *Let Assumptions 3.10 and 3.14 hold. Then the steady-state solution x_s is an asymptotically stable equilibrium point of the nonlinear system* (3.37) *with a region of attraction $\mathcal{X}_N^\beta$.*

Proof. Analogous to the proof of Theorem 3.21, using Lemma 3.37 we have

$$\begin{aligned}\overline{V}_N^{0,\beta}(x^+) - \overline{V}_N^{0,\beta}(x) &\leq -L(x, u^\beta(0;x)) \\ &\leq -\gamma(|x - x_s|), \quad \forall x \in \mathcal{X}_N^\beta\end{aligned}$$

Due to Lemmas 3.16, 3.19 and 3.37, $\gamma(|x - x_s|) \leq \overline{V}_N^{0,\beta}(x) \leq \overline{\gamma}(|x - x_s|)$ for all $x \in \mathcal{X}_N$ (Rawlings and Mayne, 2009, Propositions 2.17 and 2.18), where $\overline{\gamma}(|x - x_s|$ is a class $\mathcal{K}$ function. Hence $\overline{V}_N^{0,\beta}(x)$ is a Lyapunov function and x_s is an asymptotically stable equilibrium point of (3.37) with a region of attraction $\mathcal{X}_N^\beta$. □

Lemma 3.40 (Nesting property of admissible sets)**.** *Let Assumptions 3.10 and 3.14 hold. Define the following two sublevel sets*

$$\mathbb{X}_1 = \left\{x \mid \overline{V}_N^{0,\beta_1}(x) \leq V_1\right\}, \quad \mathbb{X}_2 = \left\{x \mid \overline{V}_N^{0,\beta_2}(x) \leq V_2\right\},$$

where $\overline{V}_N^{0,\beta}$ is defined by (3.35) *and $\overline{V}_f(x) \leq a$, $a > 0$.*

1. *Let $\beta_1 = \max\{1, V_1/a\}$ and $\beta_2 = \max\{1, V_2/a\}$. If $V_1 \leq V_2$, then $\mathbb{X}_1 \subseteq \mathbb{X}_2$.*

2. *Let $V_1 = V_2 = \overline{V}$. If $\max\{1, \overline{V}/a\} \leq \beta_1 \leq \beta_2$, then $\mathbb{X}_2 \subseteq \mathbb{X}_1$.*

Proof.

(a) In order to prove that $\mathbb{X}_1 \subseteq \mathbb{X}_2$, we show that $x \in \mathbb{X}_1$ implies $x \in \mathbb{X}_2$. For all $x \in \mathbb{X}_1$, we have

$$\begin{aligned}
\overline{V}_N^{0,\beta_2}(x) &= \sum_{k=0}^{N-1} L(x^{\beta_2}(k;x), u^{\beta_2}(k;x)) + \beta_2 \overline{V}_f(x^{\beta_2}(N;x)) \\
&\leq \sum_{k=0}^{N-1} L(x^{\beta_1}(k;x), u^{\beta_1}(k;x)) + \beta_2 \overline{V}_f(x^{\beta_1}(N;x)) \\
&= \sum_{k=0}^{N-1} L(x^{\beta_1}(k;x), u^{\beta_1}(k;x)) + \beta_2 \overline{V}_f(x^{\beta_1}(N;x)) - \\
&\quad \beta_1 \overline{V}_f(x^{\beta_1}(N;x)) + \beta_1 \overline{V}_f(x^{\beta_1}(N;x)) \\
&= \overline{V}_N^{0,\beta_1}(x) + (\beta_2 - \beta_1) \overline{V}_f(x^{\beta_1}(N;x)) \\
&\leq V_1 + (\beta_2 - \beta_1) a
\end{aligned}$$

The inequality follows from the fact that $\overline{V}_N^{0,\beta_1}(x) \leq V_1$ and $\overline{V}_f(x(N)) \leq a$. Now consider the three possible scenarios for the values of V_1 and V_2.

- Case 1: $a \leq V_1 \leq V_2$. Then $\beta_1 = V_1/a$, $\beta_2 = V_2/a$

$$V_1 + (\beta_2 - \beta_1)a = V_1 + V_2 - V_1 = V_2$$

- Case 2: $V_1 \leq a \leq V_2$. Then $\beta_1 = 1$, $\beta_2 = V_2/a$

$$V_1 + (\beta_2 - \beta_1)a = V_2 + (V_1 - a) \leq V_2$$

- Case 3: $V_1 \leq V_2 \leq a$. Then $\beta_1 = \beta_2 = 1$

$$V_1 + (\beta_2 - \beta_1)a = V_1 \leq V_2$$

Hence for all $x \in \mathbb{X}_1$ we have $\overline{V}_N^{0,\beta_2}(x) \leq V_2$ for the three possible cases. Hence $x \in \mathbb{X}_1$ and $V_1 \leq V_2$ imply $x \in \mathbb{X}_2$ and hence $\mathbb{X}_1 \subseteq \mathbb{X}_2$.

(b) For all $x \in \mathbb{X}_2$, we have

$$\begin{aligned}
\overline{V}_N^{0,\beta_1}(x) &= \sum_{k=0}^{N-1} L(x^{\beta_1}(k;x), u^{\beta_1}(k;x)) + \beta_1 \overline{V}_f(x^{\beta_1}(N,x)) \\
&\leq \sum_{k=0}^{N-1} L(x^{\beta_2}(k;x), u^{\beta_2}(k;x)) + \beta_1 \overline{V}_f(x^{\beta_2}(N,x)) \\
&= \sum_{k=0}^{N-1} L(x^{\beta_2}(k;x), u^{\beta_2}(k;x)) + \beta_2 \overline{V}_f(x^{\beta_2}(N,x)) + \\
&\quad (\beta_1 - \beta_2)\overline{V}_f(x^{\beta_2}(N,x)) \\
&= \overline{V}_N^{0,\beta_2}(x) + (\beta_1 - \beta_2)\overline{V}_f(x^{\beta_2}(N,x)) \\
&\leq \overline{V}_N^{0,\beta_2}(x)
\end{aligned}$$

where the last inequality follows from the fact that $\beta_1 \leq \beta_2$ and Lemma 3.17. Hence we have

$$\overline{V}_N^{0,\beta_1}(x) \leq \overline{V}_N^{0,\beta_2}(x) \leq \overline{V} \tag{3.38}$$

Hence $x \in \mathbb{X}_2$ and $\beta_1 \leq \beta_2$ imply $x \in \mathbb{X}_1$ and hence $\mathbb{X}_2 \subseteq \mathbb{X}_1$.

□

Hence we have established that by appropriately modifying the terminal penalty, we can remove constraints on the terminal state. The modification of the terminal cost ensures that the terminal state lies in the terminal region, and under appropriate assumptions, the closed-loop system is asymptotically stable.

Chapter 4

Suboptimal control

4.1 Introduction

All of the stability theory in Chapter 3 assumes that we are able solve our dynamic optimization problem to global optimality. When solving nonconvex optimization problems, which is usually the case when solving nonlinear problems, it is hard to guarantee global optimality of the solution, even within a pre-specified tolerance margin. The solution that the nonlinear solvers converge to are local optimums, where the optimality conditions are satisfied. In this chapter we show that global optimality is not required for the stability properties stated in Chapter 3 to hold. We develop stability results for suboptimal economic MPC in parallel to the results for suboptimal MPC with convex costs in Pannocchia, Rawlings, and Wright (2011).

4.2 Suboptimal MPC solution

We consider the terminal penalty formulation (Section 3.4) to develop our results and then extend them to the terminal constraint formulation. We assume throughout this chapter that the nonlinear system $x^+ = f(x, u)$, is dissipative with respect to the shifted economic cost (Assumption 3.9). Hence for this class of systems, optimal MPC driven nonlinear system is asymptotically stable (Theorem 3.21).

Consider the problem $\mathbb{P}_{N,p}$ as defined in (3.20).

$$\mathbb{P}_{N,p}(x): \qquad V^0_{N,p}(x) := \min_{\mathbf{u}}\{V_{N,p}(x, \mathbf{u}) \mid \mathbf{u} \in \mathcal{U}_{N,p}(x)\}$$

Instead of solving the problem to global optimality, we consider using any suboptimal algorithm that has the following properties: Let $\mathbf{u} \in \mathcal{U}_{N,p}(x)$ denote the (suboptimal) control sequence for the initial state x, where $\mathcal{U}_{N,p}(x)$ is the input constraint set defined in (3.14), and let $\mathbf{u}$ denote a *warm start* for the successor initial state $x^+ = f(x, u(0; x))$, obtained from $(x, \mathbf{u})$ by setting

$$\mathbf{u} = \{u(1; x), u(2; x), \dots, u(N-1; x), u_+\} \tag{4.1}$$

in which $u_+ \in \mathbb{U}$ is any input that satisfies the invariance conditions of Assumption 3.14 for $x = \phi(N; x, \mathbf{u}) \in \mathbb{X}_f$. We observe that the warm start is feasible for the successor state, i.e.

$$\mathbf{u} \in \mathcal{U}_{N,p}(x^+)$$

The suboptimal solution for the successor state is defined as any input sequence $\mathbf{u}^+$ that satisfies the following:

$$\mathbf{u}^+ \in \mathcal{U}_{N,p}(x^+) \tag{4.2a}$$

$$V_{N,p}(x^+, \mathbf{u}^+) \leq V_{N,p}(x^+, \mathbf{u}) \tag{4.2b}$$

$$V_{N,p}(x^+, \mathbf{u}^+) \leq V_f(x^+) + N\ell(x_s, u_s) \qquad \text{when } x^+ \in r\mathbb{B} \tag{4.2c}$$

in which $V_{N,p}$ is the regulator cost function as defined in (3.13), and r is a positive scalar sufficiently small that $r\mathbb{B} \subseteq \mathbb{X}_f$. Notice that the constraint (4.2c) is required to hold only if $x^+ \in r\mathbb{B}$. We now state some properties of the suboptimal MPC solution satisfying the above properties.

4.2.1 Properties

We first state the rotated cost equivalent of (4.2). We can then use the properties of the rotated costs stated in Section 3.4.3, to develop our results.

Lemma 4.1. *Suboptimal solution conditions* (4.2) *can be equivalently stated as following*

$$\mathbf{u}^+ \in \mathcal{U}_{N,p}(x^+) \tag{4.3a}$$

$$\overline{V}_{N,p}(x^+, \mathbf{u}^+) \leq \overline{V}_{N,p}(x^+, \mathbf{u}) \tag{4.3b}$$

$$\overline{V}_{N,p}(x^+, \mathbf{u}^+) \leq \overline{V}_f(x^+) \qquad \textit{when } x^+ \in r\mathbb{B} \tag{4.3c}$$

Proof. From Proposition 3.20, we know that $V_{N,p}(x, \mathbf{u}) = \overline{V}_{N,p}(x, \mathbf{u}) + N\ell(x_s, u_s) + \lambda(x_s) + V_f(x_s) - \lambda(x)$, and from the definition of $\overline{V}_f(x)$ (3.18), we have $V_f(x) = \overline{V}_f(x) + V_f(x_s) + \lambda(x_s) - \lambda(x)$. Substituting these in (4.2), we get (4.3). $\square$

Next we show that the globally optimal solution of the MPC problem satisfies the suboptimal MPC solution conditions (4.3).

Lemma 4.2. *The optimal solution to the problem $\mathbb{P}_{N,p}(x^+)$, $u^0(x^+)$, satisfies* (4.3a) *and* (4.3b) *for all $x^+ \in \mathcal{X}_{N,p}$. Moreover* (4.3c) *is satisfied by $u^0(x^+)$ for all $x^+ \in \mathbb{X}_f$.*

Proof. Since the original optimization problem $\mathbb{P}_{N,p}$ is equivalent to the auxiliary optimization problem $\overline{\mathbb{P}}_{N,p}$ (Proposition 3.20), and $\mathbf{u} \in \mathcal{U}_{N,p}$, the optimal solution $u^0(x^+)$ satisfies (4.3a) and (4.3b) due to optimality. Now consider any $x^+ \in \mathbb{X}_f$, define $x(0) = x^+$ and choose a $u(0)$ satisfying Assumption 3.14. Due to the invariance property of $\mathbb{X}_f$, $x(k) \in \mathbb{X}_f$ for all $k \in \mathbb{I}_{>0}$, and we can choose corresponding $u(k)$ satisfying Assumption 3.14. Due to lemma 3.16, we have

$$\overline{V}_f(x(k+1)) - \overline{V}_f(x(k)) \leq -L(x(k), u(k)), \quad \forall k \in \mathbb{I}_{\geq 0} \tag{4.4}$$

Denote the sequence of $u(k)$ as $\mathbf{u}_f = \{u(0), u(1), \cdots, u(N-1)\}$. Adding (4.4) for $k \in \mathbb{I}_{0:N-1}$, we get

$$\overline{V}_{N,p}(x^+, \mathbf{u}_f) = \sum_{k=0}^{N-1} L(x(k), u(k)) + \overline{V}_f(x(N)) \leq \overline{V}_f(x^+) \quad \forall x^+ \in \mathbb{X}_f$$

which completes the proof. □

We note that $\mathbf{u}$ is a set-valued map of the state x, and so too is the associated first component $u(0; x)$. If we denote the latter map as $\kappa_{N,p}(\cdot)$, we can write the evolution of the system (3.1) in closed-loop with suboptimal MPC as the following difference inclusion:

$$x^+ \in F(x) = \{f(x, u) \mid u \in \kappa_{N,p}(x)\} \tag{4.5}$$

A similar difference inclusion approach could be used to describe the evolution of the closed-loop system under optimal MPC where the optimal solution is nonunique.

Lemma 4.3. *We have that* $\kappa_{N,p}(x_s) = \{u_s\}$ *and* $F(x_s) = \{x_s\}$.

Proof. We know that $L(x,u) \geq \gamma(|x - x_s|)$ (3.6) for all $(x,u) \in \mathbb{Z}$. We also know that $V_f(x) \geq \gamma(|x - x_s|)$ for all $x \in \mathbb{X}_f$ (Lemma 3.19). Hence we can write

$$\overline{V}_{N,p}(x,\mathbf{u}) = \sum_{k=0}^{N-1} L(x(k),u(k)) + V_f(x(N)) \geq L(x,u(0;x)) \geq \gamma(|x - x_s|), \quad \forall (x,\mathbf{u}) \in \mathbb{X} \times \mathbb{U}^N$$

Since $\mathbb{X}_f$ contains x_s (Assumption 3.14), from (4.3c) we have $\gamma(0) \leq \overline{V}_{N,p}(x_s,\mathbf{u}) \leq \overline{V}_f(x_s) = 0$. Hence $\overline{V}_{N,p}(x_s,\mathbf{u}) = 0$. Since $L(x_s,u(k)) \geq 0$ for all $k \in \mathbb{I}_{0:N-1}$, it follows that $u(k) = u_s$ and hence $\kappa_{N,p}(x_s) = \{u_s\}$. Consequently, $F(x_s) = f(x_s,u_s) = x_s$. $\square$

4.3 Extended state and difference inclusions

It is now clear that in suboptimal MPC, we must keep track of the input $\mathbf{u}$ as well as the state x, because the input is not determinable solely by the state as in optimal MPC. Hence we define an *extended* state $z = (x,\mathbf{u})$ and observe that it evolves according to the difference inclusion

$$z^+ \in H(z) = \{(x^+,\mathbf{u}^+) \mid x^+ = f(x,u(0;x)),\ \mathbf{u}^+ \in G(z)\} \tag{4.6}$$

in which (noting that both x^+ and $\mathbf{u}^+$ depend on z):

$$G(z) = \{\mathbf{u}^+ \mid \mathbf{u}^+ \in \mathcal{U}_{N,p}(x^+),\ \overline{V}_{N,p}(x^+,\mathbf{u}^+) \leq \overline{V}_{N,p}(x^+,\mathbf{u}), \text{and } \overline{V}_{N,p}(x^+,\mathbf{u}^+) \leq \overline{V}_f(x^+) \text{ if } x^+ \in r\mathbb{B}\}$$

We also define the following set (notice that $r\mathbb{B} \subseteq \mathbb{X}_f$):

$$\mathcal{Z}_r = \{(x, \mathbf{u}) \in \mathbb{Z}_{N,p} \mid \overline{V}_{N,p}(x, \mathbf{u}) \leq \overline{V}_f(x) \text{ if } x \in r\mathbb{B}\}.$$

Given the difference inclusion (4.6), we denote by $\psi(k; z) = z(k)$ a solution at time $k \in \mathbb{I}_{\geq 0}$ starting from the initial state $z(0) = z$. We now define Asymptotic stability and Lyapunov functions for the difference inclusion (4.6).

Definition 4.4 (Asymptotic stability)**.** *The steady state z_s of the difference inclusion $z^+ \in H(z)$ is* asymptotically stable *(AS) on $\mathcal{Z}$, $z_s \in \mathcal{Z}$, if there exist a class $\mathcal{K}$ function $\gamma(\cdot)$ such that for any $z \in \mathcal{Z}$,* all *solutions $\psi(k; z)$ satisfy:*

$$\psi(k; z) \in \mathcal{Z}, \quad |\psi(k; z) - z_s| \leq \gamma(|z - z_s|, k) \quad \textit{for all } k \in \mathbb{I}_{\geq 0}.$$

Definition 4.5 (Lyapunov function)**.** *$V(z)$ is an* Lyapunov *function on the set $\mathcal{Z}$ for the difference inclusion $z^+ \in H(z)$ if there exist class $\mathcal{K}$ functions $\gamma_1(\cdot)$, $\gamma_2(\cdot)$, and $\gamma_3(\cdot)$ such that the following holds for all $z \in \mathcal{Z}$:*

$$\gamma_1(|z - z_s|) \leq V(z) \leq \gamma_2(|z - z_s|), \quad \max_{z^+ \in H(z)} V(z^+) \leq V(z) - \gamma_3(|z - z_s|).$$

Lemma 4.6. *If the set $\mathcal{Z}$ is positively invariant for the difference inclusion $z^+ \in H(z)$, $H(0) = \{0\}$, and there exists a Lyapunov function V on $\mathcal{Z}$, then z_s is asymptotically stable on $\mathcal{Z}$.*

Proof. From the definition of V, for all $z \in \mathcal{Z}$ we have

$$\max_{z \in H(z)} V(z^+) \leq V(z) - \gamma_3(|z - z_s|) \leq V(z)$$

Hence we can write $V(\psi(k;z)) \leq V(z)$ for all $k \in \mathbb{I}_{\geq 0}$. Since $\psi(k;z) \in \mathcal{Z}$ for all $k \in \mathbb{I}_{\geq 0}$, we can write

$$\gamma_1(|\psi(k;z) - z_s|) \leq V(\psi(k;z)) \leq V(z) \leq \gamma_2(|z - z_s|)$$

Thus we obtain $|\psi(k;z) - z_s| \leq \gamma_1^{-1}(\gamma_2(|z - z_s|))$. We note that $\overline{\gamma}(\cdot) = \gamma_1^{-1}(\gamma_2(\cdot))$ is also a class $\mathcal{K}$ function (Khalil, 2002, Lemma 4.2). Hence we have $|\psi(k;z) - z_s| \leq \overline{\gamma}(|z - z_s|)$ for all $z \in \mathcal{Z}$, and hence z_s is asymptotically stable on $\mathcal{Z}$. □

4.4 Nominal stability

We now show that the nonlinear system $x^+ = f(x,u)$ driven by a suboptimal algorithm MPC satisfying (4.3) is asymptotically stable.

Lemma 4.7. *There exists a class $\mathcal{K}$ function $\gamma_m(\cdot)$ such that $|\mathbf{u} - \mathbf{u}_s| \leq \gamma_m(|x - x_s|)$ for any $(x, \mathbf{u}) \in \mathcal{Z}_r$.*

Proof. We first show that $|\mathbf{u} - \mathbf{u}_s| \leq \gamma_s|x - x_s|$ holds, for some class $\mathcal{K}$ function $\gamma_s(\cdot)$, if $x \in r\mathbb{B} \subseteq \mathbb{X}_f$. From the definition of $\overline{V}_{N,p}(\cdot)$ and (3.6) we have

$$\begin{aligned} \overline{V}_{N,p}(x,\mathbf{u}) &\geq \sum_{k=0}^{N-1} \rho((\phi(k;x,\mathbf{u}) - x_s, u - u_s)), \quad \forall (x,\mathbf{u}) \in \mathbb{X} \times \mathbb{U}^N \\ &= \rho_s(x - x_s, \mathbf{u} - \mathbf{u}_s) \\ &\geq \gamma_s\big(\,|(x - x_s, \mathbf{u} - \mathbf{u}_s)|\,\big) = \gamma_s(|z - z_s|) \qquad \text{(Lemma 3.3)} \qquad (4.7) \end{aligned}$$

where $\rho(\cdot)$ and $\rho_s(\cdot)$ are positive definite functions and $\gamma_s(\cdot)$ is a class $\mathcal{K}$ function. From Lemma 3.19 we know that there exists a class $\mathcal{K}$ function $\gamma(\cdot)$ such that, $\overline{V}_f(x) \leq \gamma(|x - x_s|)$

for all $x \in \mathbb{X}_f$. Hence for all $x \in r\mathbb{B} \subseteq \mathbb{X}_f \subseteq \mathbb{X}$, we can write

$$\gamma_s(|\mathbf{u} - \mathbf{u}_s|) \leq \gamma_s(|(x - x_s, \mathbf{u} - \mathbf{u}_s)|) \leq \overline{V}_{N,p}(x, \mathbf{u}) \leq \overline{V}_f(x) \leq \gamma(|x - x_s|)$$

Hence we have $|\mathbf{u} - \mathbf{u}_s| \leq \gamma_s(|x - x_s|)$ for all $x \in r\mathbb{B}$, where $\gamma_s(\cdot) = \gamma_s^{-1}(\gamma(\cdot))$ is also a class $\mathcal{K}$ function (Khalil, 2002, Lemma 4.2). Define $\mu = \max_{\mathbf{u} \in \mathbb{U}^N} |\mathbf{u}|$, and note that $\mu < \infty$ because $\mathbb{U}^N$ is compact. Define a class $\mathcal{K}$ function $\gamma_m(|x|) := \max\left\{\gamma_s(|x|), \frac{\mu}{r}|x|\right\}$. Note that since both $\gamma_s(\cdot)$ and $|\cdot|$ are continuous and strictly increasing, $\gamma_m(\cdot)$ is also continuous. Hence we have $|\mathbf{u} - \mathbf{u}_s| \leq \gamma_m(|x - x_s|)$ for all $(x, \mathbf{u}) \in \mathcal{Z}_r$. □

Lemma 4.8. *$\overline{V}_{N,p}(z)$ is a Lyapunov function for the extended closed-loop system* (4.6) *in any compact subset of $\mathcal{Z}_r$.*

Proof. As established in (4.7) in the proof of Lemma 4.7, $\overline{V}_{N,p}(z) \geq \gamma_s(|z - z_s|)$ for all $z \in \mathbb{X} \times \mathbb{U}^N$. Consider any compact set $\mathcal{C} \subseteq \mathcal{Z}_r$. From the continuity of $\ell(\cdot)$, $V_f(\cdot)$ and $\lambda(\cdot)$ (Assumption 3.10) and Lemma 3.18, we have

$$\overline{V}_{N,p}(x, \mathbf{u}) \leq \gamma_2(|(x - x_s, \mathbf{u} - \mathbf{u}_s)|), \quad \forall (x, \mathbf{u}) \in \mathcal{C} \subseteq \mathcal{Z}_r$$

where $\gamma_2(\cdot) = C|\cdot|$ is a class $\mathcal{K}$ function. From the definition of $\overline{V}_{N,p}(z)$ and (3.6) we know that $\overline{V}_{N,p}(z^+) - \overline{V}_{N,p}(z) \leq -L(x, u(0)) \leq -\gamma(|(x - x_s, u(0) - u_s)|)$. From Lemma 4.7 we can write

$$\begin{aligned} |z - z_s| &\leq |x - x_s| + |\mathbf{u} - \mathbf{u}_s| \leq |x - x_s| + \gamma_s(|x - x_s|), \quad \forall z \in \mathcal{C} \\ &= \overline{\gamma}_s(|x - x_s|) \\ &\leq \overline{\gamma}_s(|(x - x_s, u(0) - u_s)|) \end{aligned}$$

Hence we have

$$\overline{V}_{N,p}(z^+) - \overline{V}_{N,p}(z) \leq -\gamma\left(\overline{\gamma}_s^{-1}(|z - z_s|)\right) = -\gamma_3(|z - z_s|), \quad \forall z \in \mathcal{C}$$

Hence $\overline{V}_z(z)$ is a Lyapunov function for the nonlinear system (4.6) for all z in $\mathcal{C} \subseteq \mathcal{Z}_r$.

□

Theorem 4.9. *Let Assumptions 3.9, 3.10, and 3.14 hold. Then the steady-state solution x_s is an asymptotically stable equilibrium point of the nonlinear system* (4.5)*, on (arbitrarily large) compact subsets of $\mathcal{X}_{N,p}$.*

Proof. From Lemma 4.8 we have that $V_{N,p}(z)$ is a Lyapunov function for (4.6) in the set $\mathcal{Z}_r$. Let $\overline{V}$ be an arbitrary positive scalar, and consider the set

$$\mathcal{S} = \{(x, \mathbf{u}) \in \mathcal{Z}_r \mid V_{N,p}(x, \mathbf{u}) \leq V\}.$$

We observe that $\mathcal{S} \subseteq \mathcal{Z}_r$ is compact and is invariant for (4.6). By Lemma 4.6, these facts prove that z_s is asymptotically stable on $\mathcal{S}$ for the difference inclusion (4.6), i.e., there exists a class $\mathcal{K}$ function $\gamma(\cdot)$, such that for any $z \in \mathcal{S}$ we can write:

$$\psi(k; z) \in \mathcal{S} \quad \text{and} \quad |\psi(k; z) - z_s| \leq \gamma(|z - z_s|, k) \qquad \text{for all } k \in \mathbb{I}_{\geq 0}$$

in which $\psi(k; z) = z(k)$ is *a solution* of (4.6) at time k for a given initial extended state $z(0) = z$. We define $\mathcal{C} = \{x \in \mathcal{X}_{N,p} \mid \exists \mathbf{u} \in \mathcal{U}_{N,p}(x)$ such that $(x, \mathbf{u}) \in \mathcal{S}\}$ and note that $\mathcal{C} \subseteq \mathcal{X}_{N,p}$ and that $\mathcal{C}$ is compact because it is the projection onto $\mathbb{R}^n$ of the compact set $\mathcal{S}$. Thus for any $x \in \mathcal{C}$ and its associated suboptimal input sequence $\mathbf{u}$ such that $z = (x, \mathbf{u}) \in \mathcal{S}$, we denote with $\phi(k;x)$ the state component of $\psi(k;z)$ (i.e., a solution of the nonextended system (4.5)). For all $k \in \mathbb{I}_{\geq 0}$ we can write:

$$\phi(k;x) \in \mathcal{C} \quad \text{and} \quad |\phi(k;x) - x_s| \leq |\psi(k;z) - z_s| \leq \gamma(|z - z_s|) \leq \gamma(\overline{\gamma}_s|x - x_s|)$$

because from Lemma 4.8 it follows that $|z - z_s| \leq |x - x_s| + |\mathbf{u} - \mathbf{u}_s| \leq \overline{\gamma}_s|x - x_s|$. This inequality establishes that the origin of the closed-loop system is asymptotically stable on $\mathcal{C}$, and V can be chosen large enough for $\mathcal{C}$ to contain any given compact subset of $\mathcal{X}_{N,p}$. □

Corollary 4.10. *Let Assumptions 3.9, 3.10, and 3.11 hold. Then the steady-state solution x_s is an asymptotically stable equilibrium point of the nonlinear system driven by the terminal constraint MPC using a suboptimal algorithm satisfying the following:*

$$\mathbf{u}^+ \in \mathcal{U}_{N,c}(x^+) \tag{4.8a}$$

$$V_{N,c}(x^+, \mathbf{u}^+) \leq V_{N,c}(x^+, \mathbf{u}) \tag{4.8b}$$

on (arbitrarily large) compact subsets of $\mathcal{X}_{N,c}$.

Proof. The terminal constraint formulation can be viewed as a special case of the terminal penalty formulation with $\mathbb{X}_f = \{x_s\}$. □

Hence to ensure closed-loop stability in the nominal case, it is sufficient to ensure that the cost drops when the optimizer is invoked at each iteration with a feasible warm start (4.3b). The cost drop is easy to check since a feasible warm start is readily generated and when the NLP solver is initialized with a feasible warm start, it always returns a solution with a lower objective value. For very large problems, this also enables us to stop the optimizer before it converges to a local optimum, as long as the solution returned has a lower cost than the warm start. In all the simulation studies in this thesis, a drop in the cost is ensured since the NLP solver is always initialized with the warm start.

Chapter 5

Non-steady operation

Note: The text of this chapter appears in Rawlings and Amrit (2008); Angeli, Amrit, and Rawlings (2009); Angeli et al. (2011a); Angeli, Amrit, and Rawlings (2011b).

5.1 Introduction

In Chapter 3, we extended the MPC stability theory to generic nonlinear systems and cost. As established, for general nonlinear systems and/or nonconvex cost functionals, the optimal steady state x_s may not necessarily be an equilibrium point of the closed-loop system and therefore its stability cannot be expected in general. Chapter 3 establishes a class of systems - strictly dissipative systems, for which closed loop stability is established for different MPC formulations. It is in fact conceivable that the optimal path from x_s, at time 0 to x_s at time N, (that is at the end of the control horizon N), be different from the constant solution $x(k) \equiv x_s$ for all $k \in \mathbb{I}_{0:N}$, for systems which are not strictly dissipative. While this can at first sight appear to be a dangerous drawback of economic

MPC, it might be, for specific applications, one of its major strengths. Huang et al. (2011b) point out applications like simulated moving bed (SMB) and pressure swing adsorption (PSA) in which non-steady operation is desirable due to the design of the process. As we saw previously, the economic MPC formulation extracts its benefits compared to standard tracking formulation from the transient portion of process operation. Hence the processes, for which non-steady operation outperforms steady operation, have a lot of potential for extracting economic advantages.

In this chapter, we evaluate the importance of non-steady operation and discuss the possible benefits, which provide the incentive to extend MPC algorithms to control processes in non-steady fashion. Unlike Chapter 3 and 4 we do not assume that the nonlinear system $x^+ = f(x,u)$ is strictly dissipative with respect to the shifted economic cost. Hence closed loop stability is not guaranteed.

5.2 Average performance

In this section we show that even though stability is not in general guaranteed, asymptotic economic performance of the controller is preserved. We first define our performance measure.

Definition 5.1 (Average performance)**.** *The asymptotic average performance of the system $x^+ = f(x,u)$ is defined as*

$$\lim_{T\to\infty} \frac{\sum_{k=0}^{T} \ell(x(k),u(k))}{T+1}, \quad x^+ = f(x,u), \quad x(0) = x$$

where $u(k) \in \mathbb{U}$ *for all* $k \in \mathbb{I}_{\geq 0}$.

Remark 5.2. *It is important to note that the above limit may fail to exist. For example, in cyclic processes in which a recurring periodic operation is observed, the above limit does not have a finite value. However, for such cases, the asymptotic average performance can still be quantified as the following interval rather than a single value.*

$$\left[\lim_{T\to\infty} \inf \ell_{av}, \lim_{T\to\infty} \sup \ell_{av}\right], \qquad \ell_{av} = \frac{\sum_{k=0}^{T} \ell(x(k), u(k))}{T+1} \quad x^+ = f(x,u), \quad x(0) = x$$

We now show that economics optimizing MPC always outperforms the best steady-state profit in time average.

Theorem 5.3. *Consider the terminal penalty MPC formulation presented in Section 3.4. If Assumptions 3.10 and 3.14 hold, the asymptotic average performance of the closed-loop nonlinear system* (3.23) *is better, i.e., no worse, than the performance of the optimal admissible steady state.*

Proof. Consider the usual optimal input sequence (3.22) corresponding to state $x \in \mathcal{X}_N$ and the candidate sequences (3.26) and (3.27) at state $x^+ = f(x, u_p^0(0;x))$:

$$\mathbf{u}_p^0(x) = \{u_p^0(0;x), u_p^0(1;x), \cdots, u_p^0(N-1,x)\} \tag{3.22}$$

$$\mathbf{u}(x) = \{u_p^0(1;x), u_p^0(2;x), \ldots, u_p^0(N-1;x),\ \kappa_f(x^0(N;x)))\} \tag{3.26}$$

$$\mathbf{x}(x) = \left\{x_p^0(1;x), x_p^0(2;x), \ldots, x_p^0(N;x), x_p^0(N+1;x))\right\} \tag{3.27}$$

From the definition of $V_{N,p}(\cdot)$ we can write

$$V_{N,p}(x^+) = V^0(x) - \ell(x, u_p^0(0;x)) + \ell(x_p^0(N;x), K_f(x_p^0(N;x))) - V_f(x_p^0(N;x)) + V_f(x_p^0(N+1;x))$$

Using the stability assumption on $V_f(\cdot)$ (Assumption 3.14) gives

$$V_{N,p}^0(x^+) - V_{N,p}^0(x) \leq \ell(x_s, u_s) - \ell(x, u_p^0(0;x)), \quad \forall x \in \mathcal{X}_N \tag{5.1}$$

The stage cost $\ell(x,u)$ is bounded on $\mathbb{Z}$ since $\ell(\cdot)$ is continuous on $\mathbb{Z}$ and $\mathbb{Z}$ is compact. Hence $V_{N,p}^0(x^+) - V_{N,p}^0(x)$ is also bounded in the set $\mathcal{X}_N$, which in turn implies that the average,

$\frac{\sum_{k=0}^{T} V_{N,p}^0(x(k+1)) - V_{N,p}^0(x(k))}{T+1}$, is also bounded in the set $\mathcal{X}_N$. Taking averages on both sides of (5.1)

$$\begin{aligned}\liminf_{T\to+\infty} \frac{\sum_{k=0}^{T} V_{N,p}^0(x(k+1)) - V_{N,p}^0(x(k))}{T+1} &\leq \liminf_{T\to+\infty} \frac{\sum_{k=0}^{T} \ell(x_s,u_s) - \ell(x(k),u(k))}{T+1} \\ &\leq \ell(x_s,u_s) - \limsup_{T\to+\infty} \frac{\sum_{k=0}^{T} \ell(x(k),u(k))}{T+1}\end{aligned}$$

The left hand side of the inequality can be simplified as

$$\liminf_{T\to+\infty} \frac{\sum_{k=0}^{T} V_{N,p}^0(x(k+1)) - V_{N,p}^0(x(k))}{T+1} = \liminf_{T\to+\infty} \frac{V_{N,p}^0(x(T+1)) - V_{N,p}^0(x(0))}{T+1} = 0$$

which gives

$$\limsup_{T\to+\infty} \frac{\sum_{k=0}^{T} \ell(x(k),u(k))}{T+1} \leq \ell(x_s,u_s)$$

which completes the proof. □

Corollary 5.4. *Consider the system under the terminal constraint MPC presented in Section 3.3. Let Assumption 3.10 hold. The asymptotic average performance of the closed-loop nonlinear system* (3.12) *is better, i.e., no worse, than the performance of the optimal admissible steady state.*

Proof. The terminal constraint formulation can be viewed as a special case of the terminal penalty formulation with $\mathbb{X}_f = \{x_s\}$. □

5.3 Non-steady MPC algorithms

A lot of industrial criticism to nonsteady operation is the possibility of violating process safety constraints, physical system requirements and raw material constraints, during its operation, as non-steady operations can be chaotic and unpredictable. As mentioned earlier, non-steady behavior may be desired in many applications due to its economic benefit and hence this motivates the formulation of controlled non-steady operations. For a plant that is not optimally operated at steady state, it is meaningful to aim at an average asymptotic cost that is strictly less than that of the best feasible equilibrium. In these cases, to characterize the nature of operation, we introduce the following two concepts:

1. Average constraints

2. Periodic operation

In this section, we define these characterizations and propose MPC formulations to control the systems in these desired ways.

5.3.1 Average constraints

Note: The results of this section are taken from Angeli et al. (2011a).

For stable systems, the asymptotic averages of variables (typically inputs and states) are determined by the values of those variables at the equilibrium point. Therefore average constraints do not deserve special attention as they are taken into account by default in the single layer economic MPC setup or can be taken into account as static constraints in the RTO layer. But when dealing with nonsteady operation, consideration of constraints on average values of variables, besides pointwise hard bounds as discussed in the previous formulations, are necessary. In this section we first define asymptotic average of any given vector valued bounded variable, and then formulate a MPC scheme to satisfy constraints on these average quantities.

Definition 5.5 (Average vector quantity)**.** *The average of a vector valued bounded variable v is defined as*

$$Av[v] = \left\{ v \in \mathbb{R}^{n_v} \mid \exists\, t_n \to +\infty : \lim_{n \to +\infty} \frac{\sum_{k=0}^{t_n} v(k)}{t_n + 1} = v \right\}$$

Remark 5.6. *Similar to the limit in the definition of average performance, the average vector $Av[v]$ defined above may be an interval rather than a single value. The interval is always nonempty (because bounded signals have limit points). The computed value v will depend on the sequence of time points $\{t_n\}$ selected.*

Formulation

We now present a MPC algorithm that controls the system fulfilling constraints on average of desired quantities, as described above. Let $\mathbb{Y} \subseteq \mathbb{R}^p$ be a closed and *convex* set and y an auxiliary output variable defined according to:

$$y = h(x, u) \tag{5.2}$$

for some continuous map $h : \mathbb{Z} \to \mathbb{R}^p$. The following nestedness property is assumed:

$$h(x_s, u_s) \in \mathbb{Y} \tag{5.3}$$

Our goal is to design a receding horizon control strategy that ensures the following set of constraints:

$$\begin{aligned} \mathrm{Av}[\ell(x,u)] &\subseteq (-\infty, \ell(x_s,u_s)] \\ (x(k),u(k)) &\in \mathbb{Z} \quad k \in \mathbb{I}_{\geq 0} \\ \mathrm{Av}[y] &\subseteq \mathbb{Y} \end{aligned} \tag{5.4}$$

Consider the following dynamic regulation problem

$$\mathbb{P}_{N,av}(x): \qquad V^0_{N,av}(x) := \min_{\mathbf{u}} \left\{ V_{N,c}(x,\mathbf{u}) \quad | \quad \mathbf{u} \in \mathcal{U}_{N,c}(x), \quad \sum_{k=0}^{N-1} h(x(k),u(k)) \in \mathbb{Y}_t \right\} \tag{5.5}$$

where $V_{N,c}(\cdot)$ and $\mathcal{U}_{N,c}(x)$ are the terminal constraint cost function and the corresponding input constraint set defined in (3.7) and (3.8), respectively. We observe that due to Assumption 3.10 and the fact that the set $\mathbb{Y}$ is closed and convex, the above problem has a solution. The time-varying output constraint set is the new feature of this problem. To enforce the average constraints, we define the constraint sets using the following recursion

$$\mathbb{Y}_{i+1} = \mathbb{Y}_i \oplus \mathbb{Y} \ominus h(x(i),u(i)) \qquad \text{for } i \in \mathbb{I}_{\geq 0} \tag{5.6}$$

$$\mathbb{Y}_0 = N\mathbb{Y} + \mathbb{Y}_{00} \tag{5.7}$$

in which the set $\mathbb{Y}_{00} \subset \mathbb{R}^p$ is an arbitrary compact set containing the origin and the symbols $\oplus$ and $\ominus$ denote standard set addition, and subtraction, respectively. By adjusting the output constraint sets with the closed-loop behavior, we force the average constraints to be satisfied asymptotically. Denote the optimal solution of $\mathbb{P}_{N,av}(x)$ as

$$\mathbf{u}^0_{av}(x) = \{u^0_{av}(0;x), u^0_{av}(1;x), \cdots, u^0_{av}(N-1,x)\} \tag{5.8}$$

Denote the corresponding implicit MPC control law and the closed loop system as

$$x^+ = f(x, \kappa_{N,av}(x)), \qquad \kappa_{N,av}(x) = u^0_{av}(0; x) \tag{5.9}$$

Theorem 5.7 (Angeli et al. (2011a))**.** *Let Assumption 3.10 hold. Given a feasible initial condition x for the problem $\mathbb{P}_{N,av}(x)$, feasibility is ensured for all subsequent times. Moreover* (5.4) *holds for the closed loop system* (5.9).

Proof. The detailed proof is provided in Angeli et al. (2011a), and is omitted from this thesis.

□

5.3.2 Periodic operation

Note: The results of this section are taken from Angeli et al. (2009).

In many studies, it has been established that the performance of many continuous chemical processes can be improved by forced periodic operation (Lee and Bailey, 1980; Sincic and Bailey, 1980; Watanabe, Onogi, and Matsubara, 1981; Watanabe, Matsubara, Kurimoto, and Onogi, 1982). Bailey (1974) provides a comprehensive review of periodic operation of chemical reactors. Several applications in the process industry exhibit periodic/cyclic behavior due to their operational nature, such as pressure swing adsorption (PSA) (Agarwal, Biegler, and Zitney, 2009) and simulated moving bed (SMB) separation (Kawajiri and Biegler, 2006). This leads us to formulate MPC schemes that enforce periodic operation, in which the state at the beginning and at the end of the horizon are identical. Note that the steady-state solution is also a periodic solution. In this section we define *periodic solutions* that outperform the best steady solution and discuss the MPC scheme formulated by Angeli et al. (2009), that outperforms the periodic solution in time average.

Consider a situation in which there is a Q-periodic solution $x^*(k), k \in \mathbb{I}_{0:Q-1}$ that outperforms the best feasible steady state. Q, the period of the process, is assumed to be either known from process design specifications, or fixed at the time constant of the system. The periodic solution can be precomputed by solving the following optimization problem:

$$\min_{x(0),\mathbf{u}} V_Q(x(0),\mathbf{u}) = \sum_{k=0}^{Q-1} \ell(x(k),u(k))$$
$$\text{subject to} \begin{cases} x^+ = f(x,u) \\ (x(k),u(k)) \in \mathbb{Z}, \quad k \in \mathbb{I}_{0:Q-1} \\ x(Q) = x(0) \end{cases} \tag{5.10}$$

with $\mathbf{u} = \{u(0), u(1), \ldots, u(Q-1)\}$. Denote the optimal state and input sequence for this problem as $(x^*(k), u^*(k)), k \in \mathbb{I}_{0:Q-1}$.

Next we obtain a time-varying state feedback law by solving online the following optimization problem over the set of terminal constraints indexed by integer $q \in \mathbb{I}_{0:Q-1}$

$$\min_{\mathbf{v}} V_N(x, \mathbf{v}, q) \quad \text{subject to} \begin{cases} z^+ = f(z, v) \\ (z(k), v(k)) \in \mathbb{Z}, \quad k \in \mathbb{I}_{0:N-1} \\ z(N) = x^*(q) \\ z(0) = x \end{cases} \tag{5.11}$$

Let $(\mathbf{z}^0(x, q), \mathbf{v}^0(x, q))$ denote the optimal state and input of (5.11) (assumed unique) for initial state x using the qth element of the periodic terminal constraint. Next define the implicit MPC feedback control law $\kappa_N(\cdot)$ as the first element of the optimal input sequence using the qth constraint

$$\kappa_N(x, q) = v^0(0; x, q) \tag{5.12}$$

The corresponding closed loop system evolves according to

$$x^+ = f(x, \kappa_N(x, t \bmod Q)) \tag{5.13}$$

where t is the current time and x is the state at time t. This control law $\kappa_N(x, q)$ is defined on the set of x for which problem (5.11) is feasible. Notice that, due to the periodic terminal constraint, the resulting closed-loop system is also a Q-periodic nonlinear system. As in the case of optimal equilibria, asymptotic convergence to the periodic solution is not generally to be expected and can only be ensured provided suitable dissipativity assumptions are in place.

We now show that the asymptotic average cost along the closed loop system (5.13) is not worse than that of the optimal periodic solution.

Theorem 5.8 (Angeli et al. (2009)). *The average asymptotic performance of the nonlinear control system* (5.13) *fulfills:*

$$\limsup_{T\to+\infty} \frac{\sum_{k=0}^{T} \ell(x(k),u(k))}{T+1} \leq \frac{\sum_{k=0}^{Q-1} \ell(x^*(k),u^*(k))}{Q} \tag{5.14}$$

Proof. As in the proof of Theorem 5.3, we can write

$$V_{N,p}^0(x^+) - V_{N,p}^0(x) \leq \ell(x^*(q),u^*(q)) - \ell(x,u_p^0(0;x)), \quad \forall x \in \mathcal{X}_N, \quad q = t \bmod Q \tag{5.15}$$

Taking averages on both sides of (5.15)

$$\begin{aligned}\liminf_{T\to+\infty} \frac{\sum_{k=0}^{T} V_{N,p}^0(x(k+1)) - V_{N,p}^0(x(k))}{T+1} &\leq \liminf_{T\to+\infty} \frac{\sum_{k=0}^{T} \ell(x^*(k \bmod Q),u^*(k \bmod Q)) - \ell(x(k),u(k))}{T+1} \\ &\leq \frac{\sum_{k=0}^{Q-1} \ell(x^*(k),u^*(k))}{Q} - \limsup_{T\to+\infty} \frac{\sum_{k=0}^{T} \ell(x(k),u(k))}{T+1}\end{aligned}$$

The left hand side of the inequality can be simplified as

$$\liminf_{T\to+\infty} \frac{\sum_{k=0}^{T} V_{N,p}^0(x(k+1)) - V_{N,p}^0(x(k))}{T+1} = \liminf_{T\to+\infty} \frac{V_{N,p}^0(x(T+1)) - V_{N,p}^0(x(0)}{T+1} = 0$$

which gives

$$\limsup_{T\to+\infty} \frac{\sum_{k=0}^{T} \ell(x(k),u(k))}{T+1} \leq \frac{\sum_{k=0}^{Q-1} \ell(x^*(k),u^*(k))}{Q}$$

which completes the proof.

□

5.4 Enforcing convergence

As we established in the previous sections, due to potential nonconvexity of costs considered as well as nonlinearity of the underlying dynamics, convergent behaviors are not always optimal and/or desirable. In many other contexts convergence to an equilibrium is a requirement that cannot be sacrificed by trading it off with economics. Hence in this section we investigate ways to fulfill convergence requirements while still optimizing transient economic performance. In this section, two methods are discussed and compared to systematically enforce convergence to the best equilibrium provided by the static optimization layer while still employing an economic MPC scheme.

5.4.1 Regularization of objective

As established in Sections 3.3 and 3.4, satisfaction of strict dissipativity (Definition 3.8) ensures convergent behavior in the system. Angeli et al. (2011a) use this fact to propose a method to enforce convergence.

We consider the following modified stage cost in which we shall determine the function $\alpha : \mathbb{X} \times \mathbb{U} \to \mathbb{R}_{\geq 0}$

$$\bar{\ell}(x, u) = \ell(x, u) + \alpha(x, u) \tag{5.16}$$

in which $\alpha(\cdot)$ is chosen positive definite with respect to (x_s, u_s). Hence, $\bar{\ell}(\cdot)$ and $\ell(\cdot)$ share the same optimal steady state, (x_s, u_s). To achieve strict dissipativity, it is sufficient to satisfy the following inequality for some continuous $\lambda(x) : \mathbb{X} \to \mathbb{R}$ and all $(x, u) \in \mathbb{Z}$

$$\lambda(x) - \lambda(f(x, u)) \leq -\rho(x) + \ell(x, u) - \ell(x_s, u_s) + \alpha(x, u)$$

Rearranging, we must satisfy for some λ and all $(x, u) \in \mathbb{Z}$

$$\alpha(x, u) \geq h(x, u, \lambda) := \lambda(x) - \lambda(f(x, u)) + \rho(x) - \ell(x, u) + \ell(x_s, u_s)$$

The right hand side in the above inequality is continuous in (x, u) for all λ. To obtain the weakest modification to the economic stage cost, we first determine the maximum of the lower bounding function in a ball of radius r around the steady state:

$$h(r, \lambda) = \max_{\substack{(x,u)\in\mathbb{Z} \\ |(x,u)-(x_s,u_s)|\leq r}} h(x, u, \lambda), \qquad \forall r \in \mathbb{R}_{\geq 0}$$

in which the maximum exists for all $r \in \mathbb{R}_{\geq 0}$ by the Weierstrass theorem. Define $\alpha(\cdot)$ as:

$$\alpha(x, u) = h(|(x, u) - (x_s, u_s)|, \lambda) \tag{5.17}$$

For any $\lambda(x) : \mathbb{X} \to \mathbb{R}$, $\alpha(x, u)$ is positive definite with respect to (x_s, u_s) and suffices for strict dissipativity. Note that the choice of $\lambda(x)$ is critical for above analysis. In general, storage functions can be nonlinear. A special class of strictly dissipative systems are called *strongly dual* systems (Diehl et al., 2011), in which the storage function is a linear function of the state, i.e. $\lambda(x) = \lambda' x$ for $\lambda \in \mathbb{R}^n$. Angeli et al. (2011a) present the above analysis for such a choice of $\lambda(x)$.

We then have the following stability result.

Theorem 5.9 (Amrit et al. (2011)). *Consider a nonlinear control system $x^+ = f(x, u)$ and the MPC control scheme defined in Sections 3.3 and 3.4. If the stage cost is chosen according to* (5.16) *with $\alpha(x, u)$ chosen according to* (5.17) *for any $\lambda \in \mathbb{R}^n$, then x_s is an asymptotically stable equilibrium point of the closed-loop system with region of attraction $\mathcal{X}_N$.*

Proof. By construction of $\alpha(\cdot)$, strict dissipativity is satisfied and Theorems 3.13 and 3.21 apply, giving asymptotic stability of x_s. $\square$

Theorem 5.9 allows us to add *sufficiently convex* regularization terms to the economic stage cost to enforce convergent behavior, without changing the steady-state optimum. For practical purposes, the most straightforward choice of the regularization term is the following standard tracking form

$$\alpha(x, u) = (1/2)(|x - x_s|_Q^2 + |u - u_s|_R^2)$$

where the penalties Q and R are chosen as the minimum required to achieve strict dissipativity. Another choice of $\alpha(\cdot)$ is motivated from the fact that non-steady operation involves the control variables to jump between its bounds (e.g. bang-bang control). To enforce convergence this observation leads to penalizing the input moves:

$$\alpha(x, u) = (1/2)\,|u(k) - u(k-1)|_S^2$$

Note that by adding the regularization terms, the contours of objective function of the optimization problem change, and the controller is not purely economic anymore. Hence a decrease in economic performance is expected. This decrease in performance is the trade off for gain in stability.

5.4.2 Convergence constraint

As pointed in the previous section, changing the objective function changes the cost surface and the controller does not optimize purely economic cost functions. If changing the objective function is not desired, the next window for modification in the MPC regulation problem are the constraints. In this section we exploit the MPC scheme designed in

Section 5.3.1 to enforce constraints on average quantities during closed loop operation. We introduce *convergence constraints* which specifically enforce the following *zero variance constraint* on the system:

$$\mathrm{Av}[|x - x_s|^2] \in \{0\}$$

Theorem 5.10 (Angeli et al. (2011b)). *Consider the problem* $\mathbb{P}_{N,av}(x)$ *defined in* (5.5)*, with* $h(x,u) = |x - x_s|^2$ *and* $\mathbb{Y} = \{0\}$*. The corresponding closed loop system* (5.9) *asymptotically converges to the equilibrium point* x_s*.*

Proof. The detailed proof is provided in Angeli et al. (2011b), and is omitted from this thesis. □

5.5 Illustrative examples

Having established the benefits of non-steady process operation and developed MPC schemes to control these processes, we now present two chemical engineering examples from the literature to demonstrate the application of these concepts.

5.5.1 Batch process: Maximizing production rate in a CSTR

Consider a single second-order, irreversible chemical reaction in an isothermal CSTR (Sincic and Bailey, 1980)

$$\mathrm{A} \longrightarrow \mathrm{B} \qquad r = kc_A^n$$

in which k is the rate constant and n is the reaction order. The material balance for component A is

$$\begin{aligned}\frac{dc_A}{dt} &= \frac{1}{\tau}(c_{Af} - c_A) - kc_A^n \\ \frac{dx}{dt} &= \frac{1}{\tau}(u - x) - kx^n \qquad \tau = 10, \quad k = 1.2, \quad n = 2\end{aligned} \tag{5.18}$$

in which $c_A = x$ is the molar A concentration, $c_{Af} = u$ is the feed A concentration, and $\tau = 10$ is the reactor residence time. Consider the simple case in which the process economics for the reactor are completely determined by the average production rate of B. The reactor processes a mean feedrate of component A. The available manipulated variable is the instantaneous feed concentration. The constraints are that the feed rate is nonnegative, and the mean feed rate must be equal to the amount of A to be processed

$$u(t) \geq 0 \qquad \frac{1}{T}\int_0^T u(t)dt = 1 \tag{5.19}$$

in which T is the time interval considered. We wish to maximize the average production rate or minimize the negative production rate

$$V(x(0), u(t)) = -\frac{1}{T}\int_0^T kx^n(t)dt \qquad \text{subject to (5.18)} \tag{5.20}$$

The optimal control problem is then

$$\min_{u(t)} V(x(0, u(t)) \qquad \text{subject to (5.18)–(5.19)}$$

The optimal steady operation is readily determined. In fact, the average flowrate constraint admits only a single steady feed rate, $u^* = 1$, which determines the optimal steady-state reactor A concentration and production rate

$$u^* = 1 \qquad x^* = 0.25 \qquad V^* = -0.075$$

For the second-order reaction, we can easily beat this production rate with a nonsteady A feed policy. Consider the following extreme policy

$$u(t) = T\delta(t) \qquad 0 \leq t \leq T$$

which satisfies the mean feed rate constraint, and let $x(0) = 0$ be the reactor initial condition at $t = 0^-$. The impulsive feed policy gives a jump in x at $t = 0$ so $x(0^+) = T/\tau$. Solving the reactor material balance for this initial condition and $u = 0$ over the remaining time interval gives

$$x(t) = \frac{T/\tau}{(1 + 12T/\tau)e^{0.1t} - 12T/\tau} \qquad 0 \leq t \leq T$$

We see from this solution that by choosing T large, $x(T)$ is indeed close to zero, and we are approaching a periodic solution with a large period. Substituting $x(t)$ into (5.20) and performing the integral in the limit $T \to \infty$ gives

$$V^* = \lim_{T\to\infty} -\frac{1}{T}\int_0^T kx^2(t)dt = -0.1$$

The sequence of impulses has increased the average production rate by 33% compared to steady operation. Of course, we cannot implement this extreme policy, but we can understand why the production rate is higher. The impulse increases the reactor A concentration sharply. For *second-order* kinetics, that increase pays off in the production of B, and we obtain a large instantaneous production rate which leads to a large average production rate.

For an implementable policy we can add upper bounding constraints on u and

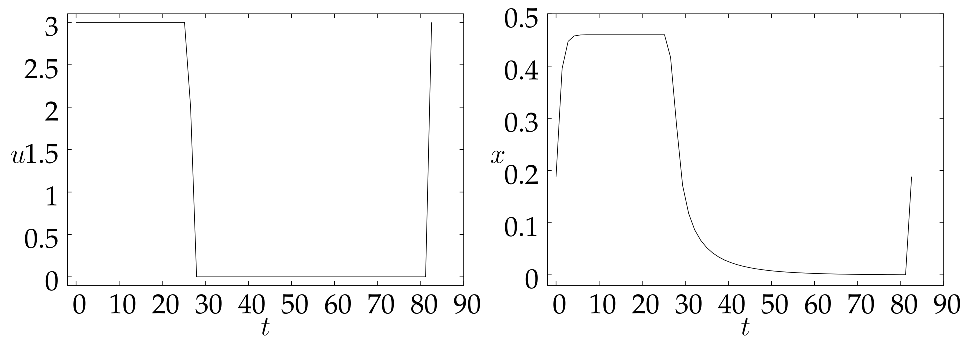

Figure 5.1: Optimal periodic input and state. The achieved production rate is $V^* = -0.0835$, an 11% improvement over steady operation.

constrain the period

$$0 \leq u(t) \leq 3 \qquad \frac{1}{T}\int_0^T u(t)dt = 1 \qquad 0 \leq T \leq 100$$

Solving the optimal control problem subject to this constraint and periodic boundary conditions on $x(t)$ gives the results in Figure 5.1. With the new constraints, switching the input between the bounds (bang bang control), yields a time average production rate of 0.0835, which is an 11% improvement over the steady-state value of 0.075. The optimal solution is similar to the extreme policy: increase the reactor A concentration to the highest achievable level by maximizing the feed concentration for as long as possible while meeting the mean constraint.

5.5.2 CSTR with parallel reactions

We consider the control of a nonlinear continuous flow stirred-tank reactor with parallel reactions (Bailey, Horn, and Lin, 1971).

$$R \rightarrow P_1$$

$$R \rightarrow P_2$$

The primary objective of such processes is a desirable distribution of products in the effluent. The dimensionless heat and mass balances for this problem are

$$x_1 = 1 - 10^4 x_1^2 e^{-1/x_3} - 400 x_1 e^{-0.55/x_3} - x_1$$

$$x_2 = 10^4 x_1^2 e^{-1/x_3} - x_2$$

$$x_3 = u - x_3$$

where x_1 is the concentration of the component R, x_2 is the concentration of the desired product P_1 and x_3 is the temperature of the mixture in the reactor. P_2 is the waste product. u, which is the heat flux through the reactor wall is the manipulated variable, and is constrained to lie between 0.049 and 0.449, while x is considered non-negative. The primary objective of the process is to maximize the amount of P_1 ($\ell(x,u) = -x_2$). Previous analysis (Bailey et al., 1971) has clearly highlighted that periodic operation can outperform steady-state operation. The steady-state problem has a solution $x_s = \begin{bmatrix} 0.0832 & 0.0846 & 0.1491 \end{bmatrix}'$ and $u_s = 0.1491$. We solve the dynamic regulation problem with the terminal state constraint.

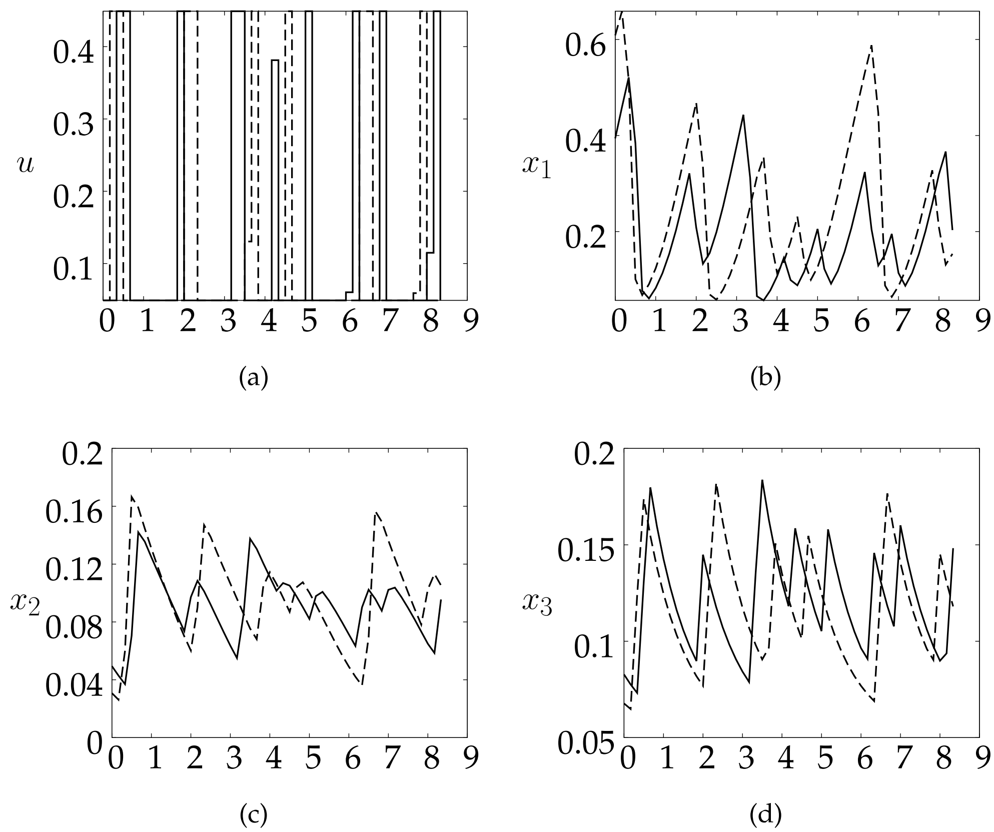

Figure 5.2: Closed-loop input (a) and state (b), (c), (d) profiles for economic MPC with different initial states

A control horizon of $N = 150$ is chosen with a sample time $T_s = 1/6$. The system is initialized at three different initial states. The closed loop system under the economic control is seen to jump between the input bounds and hence is unstable (Figure 5.2).

We observe that this system exhibits unsteady behavior and steady state convergence is not optimal. Now we demonstrate the two non-steady MPC schemes.

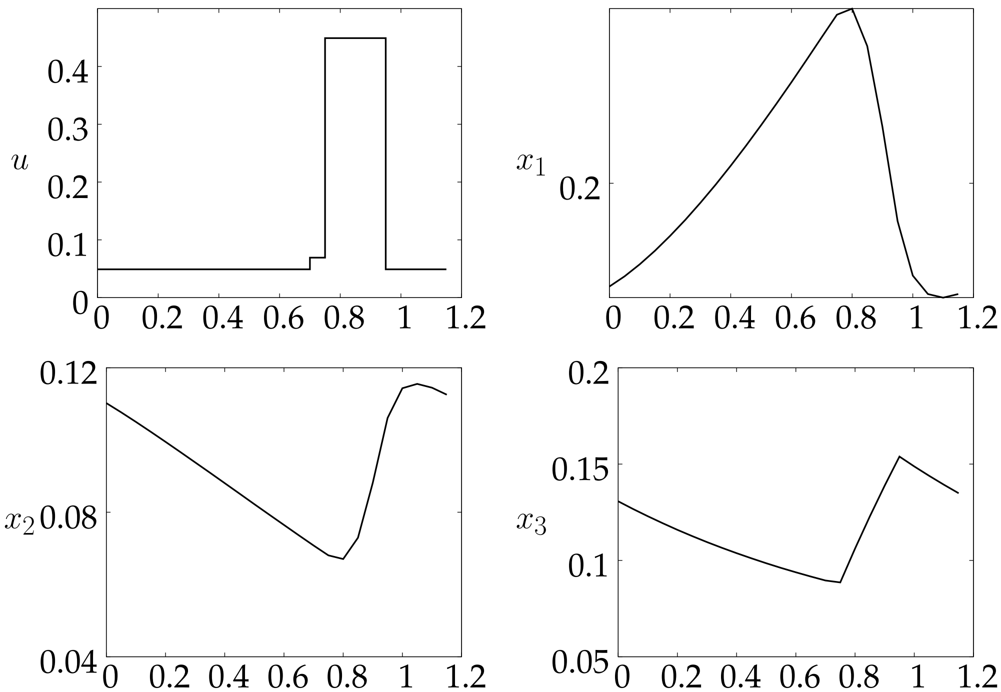

Figure 5.3: Periodic solution with period $Q = 1.2$ for CSTR with parallel reactions

Periodic operation

We first enforce periodic operation on the process. To do this, as prescribed in Section 5.3.2, we first compute the periodic steady state of the system by solving (5.10), with a fixed period $Q = 1.2$ and $x(0) = x_s$. Since we saw earlier that this system exhibits non-steady behavior, the system initialized at the steady state does not stay there. Figure 5.3 shows the periodic state of the system initialized at the best steady state. As mentioned earlier, the economic objective of the system is to maximize concentration of the desired product x_s. The periodic solution in Figure 5.3 yields a time average value of 0.092 as compared to the best steady-state value $x_{2s} = 0.084$, giving an improvement of 9.5%, which is the incentive for non-steady operation.

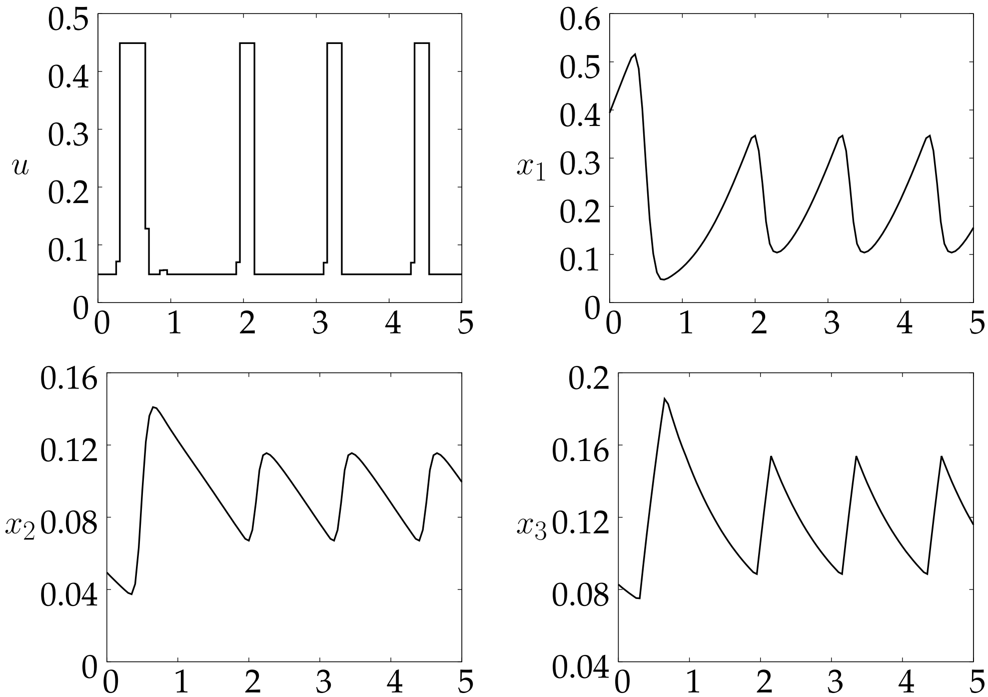

Figure 5.4: Closed loop input and state profiles of the system under periodic MPC algorithm

Next the algorithm prescribed in Section 5.3.2 for converging to a recurring periodic operation is implemented. Figure 5.4 shows the closed loop profiles of the system initialized at a random state under the periodic MPC algorithm. We see that the system transients from the initial state and settles to a recurring periodic solution.

Average constraints: Enforcing convergence

To enforce convergence, we first add a convex term in the stage cost as prescribed in Section 5.4.1.

$$V_N(x, \mathbf{u}) = \sum_{k=0}^{N} -x_2(k) + |u(k) - u(k-1)|_S^2$$

For $S = 0.17$, we observe a stable solution (Figure 5.5), and the closed loop system converges to the optimal steady state.

We can also penalize the distance from the steady state for the convex term in the objective

$$V_N(x, \mathbf{u}) = \sum_{k=0}^{N} -x_2(k) + |u(k) - u_s|_R^2$$

For $R = 0.15$, we again observe that the closed loop system converges to the optimal steady state (Figure 5.6).

Next we enforce convergence without modifying the objective function, by enforcing the zero variance constraint using the iteration scheme. Figure 5.7 shows closed loop profiles with the tuning parameter $\mathbb{Y}_{00}$ defined as

$$\mathbb{Y}_{00} = \{y \mid -w \leq y \leq w\} \tag{5.21}$$

in which $w = \begin{bmatrix} 0.5 & 0.05 & 0.018 \end{bmatrix}'$. The solution is also seen to converge to the optimal steady state.

Also note that the rate of convergence depends on the tuning parameter $\mathbb{Y}_{00}$, which is the initial variance allowance for the system. If the initial allowance is larger, iteration scheme takes a longer time to converge and hence the system is in transient for a longer time, slowing down the rate of convergence. Figure 5.8 shows closed loop profiles for $\mathbb{Y}_{00}$ defined by and $w = \begin{bmatrix} 0.5 & 0.07 & 0.07 \end{bmatrix}'$.

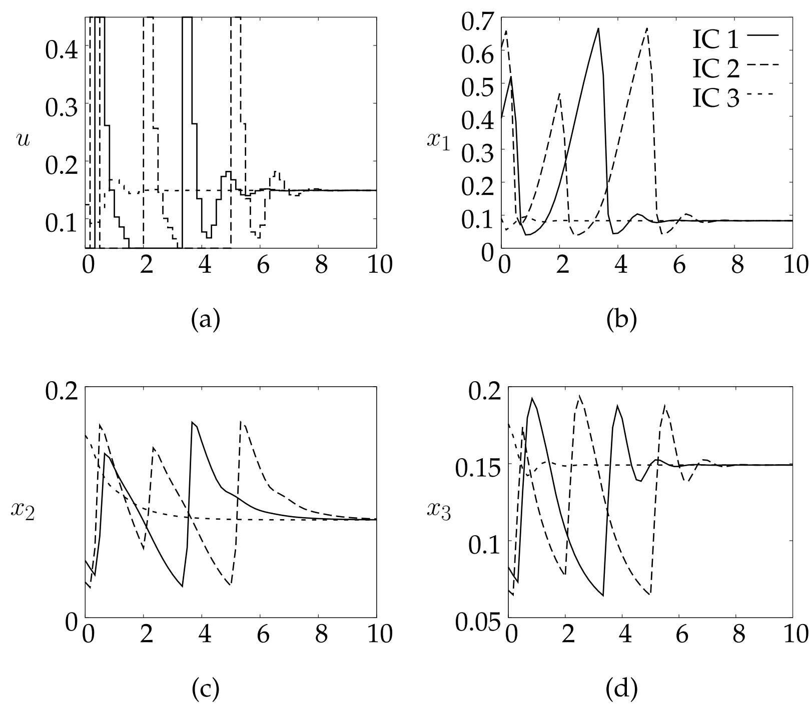

Figure 5.5: Closed-loop input (a) and state (b), (c), (d) profiles for economic MPC with a convex term, with different initial states.

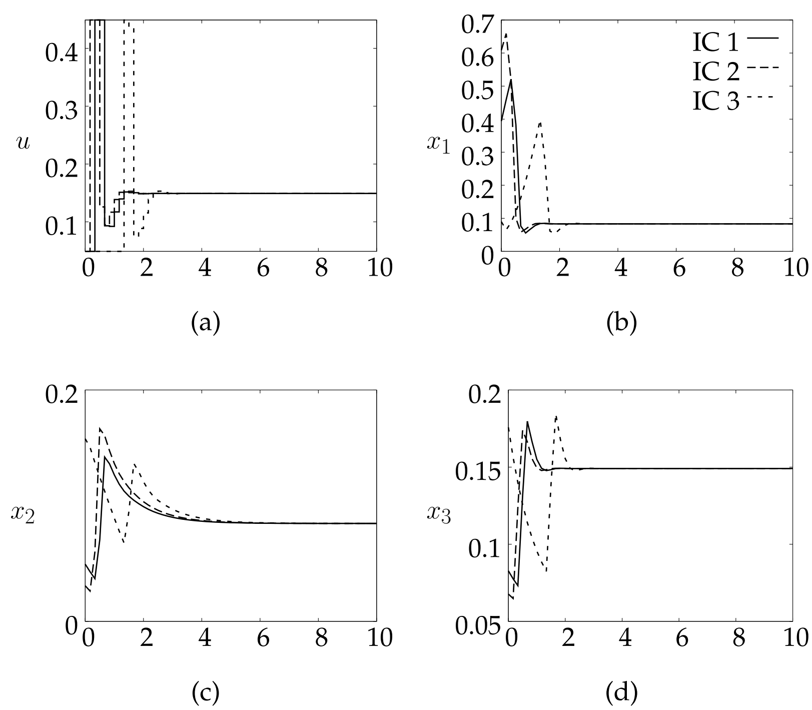

Figure 5.6: Closed-loop input (a) and state (b), (c), (d) profiles for economic MPC with a convex term, with different initial states.

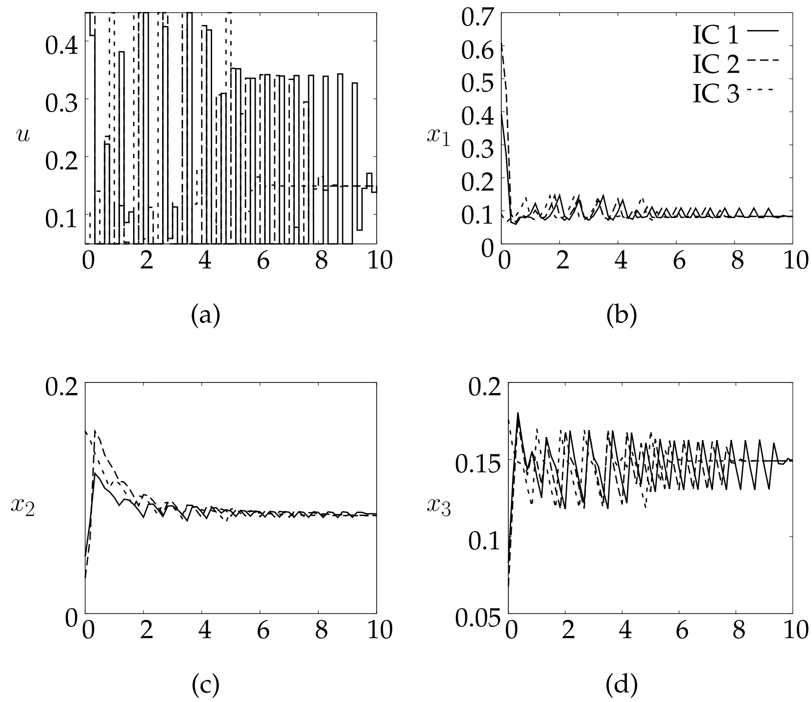

Figure 5.7: Closed-loop input (a) and state (b), (c), (d) profiles for economic MPC with a convergence constraint, with different initial states.

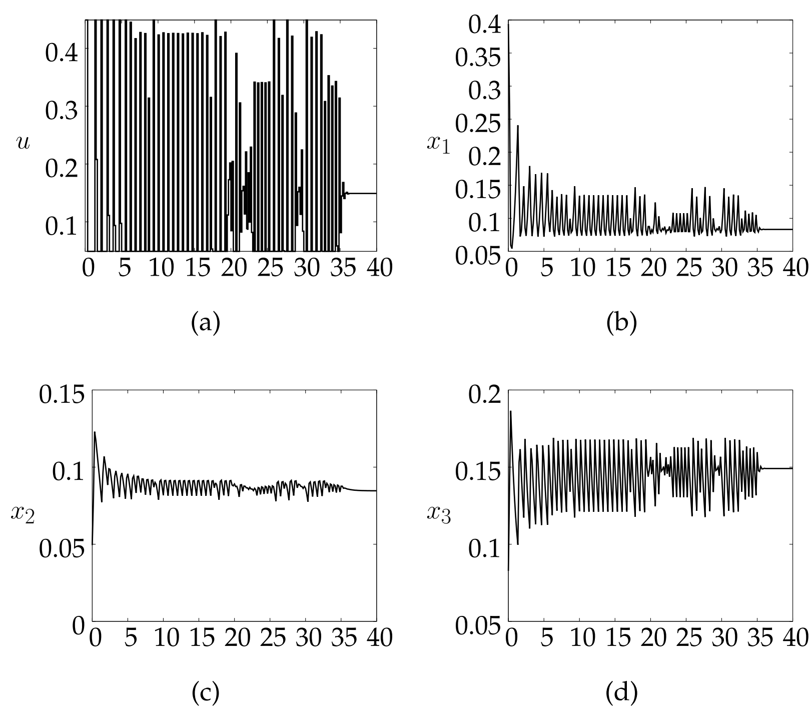

Figure 5.8: Closed-loop input (a) and state (b), (c), (d) profiles for economic MPC with a convergence constraint.

Chapter 6

Computational methods

6.1 Introduction

In the previous chapters we developed the dynamic optimization formulations for solving economic MPC problems. The standard class of problems in which the model is linear and the objective is quadratic, is a well studied class of problems, and the dynamic optimization problem is solved using well established QP algorithms (Nocedal and Wright, 2006). Economic MPC problems are, in general, nonlinear in nature and not necessarily convex. In this chapter, we discuss solution strategies to efficiently solve these nonlinear dynamic optimization problems, with focus on direct NLP strategies to solve economic dynamic MPC problems, one of which is used for all simulation studies in this thesis. First, we define the problem statement in Section 6.2. In Section 6.3 we briefly discuss the various strategies for dynamic optimization problems and introduce the direct NLP solution methods. Section 6.4 and 6.5 discuss the two direct NLP strategies, namely, the sequential and the simultaneous approach.

6.2 Problem statement

We consider the following nonlinear DAE system

$$\frac{dx_d}{dt} = f(x_d(t), x_a(t), u(t))$$
$$0 = g(x_d(t), x_a(t), u(t))$$

with state $x := \begin{bmatrix} x_d & x_a \end{bmatrix}' \in \mathbb{X} \subset \mathbb{R}^n$, control $u \in \mathbb{U} \subset \mathbb{R}^m$, and state transition maps $f : \mathbb{X} \times \mathbb{U} \to \mathbb{R}^d$ and $g : \mathbb{X} \times \mathbb{U} \to \mathbb{R}^a$, where d and a are the number of differential and algebraic variables respectively with $d + a = n$. The measurements are related to the state and input variables by the mapping $h : \mathbb{X} \times \mathbb{U} \to \mathbb{R}^p$.

$$y(t) = h(x_d(t), x_a(t), u(t))$$

We consider the discrete time domain in which time is partitioned into discrete time elements of size equal to the sample time of the problem. The problem is then parametrized in terms of the values of the state, input and measurement variables at the boundary of these finite elements. We discuss the finite horizon problem with a fixed control and prediction horizon N, which is also the number of finite elements. As mentioned previously, the constraints are imposed directly at the boundary points. As before, the system is subject to the mixed constraint

$$(x(k), u(k), y(k)) \in \mathbb{Z} \qquad k \in \mathbb{I}_{\geq 0}$$

for some compact set $\mathbb{Z} \subseteq \mathbb{X} \times \mathbb{U} \times \mathbb{Y}$. The performance measure is denoted by $\ell : \mathbb{Z} \to \mathbb{R}$.

The dynamic MPC regulation problem is set up as following:

$$\min_{\mathbf{u}} \sum_{k=0}^{N} \ell(y(k), u(k)) + V_f(y(N)) \tag{6.1a}$$

$$\frac{dx_d}{dt} = f(x_d(t), x_a(t), u(t)) \tag{6.1b}$$

$$0 = g(x_d(t), x_a(t), u(t)) \tag{6.1c}$$

$$y(t) = h(x_d(t), x_a(t), u(t)) \tag{6.1d}$$

$$g_l \leq G(y(t), u(t)) \leq g_u \tag{6.1e}$$

where the control sequence is denoted as $\mathbf{u} := \{u(0), u(1), \ldots, u(N-1)\}$. The nonlinear system is stabilized using MPC by adding either a terminal equality constraint (Section 3.3), $x(N) = x_s$ and setting $V_f(x) = 0$, or by adding a terminal inequality constraint of the form $x(N) \in \mathbb{X}_f$ for some appropriately chosen compact terminal region (Section 3.4) $\mathbb{X}_f$ and a corresponding terminal penalty $V_f(\cdot)$. The terminal constraint, along with other constraints including bounds on the state, input and measurement variables are generalized into the nonlinear constraint (6.1e).

In the standard tracking regulation, the performance measure is chosen as the distance from the optimal steady state (Rawlings and Mayne, 2009, Ch. 2). Hence $\ell_{track}(y, u) = 1/2(|y - y_s|_Q + |u - u_s|_R)$, where Q and R are the tuning parameters that govern the speed of convergence. For process economics optimizing regulation, the stage cost $\ell(\cdot)$ is chosen as the economic performance measure, like the operating cost or the negative of the profit. Note that in economic MPC $\ell(\cdot)$ is not necessarily positive definite or convex with respect to the optimal steady state as it is in the standard MPC tracking problem.

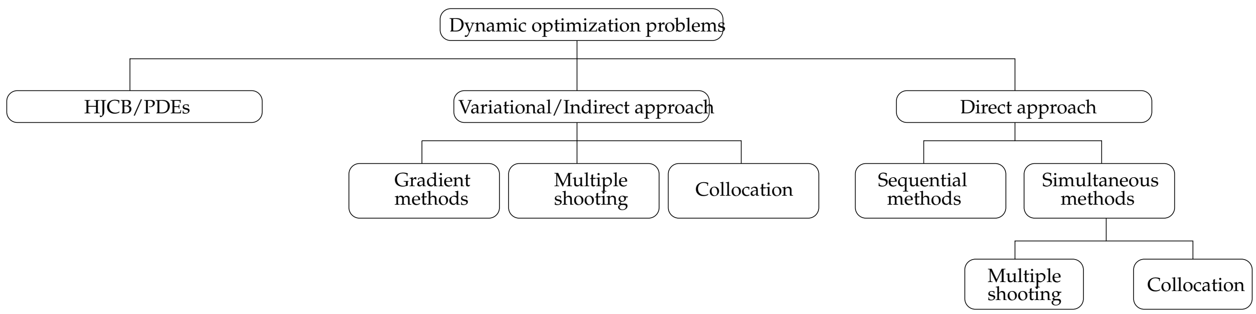

Figure 6.1: Classification of dynamic optimization solution methods

6.3 Methods for dynamic optimization

Chemical processes are modeled dynamically using differential and algebraic equations (DAEs). Dynamic equations such as mass and energy balances make up the differential equations, and physical and thermodynamic relations contribute to the algebraic part of the process model. In Model predictive control, a dynamic regulation problem is formulated in which these DAEs are used to predict the system behavior in the future. Methods to solve these dynamic optimization problems are classified into different approaches based on how the DAE's are handled (Figure 6.1).

6.3.1 Hamiltonian-Jacobi-Caratheodory-Bellman (HJCB) approach

In the Hamiltonian-Jacobi-Caratheodory-Bellman (HJCB) approach, the optimal control is obtained by solving a PDE for a value function (Pesch and Bulirsch, 1994). Solution of PDE's have two major drawbacks. Firstly, the numerical solution is possible for very small state dimensions. Secondly, the inequality constraints on the state variables as well as dynamical systems with switching points, lead to discontinuous partial derivatives and cannot be easily included. Discretization methods to compute numerical approximations of the value function by solving the first order PDE with dynamic programming has been discussed in detail by Bardi and Dolcetta (1997); Falcone and Ferretti (1994); Lions (1982). The application of this methodology is restricted to the case of continuous state systems with a maximum of three state dimensions(Binder, Blank, Bock, Bulirsch, Dahmen, Diehl, Kronseder, Marquardt, and Schloder).

6.3.2 Variational/Indirect approach

The indirect or variational approach is a common approach to optimal control problems. This approach involves defining the Hamiltonian for the problem as a function of the cost, the constraints and *adjoint variables*. The necessary conditions for optimality of solution trajectories can then be written as a boundary value problem in the states and adjoints. Early developments of the Maximum principle have been carried out by Pontryagin, Boltyanskii, Gamkrelidze, and Mishchenko (1962); Isaacs (1965). The approach has been extended to handle general constraints on the control and state variables (Hartl, Sethi, and Vickson, 1995). For problems without inequality constraints, the optimality conditions can be formulated as a set of differential algebraic equations. Often the state variables have specified initial conditions and the adjoint variables have final conditions. The resulting two-point boundary value problem (TPBVP) can be addressed with different approaches, including single shooting, invariant embedding, multiple shooting or some discretization method such as collocation on finite elements or finite differences.

A review of these approaches can be found in Cervantes and Biegler (2001).If the problem requires the handling of active inequality constraints, finding the correct switching structure as well as suitable initial guesses for state and adjoint variables is often very difficult.

6.3.3 Direct approach

In this chapter, we discuss the *Discretize then Optimize*, or the direct NLP approaches. In these approaches, the system is first discretized to form a nonlinear algebraic problem, which is then solved using an NLP algorithm. Hence we form finite dimentional problems that can use the machinery of NLP solvers. As seen in Figure 6.1, the direct NLP approaches can be separated into two groups: *Sequential* and *Simultaneous* strategies, based on which variables are discretized. Sequential strategy is discussed in Section 6.4. *Multiple shooting* serves as a hybrid between sequential and simultaneous approaches. Here the time domain is partitioned into smaller time elements and the DAE models are integrated separately in each element (Bock and Plitt, 1984; Leineweber, 1999). Control variables are parametrized in the same way as in sequential approach and gradient information is obtained for both control variables as well as initial conditions of the state variables in each element. The inequality constraints for state and control variables are imposed directly at the boundary points. The other simultaneous approach: orthogonal collocation is discussed in Section 6.5.

	Discretization scheme in the interval $t \in [t(k), t(k+1))$	Discretization control parameters
Piecewise constant	$u(t) = u(k)$	$u(k)$, $k \in \mathbb{I}_{0:N}$
Piecewise linear	$u(t) = u(k) + \left(\frac{u(k+1)-u(k)}{\Delta t}\right)(t - t(k))$	$u(k)$, $k \in \mathbb{I}_{0:N}$
Polynomial approximation	$u(t) = \sum_{q=1}^{n} \psi_q \left(\frac{t-t(k)}{\Delta t}\right) u_q(k)$ [1]	$u_q(k)$, $k \in \mathbb{I}_{0:N}, q \in \mathbb{I}_{0:n}$

Table 6.1: Discretization schemes for the control variables

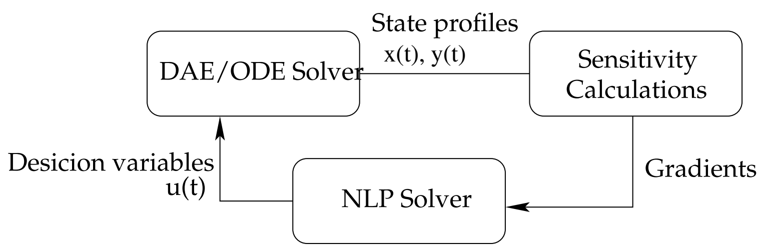

Figure 6.2: Sequential dynamic optimization strategy

6.4 Sequential methods

Also known as the control parametrization method, the sequential approach involves discretization of only the control variables. The time horizon is divided into N time stages, which is essentially the control horizon in the discrete time formulation. Different discretization schemes to parametrize the control variables are summarized in Table 6.1.

[1] $u_q(k)$ represents the value of the control variable in stage k the collocation point q. ψ_q is a Langrange polynomial of order n satisfying $\psi_q(\rho_r) = \delta_{q,r}$

Figure 6.2 provides a sketch of the sequential dynamic optimization strategy. Consider the formulation (6.1). The input profile $u(t)$, $t \geq 0$ is approximated in terms of the discretization control parameters $\mathbf{u} = \{u(k)\}$, $k \in \mathbb{I}_{0:N-1}$ according to the type of parametrization chosen (Table 6.1). Hence the optimization problem can be written in terms of the optimization variable vector $\mathbf{u}$ as

$$\min_{\mathbf{u}} \sum_{k=0}^{N-1} \ell(y(k), u(k)) + V_f(y(N)) \tag{6.2a}$$

$$\frac{dx_d}{dt} = f(x_d(t), x_a(t), \mathbf{u}) \tag{6.2b}$$

$$0 = g(x_d(t), x_a(t), \mathbf{u}), \qquad t \in (t(k-1) - t(k)], \quad k \in \mathbb{I}_{1:N} \tag{6.2c}$$

$$y(k) = h(x_d(k), x_a(k), u(k)) \tag{6.2d}$$

$$g_l \leq G(y(k), u(k)) \leq g_u \tag{6.2e}$$

A NLP solver is used to solve this optimization problem. At a given iteration of the optimization cycle, the decision variables are provided by the NLP solver. With these decision variables, the DAE/ODE system is integrated forward in time until the terminal time to compute the state profiles that determine the objective and constraint functions. Then the gradients of the objective and constraints are evaluated through solution of DAE sensitivity equations. The function and gradient information is then passed back to the NLP solver so that it can update the decision variables. The cycle continues until the NLP solver converges. Since the optimization problems in question are nonlinear and nonconvex in nature, the performance of the NLP solver depends heavily on the gradient and Hessian information. Most NLP solvers have inbuilt algorithms to compute first and second order derivatives using finite differences, but as we shall see in the next section, finite difference method is error prone and does not perform well. Hence sensitivity calculations are usually employed for the purpose, which we shall discuss in the following section.

It is also well known that sequential approaches cannot handle open loop instability (Ascher and Petzold, 1998; Flores-Tlacuahuac, Biegler, and Saldvar-Guerra, 2005). Otherwise, finding a feasible solution for a given set of control parameters may be difficult. Cervantes and Biegler (2001); Vassiliadis (1993) review these methods in detail.

6.4.1 Sensitivity strategies for gradient calculation

The most important component of the sequential approach, apart from the NLP algorithm, is the gradient calculation for the NLP solver. There are three approaches for gradient calculations

1. Perturbation
2. Forward sensitivity calculation
3. Adjoint sensitivity calculation

Gradients by perturbation

Perturbation is the easiest way to compute the gradients. Consider a standard NLP of the form

$$\min_{\mathbf{z}} f(p, \mathbf{z}) \qquad \text{s.t. } c(p, \mathbf{z}) = 0 \quad \mathbf{z}_l \le \mathbf{z} \le \mathbf{z}_u \tag{6.3}$$

where p is the parameter, which in our case would be the initial state, and $\mathbf{z}$ is the optimization variable vector. The derivatives of the objective $f(\cdot)$ and the constraints $c(\cdot)$, need to be computed implicitly from the DAE model, often in tandem with the DAE solution. To compute the gradients with respect to the decision vector $\mathbf{z}$, we apply forward difference perturbation to the vector $\mathbf{z}$

$$\mathbf{z}_i = \mathbf{z} + \delta e_i, \quad i \in \mathbb{I}_{1:n_z}$$

where the ith element of vector e_i is 1 and the other elements are zero, and δ is a small perturbation size. the approximate gradients are

$$\frac{1}{\delta}\left(f(p, \mathbf{z}_i) - f(p, \mathbf{z})\right) = \nabla_{\mathbf{z}_i} f(p, \mathbf{z}) + \mathcal{O}(\delta) + \mathcal{O}(\delta^{-1})$$
$$\frac{1}{\delta}\left(c(p, \mathbf{z}_i) - c(p, \mathbf{z})\right) = \nabla_{\mathbf{z}_i} c(p, \mathbf{z}) + \mathcal{O}(\delta) + \mathcal{O}(\delta^{-1})$$

It is well known that gradients evaluated by perturbation are often plagued by truncation errors and roundoff errors. Truncation errors result from neglect of higher order Taylor series terms that vanish as $\delta \to 0$. On the other hand, roundoff errors that result from internal calculation loops (i.e. convergence noise from the DAE solver) are independent of δ and lead to large gradient errors as $\delta \to 0$. While δ can be selected carefully and roundoff errors can be controlled, the gradient error cannot be eliminated completely. Biegler (2010, Ch. 7) show that this can lead to inefficient and unreliable performance by the NLP solver.

Forward sensitivity calculation

Consider the DAE system defined by (6.2a) and (6.2b). Assuming the functions $f(\cdot)$ and $g(\cdot)$ are sufficiently smooth in all of their arguments, we differentiate the system with respect to the decision variable $\mathbf{u}$ using chain rule as following

$$\frac{d}{d\mathbf{u}}\begin{cases} \frac{dx_d}{dt} = f(x_d(t), x_a(t), u(t)), \quad x_d(0) = x_0 \\ g(x_d(t), x_a(t), u(t)) = 0 \end{cases}$$

Defining sensitivity matrices $S(t) = \frac{dx_d}{d\mathbf{u}}^T$ and $R(t) = \frac{dx_a}{d\mathbf{u}}^T$, we obtain the following sensitivity equations

$$\begin{aligned} \frac{dS}{dt} &= \frac{\partial f}{\partial x_d}^T S(t) + \frac{\partial f}{\partial x_a}^T R(t) + \frac{\partial f}{\partial \mathbf{u}}^T, \qquad S(0) = \frac{\partial x_0}{\partial \mathbf{u}} \\ 0 &= \frac{\partial g}{\partial x_d}^T S(t) + \frac{\partial g}{\partial x_a}^T R(t) + \frac{\partial g}{\partial \mathbf{u}} \end{aligned}$$

For n states and N decision variables, we have $n \times N$ sensitivity equations. These sensitivity equations are index-1 DAE's. To avoid the need to store the state profiles, the sensitivity equations are usually solved simultaneously with the state equations. Once the sensitivities are determined, we compute the gradients for the objective and constraint functions as following

$$\nabla_{\mathbf{u}} f = S(t_f)\frac{\partial f}{\partial x} + \frac{\partial f}{\partial \mathbf{u}}$$

Hence we can compute the gradients by solving a larger augmented system of DAE's and these estimated gradients are passed to the NLP solver to compute its next iteration.

6.4.2 Adjoint sensitivity calculation

The Adjoint method is rooted in calculus of variations and the Euler-Lagrange approach to optimal control (Bryson and Ho, 1975; Bryson Jr, 1996; Bryson, 1999). However, the adjoint approach to sensitivity analysis has recently had a renaissance as dynamic optimization problems of large size and with a large number of parameters appear in engineering applications. Petzold, Li, Cao, and Serban (2006) provide an overview of sensitivity analysis in differential algebraic systems by the adjoint approach. Cao, Li, Petzold, and Serban (2003) analyze the numerical stability properties of the adjoint system. They show that the stability of the adjoint system is identical to the stability of the original system for systems of ordinary differential equations as well as for semi- explicit index-1 differential algebraic equations. For general index-0 and index-1 DAE systems, they define an augmented adjoint system that is stable if the original DAE system is stable.

As we observed, forward sensitivity setup requires integration of $n+(n\times N)$ DAE's equation. This number grows if the number of optimization variables and/or the number of states become large and hence the method becomes inefficient. A complementary approach can be derived based on variational approach. In this approach to derive the sensitivities, we consider the sensitivity of the objective and constraint functions separately. Denote Ψ as an element of $\Psi(\mathbf{u})$, which represents either the objective or constraint function at the end of the sample time ($t = t_s$).

Consider the DAE system defined by (6.1b) and (6.1c). We define adjoint variables as follows

$$\begin{aligned}\Psi(x_d(t), x_a(t), \mathbf{u}) = \Psi(x_d(t_s), x_a(t_s), \mathbf{u}) + \\ \int_0^{t_s} \left[\lambda_d(t)' \left(f(x_d(t), x_a(t), \mathbf{u}) - \frac{dx_d}{dt}(t) \right) + \lambda_a(t)' g(x_d(t), x_a(t), \mathbf{u}) \right] dt \end{aligned} \tag{6.4}$$

where $\lambda_d(t)$ and $\lambda_a(t)$ are the differential and algebraic *adjoint variables* respectively. They can also be seen as the Langrange multipliers of 6.1b and 6.1c, i.e the constraints due the system dynamics, in the optimization problem (6.1). Integrating (6.4) we get

$$\begin{aligned}\Psi(x_d(t), x_a(t), \mathbf{u}) = \Psi(x_d(t_s), x_a(t_s), \mathbf{u}) - x_d(t_s)'\lambda_d(t_s) + x_d(0)'\lambda_d(0) + \\ \int_0^{t_s} \left[\lambda_d(t)' f((x_d(t), x_a(t), \mathbf{u}) + x_d(t)' \frac{d\lambda_d}{dt}(t) + \lambda_a(t)' g(x_d(t), x_a(t), \mathbf{u}) \right] dt\end{aligned}$$

Applying perturbations to this equation we get

$$\begin{aligned}d\Psi = \left[\frac{\partial \Psi}{\partial x_d} - \lambda_d(t_s)\right]' \delta x_d(t_s) + \lambda_d(0)'\delta x_d(0) + \frac{\partial \Psi'}{\partial \mathbf{u}} d\mathbf{u} + \\ \int_0^{t_s} \left[\frac{\partial f}{\partial x_d}\lambda_d - \frac{d\lambda_d}{dt} + \frac{\partial g}{\partial \lambda_a}\right]' \delta x_d(t) + \left[\frac{\partial f}{\partial x_a}\lambda_d + \frac{\partial g}{\partial x_a}\lambda_a\right]' \delta x_a(t) + \\ \left[\frac{\partial f}{\partial \mathbf{u}}\lambda_d + \frac{\partial g}{\partial \mathbf{u}}\lambda_a\right]' d\mathbf{u} dt\end{aligned}$$

We set all the terms which are not influenced by $d\mathbf{u}$ to zero so that only $d\mathbf{u}$ has a direct influence on $d\Psi$. This gives us the following

$$\frac{d\lambda_d}{dt} = -\frac{\partial f}{\partial x_d}\lambda_d - \frac{\partial g}{\partial x_d}\lambda_a \tag{6.5a}$$

$$0 = \frac{\partial f}{\partial x_a}\lambda_d + \frac{\partial g}{\partial x_a}\lambda_a \tag{6.5b}$$

$$\lambda_d(t_s) = \frac{\partial \Psi}{\partial x_d} \tag{6.5c}$$

$$\delta x_d(0) = 0 \tag{6.5d}$$

In the above system, (6.5a) and (6.5b) give us a DAE system in the adjoint variables with a terminal boundary condition (6.5c). (6.5d) comes from the fact that in our problem, the initial state is a fixed parameter. Hence we get

$$\frac{d\Psi}{d\mathbf{u}} = \left[\frac{\partial \Psi}{\partial \mathbf{u}}\right]' + \int_0^{t_s} \left[\frac{\partial f}{\partial \mathbf{u}}\lambda_d + \frac{\partial g}{\partial \mathbf{u}}\lambda_a\right]' dt$$

Hence calculation of adjoint sensitivities requires the solution of a DAE system (6.5) with a terminal condition instead of an initial condition. Once the state and adjoint variables are obtained, the integrals allow direct calculation of the gradients $\nabla_{\mathbf{u}}\Psi$. The adjoint sensitivity approach is more difficult to implement as compared to the forward sensitivity approach since the solution requires storage of state profiles, which are used later for backward integration of the adjoint DAE system. To avoid the storage requirement, especially for large systems, the adjoint approach is usually implemented with a *checkpointing scheme*. At the cost of at most one additional forward integration, this approach offers the best possible estimate of memory requirements for adjoint sensitivity analysis (Hindmarsh, Brown, Grant, Lee, Serban, Shumaker, and Woodward, 2005). Here the state variables are stored at only a few *checkpoints* in time. Starting from the checkpoint closest to t_s, the state profile is reconstructed by integrating forward from the checkpoint and the adjoint variable is calculated by integrating backward up to this checkpoint. Once the adjoint is calculated at this point, we back up to an earlier checkpoint and the state and adjoint calculation is repeated until the beginning of the time horizon. The checkpointing scheme offers a trade-off between repeated adjoint calculation and state variable storage. Moreover, strategies have been developed for the optimal distribution of checkpoints that lead to efficient adjoint sensitivity calculations (Griesse and Walther, 2004).

6.5 Simultaneous approach

In this thesis, we will focus on the simultaneous approach, also known as direct transcription approach. In this technique both the state and control variables are discretized, which leads to a large number of optimization variables. These large scale NLP's require special solution strategies (Betts and Huffman, 1990; Betts and Frank, 1994; Cervantes and Biegler, 1998, 2000; Cervantes, Wachter, Tutuncu, and Biegler, 2000). The simultaneous approach has a number of advantages over other approaches to dynamic optimization.

1. Control variables are discretized at the same level as the state variables. The Karush Kuhn Tucker (KKT) conditions of the simultaneous NLP are consistent with the optimality conditions of the discretized variational problem, and, under mild conditions, convergence rates can be shown (Reddien, 1979; Cuthrell and Biegler, 1989; Hager, 2000; Kameswaran and Biegler, 2006, 2008).

2. As with multiple shooting approaches, simultaneous approaches can deal with instabilities that occur for a range of inputs. Because they can be seen as extensions of robust boundary value solvers, they are able to "pin down" unstable modes (or increasing modes in the forward direction). This characteristic has benefits on problems that include transitions to unstable points, optimization of chaotic systems (Bock and Plitt, 1984) and systems with limit cycles and bifurcations, as illustrated in Flores-Tlacuahuac et al. (2005).

3. Simultaneous methods also allow the direct enforcement of state and control variable constraints, at the same level of discretization as the state variables of the DAE system. As was discussed in Kameswaran and Biegler (2006), these can present some interesting advantages on large-scale problems.

4. Finally, recent work has shown (Kameswaran and Biegler, 2006, 2005) that simultaneous approaches have distinct advantages for singular control problems and problems with high index path constraints.

Nevertheless, simultaneous strategies require the solution of large non-linear programs, and specialized methods are required to solve them efficiently. These NLPs are usually solved using variations of Successive Quadratic Programming (SQP). Both full-space and reduced-space options exist for these methods. Full-space methods take advantage of the sparsity of the DAE optimization problem. They are best suited for problems where the number of discretized control variables is large (Betts and Huffman, 1990). Here, second derivatives of the objective function and constraints are usually required, as are measures to deal with directions of negative curvature in the Hessian matrix (Wachter and Biegler, 2006). Betts (2000) provides a detailed description of the simultaneous approach with full-space methods, along with mesh refinement strategies and case studies in mechanics and aerospace. On the other hand, reduced-space approaches exploit the structure of the DAE model and decompose the linearized KKT system; second derivative information is often approximated here with quasi-Newton formulae. This approach has been very efficient on many problems in process engineering that have few discretized control variables. The NLP algorithm used for our computation is IPOPT. The details of the algorithm are sketched and discussed in Wachter and Biegler (2006); Biegler (2007).

6.5.1 Formulation

The DAE optimization problem (6.1), which has the system dynamics in continuous time, is converted into a discrete time NLP by approximating the state and control profiles by a family of polynomials on finite elements. These polynomials can be represented as power series, sums of orthogonal polynomials or in Lagrange form. Here, we use the following monomial basis representation for the differential profiles, which is popular for Runge-Kutta discretizations:

$$x(t) = x(k-1) + h(k) \sum_{q=1}^{K} \Omega_q \left(\frac{t - t(k)}{h(k)} \right) \frac{dx}{dt}_{k,q} \tag{6.6}$$

Here $x(k-1)$ is the value of the differential variable at the beginning of element k, $h(k)$ the length of element k, $dx/dt_{k,q}$ the value of its first derivative in element k at the collocation point q, and Ω_q is a polynomial of order K, satisfying

$$\Omega_q(0) = 0 \qquad \text{for } q = 1, \cdots, K$$

$$\Omega_q'(\rho_r) = \delta_{q,r} \quad \text{for } q, r = 1, \cdots, K$$

where ρ_r is the location of the r^{th} collocation point within each element. Continuity of the differential profiles is enforced by

$$x(k) = x(k-1) + h(k) \sum_{q=1}^{K} \Omega_q(1) \frac{dx}{dt}_{k,q} \tag{6.7}$$

Based on the recommendation by Biegler (2007), we use Radau collocation points because they allow constraints to be set at the end of each element and to stabilize the system more efficiently if high index DAEs are present. In addition, the control and algebraic profiles are approximated using a Lagrange basis representation which takes the form

$$y(t) = \sum_{q=1}^{K} \Psi_q \left(\frac{t - t(k-1)}{h(k)} \right) y_{k,q} \tag{6.8}$$

$$u(t) = \sum_{q=1}^{K} \Psi_q \left(\frac{t - t(k-1)}{h(k)} \right) u_{k,q} \tag{6.9}$$

Here $y_{k,q}$ and $u_{k,q}$ represent the values of the algebraic and control variables, respectively, in element k at collocation point q. Ψ_q is the Lagrange polynomial of degree K satisfying

$$\Psi_q(\rho_r) = \delta_{q,r}, \quad \text{for } q, r = 1, \cdots, K$$

Note that $u_{k,K} = u(k)$ and $y_{y,K} = y(K)$, i.e. the last collocation point in each finite element lies on the boundary of that element (see Figure 6.3). Substituting (6.6)-(6.9) into

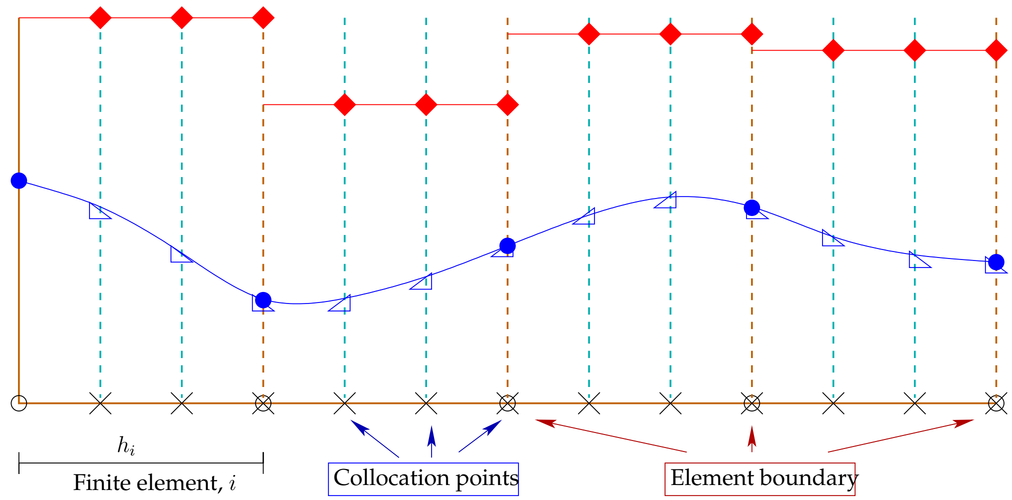

Figure 6.3: Sequential dynamic optimization strategy

(6.1b)-(6.1e) gives the following NLP

$$\min_{(dx/dt_{k,q}, u_{k,q}, y_{k,q}, z_{k,q})} \sum_{k=0}^{N-1} \ell(y(k), u(k)) + V_f(y(N)) \tag{6.10a}$$

$$\frac{dx}{dt}_{k,q} = f(x_{k,q}, u_{k,q}) \tag{6.10b}$$

$$x_{k,q} = x(k-1) + h(k) \sum_{q=1}^{K} \Omega_{q'}(\rho_q) \frac{dx}{dt}_{k,q} \tag{6.10c}$$

$$x(k) = x(k-1) + h(k) \sum_{q=1}^{K} \Omega_q(1) \frac{dx}{dt}_{k,q} \tag{6.10d}$$

$$0 = g(x_{k,q}, u_{k,q}) \qquad k = 1, \cdots, N \quad q = 1, \cdots, K \tag{6.10e}$$

$$y_{k,q} = h(x_{k,q}, u_{k,q}) \qquad k = 1, \cdots, N \quad q = 1, \cdots, K \tag{6.10f}$$

$$g_l \leq G(y_{k,q}, u_{k,q}) \leq g_u \qquad k = 1, \cdots, N \quad q = 1, \cdots, K \tag{6.10g}$$

This is a standard NLP of the form

$$\min_z f(z) \qquad \text{s.t. } c(z) = 0 \quad z_l \leq z \leq z_u$$

where $z = (dx/dt_{k,q}, u_{k,q}, y_{k,q}, z_{k,q})$, and is solved using a nonlinear solver. Hence the differential variables are required to be continuous throughout the time horizon, while the control and algebraic variables are allowed to have discontinuities at the boundaries of the elements. As seen from Figure 6.3. Bounds are imposed directly on the differential variables at element boundaries. These can also be enforced at all collocation points by writing additional point constraints. We use IPOPT as the nonlinear solver for our simulations.

6.6 Software tools

In this section, we describe the structure of the software tool: NLMPC, that was developed during this thesis. Of the two direct NLP approaches described above, the direct collocation approach formulated in Section 6.5 has been most efficient in solving our nonlinear nonconvex dynamic regulation problems. The two most important ingredients of the direct NLP strategy are

1. NLP solver
2. Derivative calculator

As mentioned above we use IPOPT (Wachter and Biegler, 2006) as the NLP solver for our simulations. IPOPT is a primal-dual interior-point algorithm with a filter line-search method tailored specifically for large scale problems, and takes advantage of sparse

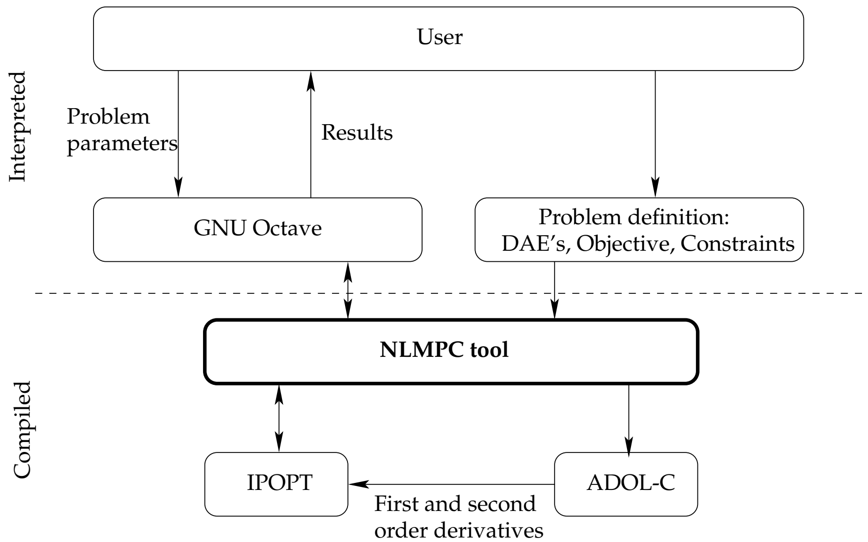

Figure 6.4: Structure of NLMPC tool

matrix memory management capabilities to efficiently implement the NLP solution algorithm. The solver is written in C++.

In the direct collocation approach, the system of DAE's is converted into a system of explicit nonlinear algebraic equations. Hence we can use direct differentiation to compute the first and second order derivatives instead of sensitivity calculations, which are prone to integration and round-off errors as described in Section 6.4.1. We use ADOL-C (Wagner, Walther, and Schaefer, 2010; Walther, 2008), which is an open-source package for the automatic differentiation of C and C++ programs, for computing first and second order derivative information of the NLP resulting from the collocation formulation (6.10).

Both NLP solver and derivative calculator being in C++, enables us to write an interface between IPOPT and ADOL-C in C++. We call this interface, the NLMPC tool. This tool has two plugs for interaction with the user (Figure 6.4). The first one reads the problem information i.e., the DAE's, the objective function and the constraints for the dynamic regulation problem from a C++ file provided by the user. The second one is an interface with GNU Octave, that allows the user to pass problem parameters and read back the results of the optimization problem in a high-level interpreted language for further analysis.

The interface does the following operations:

1. Formulates the corresponding NLP according to the scheme derived in Section 6.5.1
2. Calls ADOL-C to compute the first and second order derivatives of the objective and the constraints
3. Passes the NLP and the derivative information to IPOPT to optimize
4. Returns the optimal solution back to the user through the Oct interface with GNU Octave.

The derivative information is very crucial to the performance of IPOPT's NLP algorithm and hence providing the problem definition, i.e. the DAE's, objective and the constraints, as a C++ code allows us to use automatic differentiation via ADOL-C, which gives us exact derivatives, and greatly improves the performance of IPOPT. Once the problem definition has been provided, the NLMPC tool compiles the source along with the problem definition to transform the toolbox's algorithm, coupled with IPOPT and ADOL-C, into compiled code for faster execution. GNU Octave's OCT interface allows the toolbox to interact with this compiled code directly. It allows the user to easily pass problem parameters and read the results for further analysis, without having to recompile the code, and hence enables the use of the tool for simulation studies with great ease. Appendix B provides a brief user manual of the NLMPC tool.

Chapter 7

Case studies

7.1 Introduction

The motivation behind extending the MPC framework to handle generic nonlinear non-convex economic objectives is to gain economic benefit during the transient operation of the processes controlled using MPC. We developed economic MPC algorithms for both stable and unstable operation, and the corresponding theory, in the proceeding chapters. In this chapter we present some case studies to demonstrate the application of the economic dynamic regulation and show the benefits of optimizing process economics directly in the dynamic regulation problem. To gauge the benefit of using economics based MPC over the standard tracking MPC, we define the following performance measure

$$G = \frac{P_{T,\text{eco}} - P_{T,\text{track}}}{T P_s} \times 100\%$$

where $P_{T,\text{eco}}$ and $P_{T,\text{track}}$ are the cumulative profits over T time steps, of the closed loop systems under the economics and tracking MPC respectively, and P_s is the steady state profit.

7.2 Evaporation process

We first consider an evaporation process that removes a volatile liquid from a nonvolatile solute, thus concentrating the solution. It consists of a heat exchange vessel with a recirculating pump. The overhead vapor is condensed by the use of a process heat exchanger. The details of the mathematical model can be found in Newell and Lee (1989, Ch. 2). We use the following modified process model

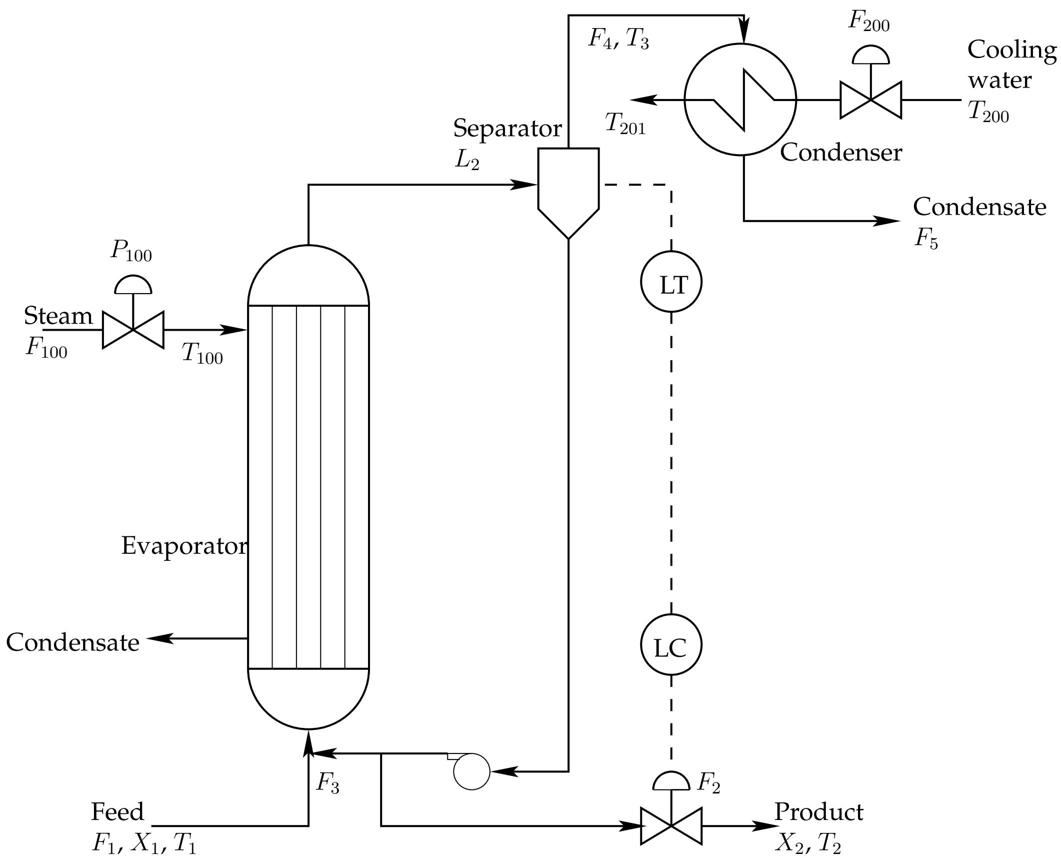

Figure 7.1: Evaporator system

Differential equations:

$$M\frac{dX_2}{dt} = F_1X_1 - F_2X_2$$
$$C\frac{dP_2}{dt} = F_4 - F_5$$

Process liquid energy balance

$$T_2 = 0.5616P_2 + 0.3126X_2 + 48.43$$

$$T_3 = 0.507P_2 + 55$$

$$F_4 = (Q_{100} - F_1C_p(T_2 - T_1))/\lambda$$

Heat steam jacket

$$T_{100} = 0.1538P_{100} + 90$$

$$Q_{100} = UA_1(T_{100} - T_2)$$

$$UA_1 = 0.16(F_1 + F_3)$$

$$F_{100} = Q_{100}/\lambda_s$$

Condenser

$$Q_{200} = \frac{UA_2(T_3 - T_{200})}{1 + UA_2/(2C_pF_{200})}$$

$$F_5 = Q_{200}/\lambda$$

Level controller

$$F_2 = F_1 - F_4$$

In the above equations, $M = 20$ kg/m is the liquid holdup in the evaporator, $C = 4$ kg/kPa is a constant, UA_1 and $UA_2 = 6.84$ kW/K are the products of the heat transfer coefficients and the heat transfer area in the evaporator and condenser respectively, $C_p = 0.07$ kW/kg·min is the heat capacity of water, $\lambda = 38.5$ kW/kg·min is the latent heat of evaporation of water and $\lambda_s = 36.6$ kW/kg·min is the latent heat of steam at saturated conditions.

The economic objective of the evaporator process is to minimize the following operating cost (in 10^{-3} \$/h), which consists of the cost of electricity, steam and cooling water (Wang and Cameron, 1994; Govatsmark and Skogestad, 2001).

$$J = 1.009(F_2 + F_3) + 600F_{100} + 0.6F_{200}$$

The product composition X_2 and the operating pressure P_2 are the state variables as well as the available measurements, and the steam pressure P_{100} and the cooling water flow rate F_{200} are the manipulated variables. The following variables are the source of disturbances in the system. The following bounds are imposed.

$$X_2 \geq 25\% \qquad 40 \text{ kPa} \leq P_2 \leq 80 \text{ kPa}$$

$$P_{100} \leq 400 \text{ kPa} \qquad F_{200} \leq 400 \text{ kg/min}$$

At the best steady state under nominal conditions, the input and output variables have

Variable	Description	Value
F_1	Feed flow rate	10 kg/min
C_1	Feed composition	5 $\%$
F_3	Circulating flowrate	50 kg/min
T_1	Feed temperature	40 C
T_{200}	Cooling water inlet temperature	25 C

Table 7.1: Disturbance variables in the evaporator system and their nominal values

the following values

$$X_2 = 25 \qquad P_2 = 50.57 \qquad P_{100} = 193.45 \qquad F_{200} = 207.33$$

We set up the dynamic MPC problems with a sample time of $\Delta = 1$ min and a control horizon of $N = 200$. The economic MPC problem is set up with the operating cost as the stage cost and the tracking problem uses $\ell = |x - x_s|_Q + |u - u_s|_R$, where Q =diag$(0.92, 0.3)$ and R =diag$(1, 1)$, as the stage cost. Both controllers are implemented with a terminal state constraint.

We first subject the system to a disturbance in the operating pressure P_2. A periodic drop in the pressure was injected into the system and the performance of the two controllers was compared. Figure 7.2 shows the input and state profiles as well as the corresponding instantaneous operating costs of the two closed loop systems. A pressure drop of 8 kPa was injected with a repetition period of 20 mins. A drop in the operating pressure decreases the instantaneous operating cost and hence the system under economic MPC tends to stay at a lower pressure as compared to the tracking MPC during its transient back to the optimal steady state. The corrective control action resulting from this disturbance also increases the product composition, which in turn, increases the operating cost. Hence the economic MPC drives the system back to the steady state composition faster than tracking MPC. The benefit obtained from economic MPC as compared to the tracking controller is $G = 6.15\%$ of the steady state operating cost.

Next we subject the system to a measured disturbance in the feed flow rate (F_1), the feed temperature (T_1) and the coolant water inlet temperature (T_{100}). Figure 7.3 shows the input and state profiles as well as the corresponding instantaneous operating costs of the two closed loop systems. An increase in the feed flow rate drops the product concentration. To counter this disturbance both controllers raise the steam pressure and the cooling water flow rate raising the the product concentration and the operating pressure, increasing the operating cost. The economic controller keeps the system at a lower concentration and pressure as compared to the tracking controller. In order to drop the instantaneous operating cost, the economic controller drops the inlet water flow rate when there is a disturbance in the cooling water inlet temperature causing it to rise. The economic controller drops the water flow more than the tracking controller making higher instantaneous profit. In this scenario the benefit obtained from economic MPC as compared to the tracking controller is $G = 2.2\%$ of the steady state operating cost.

Table 7.2 shows the average operating cost of the evaporator process under the two controllers in the two disturbance scenarios discussed above. The economic MPC's bene-

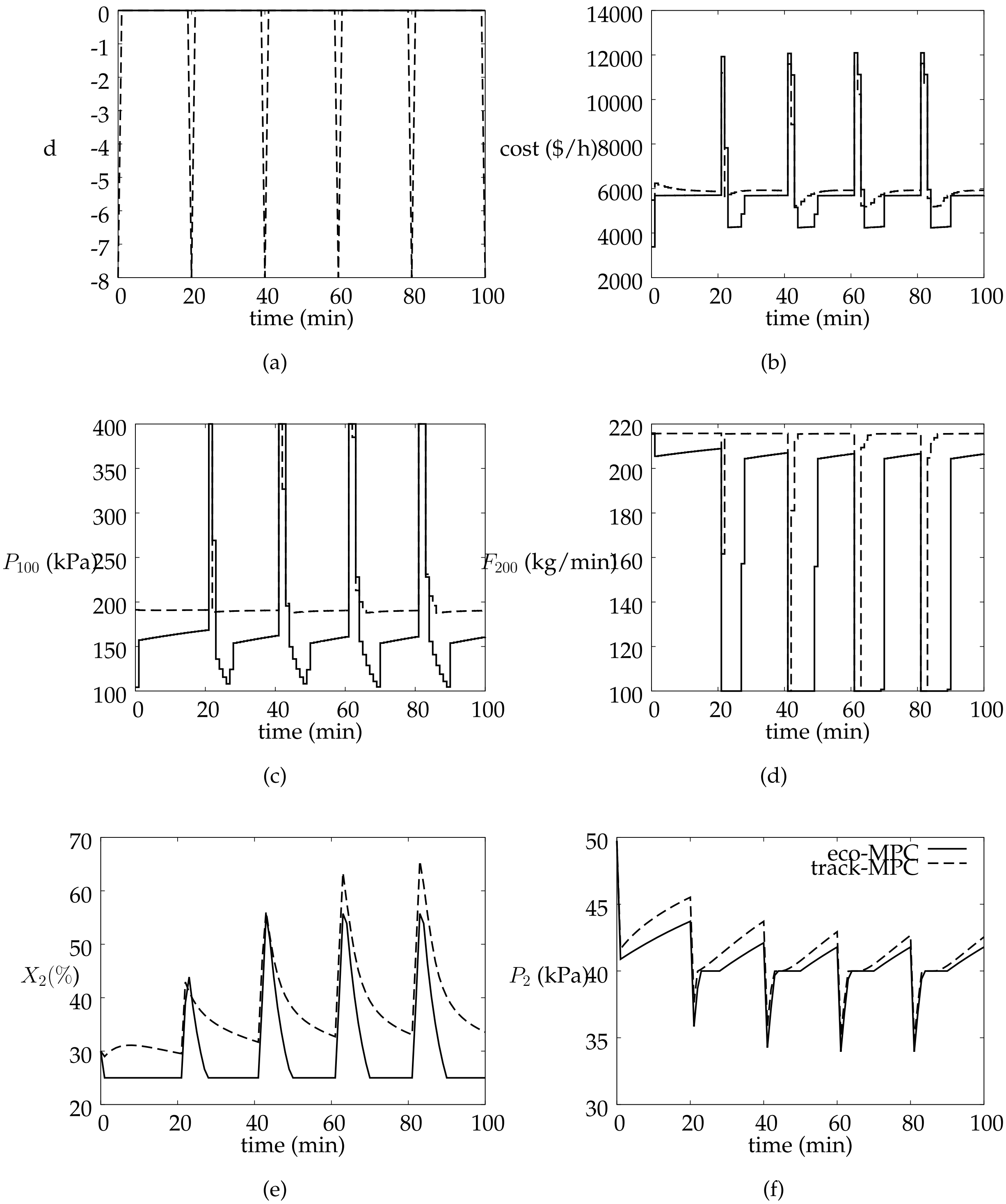

Figure 7.2: Closed-loop input (c),(d) and state (e),(f) profiles, and the instantaneous profit (b) of the evaporator process under unmeasured disturbance (a) in the operating pressure.

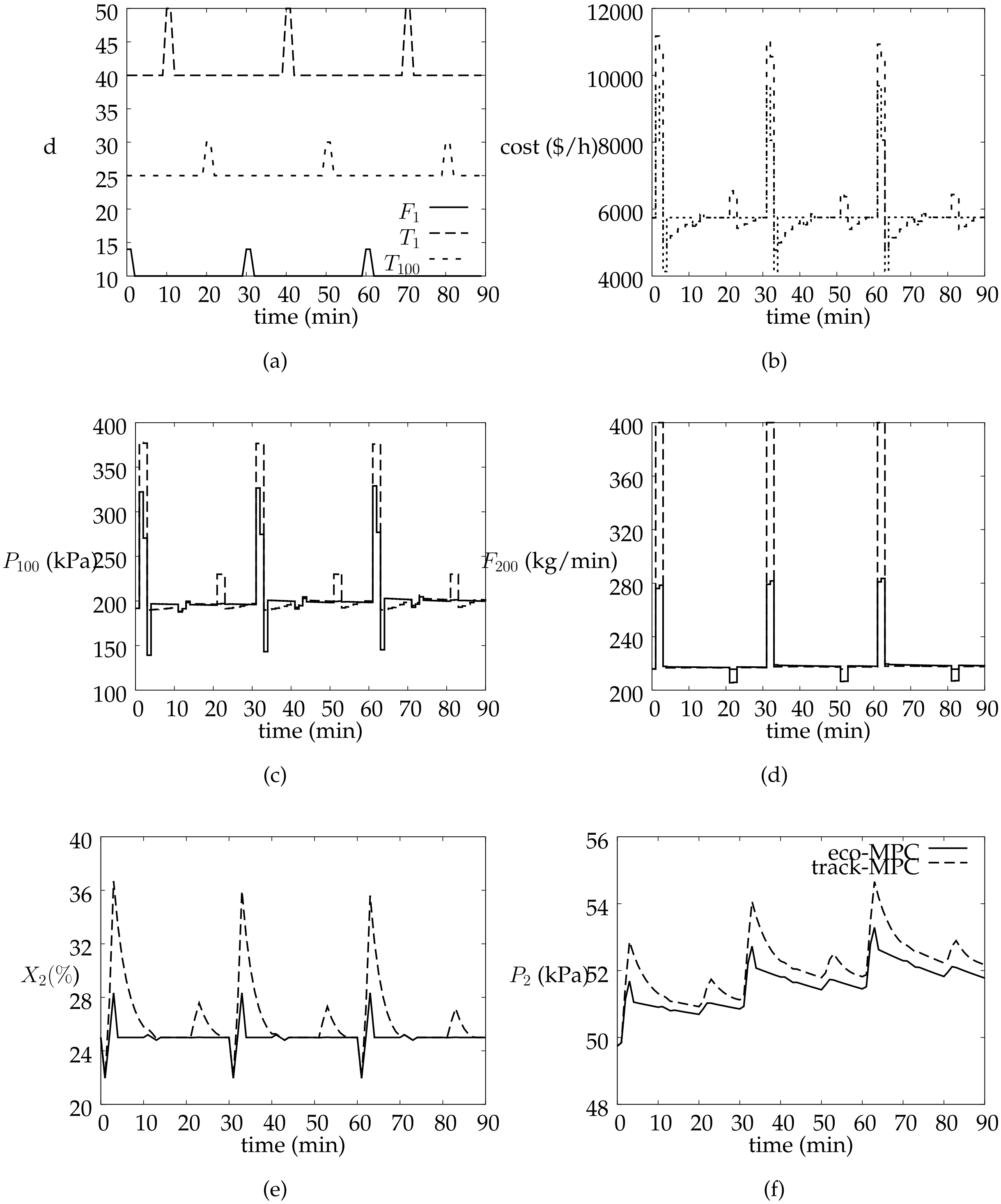

Figure 7.3: Closed-loop input (c),(d) and state (e),(f) profiles, and the instantaneous profit (b) of the evaporator process under measured disturbances (a)

fit is seen to be 6.15% of the nominal steady state profit under unmeasured disturbances.

Disturbance	Avg. operating cost (eco-MPC)	Avg. operating cost (track-MPC)	G
Measured	5894.3	5965.5	2.2 $\%$
Unmeasured	5804.1	6154.8	6.15 $\%$

Table 7.2: Performance comparison of the evaporator process under economic and tracking MPC

7.3 Williams-Otto reactor

The Williams-Otto reactor is one unit of the Williams-Otto plant model (Williams and Otto, 1960). The reactor is a CSTR with mass holdup 2104.7 kg and temperature T_R. The reactor is fed with two pure component reactant streams F_A and F_B. The following three simultaneous reactions involving 6 components occur inside the reactor.

$$\mathrm{A} + \mathrm{B} \longrightarrow \mathrm{C} \qquad \mathrm{k_1} = 1.6599 \times 10^6 \mathrm{e}^{\frac{-6666.7}{\mathrm{T_R}}} \mathrm{s}^{-1}$$

$$\mathrm{B} + \mathrm{C} \longrightarrow \mathrm{P} + \mathrm{E} \qquad \mathrm{k_2} = 7.2117 \times 10^8 \mathrm{e}^{\frac{-8333.3}{\mathrm{T_R}}} \mathrm{s}^{-1}$$

$$\mathrm{C} + \mathrm{P} \longrightarrow \mathrm{G} \qquad \mathrm{k_3} = 2.6745 \times 10^{12} \mathrm{e}^{\frac{-11111}{\mathrm{T_R}}} \mathrm{s}^{-1}$$

the following dynamic mass balances represent the plant behavior

$$W\frac{dX_A}{dt} = F_A - (F_A + F_B)X_A - r_1$$
$$W\frac{dX_B}{dt} = F_B - (F_A + F_B)X_B - r_1 - r_2$$
$$W\frac{dX_C}{dt} = -(F_A + F_B)X_C + 2r_1 - 2r_2 - r_3$$
$$W\frac{dX_E}{dt} = -(F_A + F_B)X_E + r_2$$
$$W\frac{dX_G}{dt} = -(F_A + F_B)X_G + 1.5r_3$$
$$W\frac{dX_P}{dt} = -(F_A + F_B)X_P + r_2 - 0.5r_3$$

where X_A, X_B, X_C, X_E, X_G and X_P are the mass fractions of the respective components and $r_1 = k_1X_AX_BW$, $r_2 = k_2X_BX_CW$ and $r_1 = k_3X_CX_PW$ are the three reaction rates. The economic objective of the process is to maximize the profit, which is the difference between the sales of the products E and P and the costs of raw materials A and B (Xiong and Jutan, 2003).

$$P = 5554.1(F_A + F_B)X_P + 125.91(F_A + F_B)X_E - 370.3F_A - 555.42F_B$$

The mass fractions of all the components are the state variables as well as the available measurements and the input flow rate of component B (F_B) and the reactor temperature (T_R) are the control variables. The flow rate of component A (F_A) is the source of disturbance with a nominal value 1.8 kg/sec.

We first subject the system to periodic step changes in the feed flow rate of A (F_A). The economic controller tries to extract more profit from the disturbance by raising the product concentrations (X_P and X_E) more than the tracking controller. Figure 7.4 shows

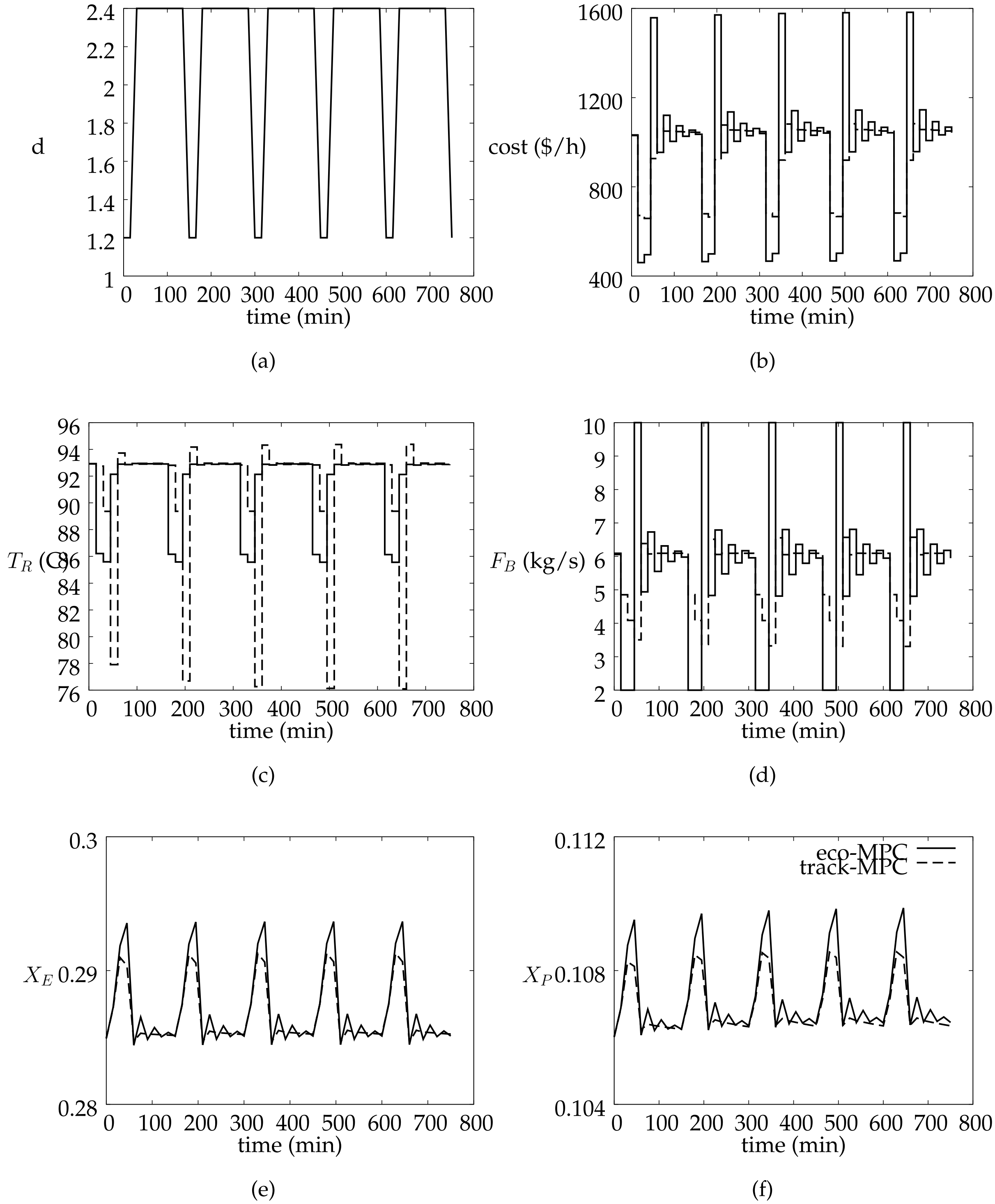

Figure 7.4: Closed-loop input (c),(d) and state (e),(f) profiles, and the instantaneous profit (b) of the Williams-Otto reactor under step disturbance in the feed flow rate of A (a)

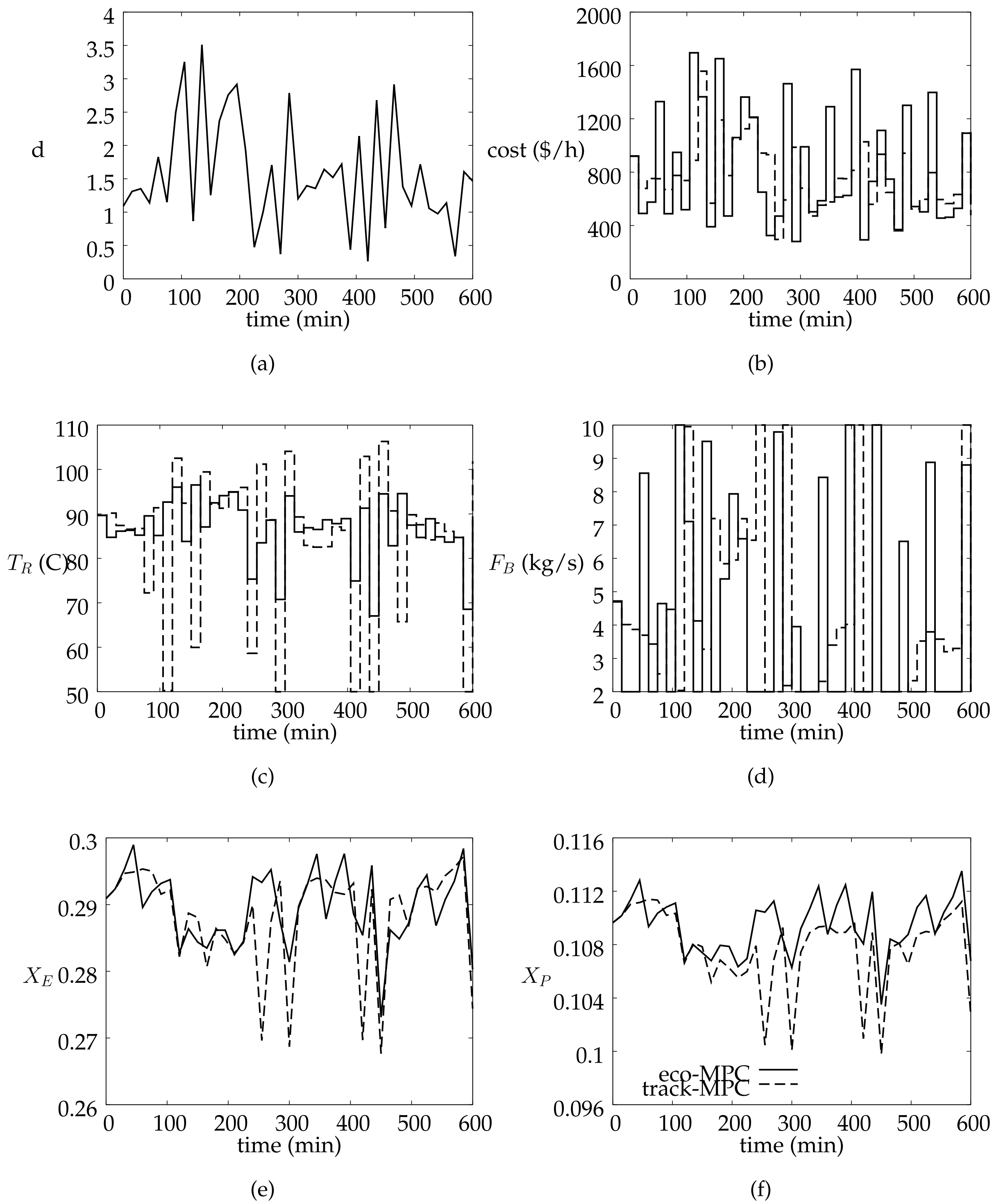

Figure 7.5: Closed-loop input (c),(d) and state (e),(f) profiles, and the instantaneous profit (b) of the Williams-Otto reactor under large random disturbances in the feed flow rate of A (a)

the control moves and the mass fractions of the product P and E of the two closed loop systems.

To simulate more transient behavior, F_A, which is a measured disturbance variable, is disturbed with large variations. Figure 7.5 shows the control moves and the mass fractions of the product P and E of the two closed loop systems.

Table 7.3 shows the average operating cost of the Williams-Otto reactor under the two controllers in the two disturbance scenarios discussed above. The economic MPC's benefit is seen to be 5.8% of the nominal steady state profit under large random measured disturbances.

Disturbance	Avg. Profit (eco-MPC)	Avg. Profit (track-MPC)	G
Step	986.60	966.47	2 $\%$
Random	827.64	622.26	5.8 $\%$

Table 7.3: Performance comparison of the Williams-Otto reactor under economic and tracking MPC

7.4 Consecutive-competitive reactions

We consider next the control of a nonlinear isothermal chemical reactor with consecutive-competitive reactions (Lee and Bailey, 1980). Such networks arise in many chemical and biological applications such as polymerizations, and are characterized by a set of reactions of the following form:

$$
\begin{aligned}
P_{i-1} + B \quad &\rightarrow \quad P_i \\
i \quad &\in \quad \{1, 2, \ldots, R\}.
\end{aligned} \tag{7.1}
$$

Typically a desirable distribution of products in the effluent is a primary objective in the reactor design for these processes. For simplicity we consider the case of two reactions:

$$P_0 + B \longrightarrow P_1$$

$$P_1 + B \longrightarrow P_2$$

The dimensionless mass balances for this problem are:

$$x_1 = u_1 - x_1 - \sigma_1 x_1 x_2$$

$$x_2 = u_2 - x_2 + \sigma_1 x_1 x_2 - \sigma_2 x_2 x_3$$

$$x_3 = -x_3 + \sigma_1 x_1 x_2 - \sigma_2 x_2 x_3$$

$$x_4 = -x_4 + \sigma_2 x_2 x_3$$

where x_1, x_2, x_3 and x_4 are the concentrations of P_0, B, P_1, and P_2 respectively, while u_1 and u_2 are inflow rates of P_0 and B and are the manipulated variables. The parameters σ_1 and σ_2 have values 1 and 0.4 respectively. The time average value of u_1 is constrained to lie between 0 and 1.

$$Av[u_1] \subseteq [0, 1].$$

The primary objective for this system is to maximize the average amount of P_1 in the effluent flow ($\ell(x, u) = -x_3$). Previous analysis has clearly highlighted that periodic operation can outperform steady-state operation (Lee and Bailey, 1980). The steady-state problem has a solution $x_s = \begin{bmatrix} 0.3874 & 1.5811 & 0.3752 & 0.2373 \end{bmatrix}'$ with the optimal input $u_s = \begin{bmatrix} 1 & 2.4310 \end{bmatrix}'$.

We solve the dynamic regulation problem using the simultaneous approach (Flores-Tlacuahuac, Moreno, and Biegler, 2008). The state space is divided into a fixed number of finite elements. The input is parametrized according to zero order hold with the input value constant across a finite element. An additional upper bound of 10 is imposed on $u_1(t)$. A terminal state constraint is used in all the simulations.

The system is first initialized at the steady state to check suboptimality of steady-state operation. A horizon of 100 is chosen with a sample time $T_s = 0.1$. The steady-state solution is used as the initial guess for the nonlinear solver. The solution of the dynamic problem is seen to be unstable (Figure 7.6). The solution returned by the optimizer shows the inputs jumping between the upper and lower bounds. Different initial guesses gave different locations of these jumps suggesting that these solutions are local optima, with a negligible cost difference.

In order to stabilize the system a convex term is added to the objective and the penalties are varied.

$$\ell(x, u) = -x_3 + (1/2)\big(|x - x_s|_Q^2 + |u - u_s|_R^2 \big)$$

Next the R penalty is tuned up to 0.04. The optimal solution now converges to the steady state. The system is initialized at a random initial state, and three different simulations are carried out under the influence of three different controllers: the purely

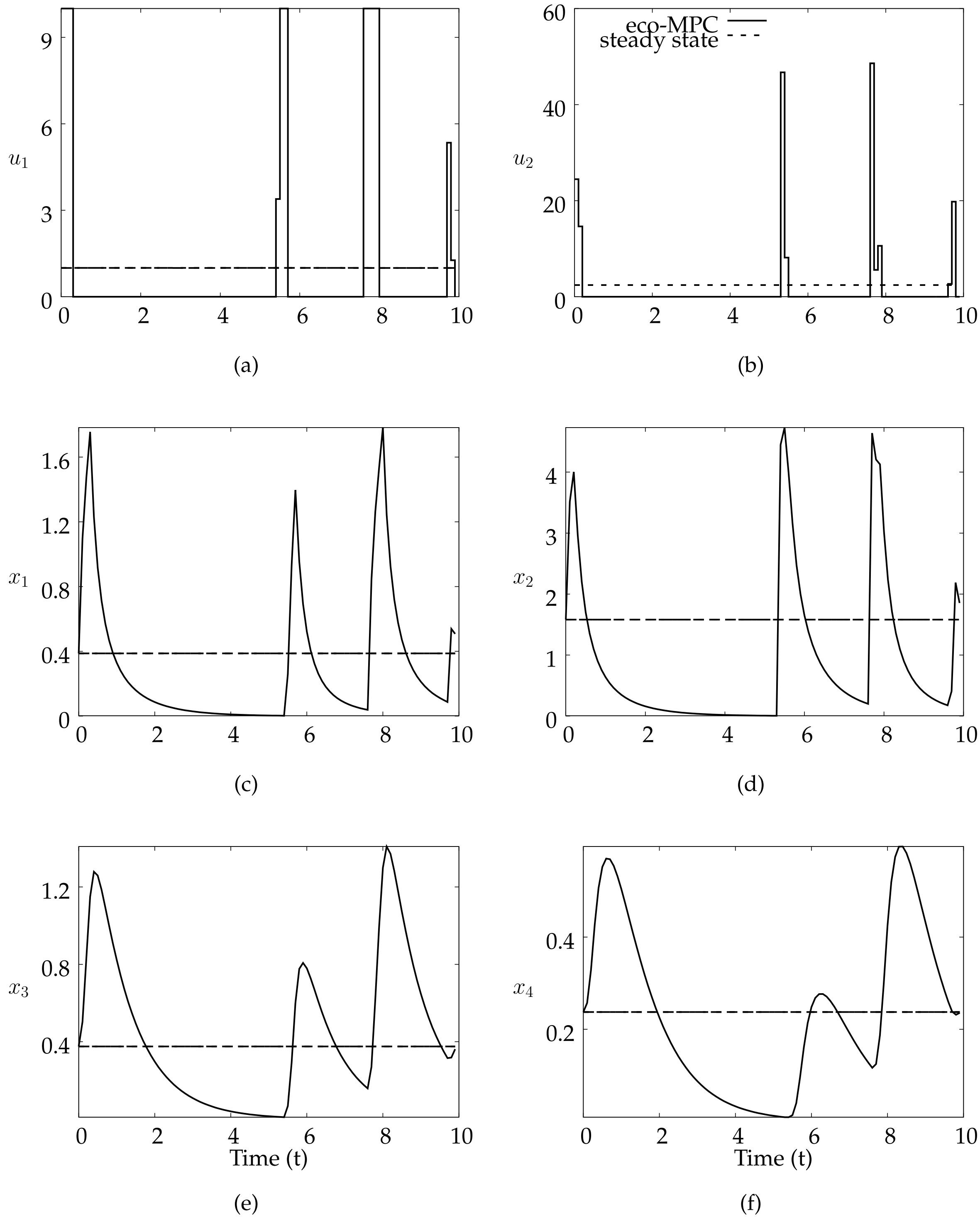

Figure 7.6: Open-loop input (a), (b) and state (c), (d), (e), (f) profiles for system initialized at the steady state

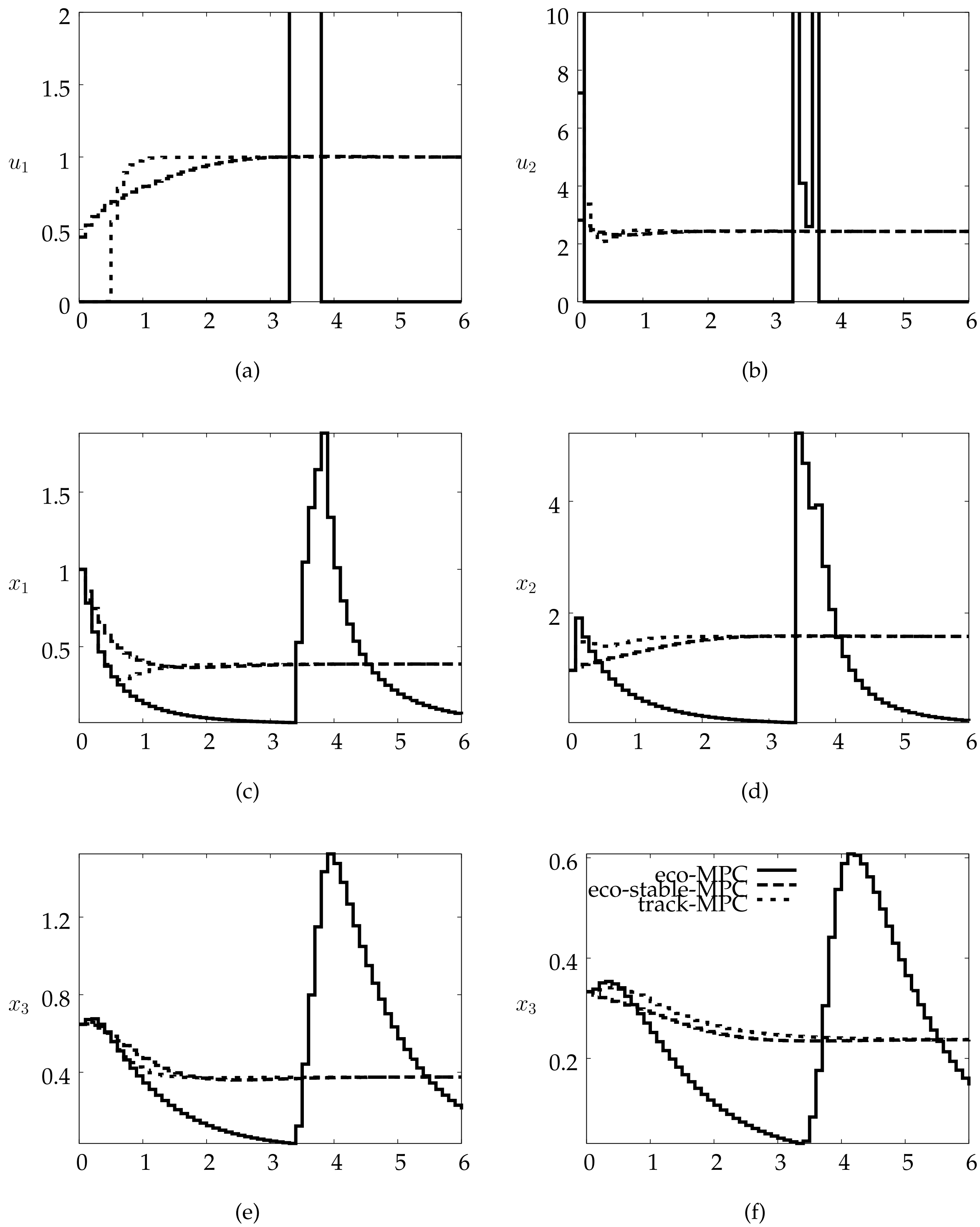

Figure 7.7: Closed-loop input (a), (b) and state (c), (d), (e), (f) profiles for system under the three controllers, initialized at a random state

economic controller, the regularized controller with $R = 0.04$ and a tracking type controller with $Q = 0.36 I_4$ and $R = 0.002 I_2$. The closed loop solutions are compared in Figure 7.7.

Controller	Avg. Profit (eco-MPC)	Avg. profit (track-MPC)	G
Economic	0.44	0.38	15 %
Economic-stable	0.39	0.38	2 %

Table 7.4: Performance comparison of the CSTR with consecutive competitive reactions under economic and tracking MPC

Table 7.4 lists the performance comparison for the two economic controllers presented. It is seen that unsteady operation gains significant profit over steady operation and the purely economic MPC scores 15% of the steady state benefit as compared to the tracking controller. When convergence is forced, this benefit it reduced to 2% of the steady state profit.

Chapter 8

Conclusions and future work

In this chapter we conclude the thesis by highlighting the contributions and suggest future research directions in the topic.

8.1 Contributions

Stability theory for nonlinear MPC: The stability theory for model predictive control was extended to generic nonlinear systems and costs in Chapter 3. For general nonlinear problems, the stability of the closed loop system cannot be always expected. Chapter 3 identifies a class of systems: strictly dissipative systems, for which closed-loop stability is guaranteed. The two standard MPC formulations, namely the terminal constraint and the terminal control/penalty formulations, are extended to the economic MPC framework. Asymptotic stability is established for both the formulations by proposing Lyapunov functions based on a modified cost. A third formulation, which does not have any constraint on the terminal state, is also proposed and asymptotic stability is established.

These results were extended to suboptimal MPC algorithm in Chapter 4, which relaxes the requirement of global optimality of the dynamic optimization problem to maintain asymptotic closed-loop stability. This fits the simulation studies into the developed theoretical framework as numerical NLP solvers do not guarantee global optimality.

Theory and algorithms supporting non-steady operation: It is established that optimizing economic performance may prescribe non-steady operation. In Chapter 5 it is established that irrespective of the nature of operation, optimizing economic performance always performs better in time average as compared to the best steady state solution. For non-steady operation, a MPC algorithm is presented that ensures satisfaction of constraints on average quantities during the closed-loop operation. To characterize non-steady operation, the concept of periodic/cyclic operation is introduced and an algorithm to enforce periodic operation in closed-loop is also presented. For cases where convergence to an equilibrium is a requirement that cannot be sacrificed by trading it off with economics, methods to enforce convergence are presented and demonstrated my means of a chemical process example from literature.

Solution methods and software tools for implementation: The economic regulation problems discussed in the thesis are usually nonlinear and nonconvex in nature and hence numerical solution of these problems poses a challenge. Chapter 6 reviews the various solution methods for dynamic optimization problems and describes the direct NLP approaches in detail. Collocation simultaneous strategy described in Chapter 6 is implemented in C and interfaced with GNU Octave to provide a tool for numerically solving economics optimizing dynamic regulation problems. Open source NLP solvers and differentiation packages were used and the software allows to solve the optimization problem in compiled executable form for efficient memory management and higher computational speed.

Demonstration of economic benefit: The motivation behind developing theory and numerical solution tools for economic dynamic optimization is the potential economic benefit during the process transients, that is ignored by the standard tracking approach. A number of case studies are presented in Chapter 7, which demonstrate how optimizing process economics in the dynamic regulation, exploits this potential to provide economic benefits. Performance comparison between the economic MPC and tracking type MPC is computed with respect to the steady state profit. The examples also demonstrate non-steady operation and methods to enforce convergence. The drop in performance is demonstrated for these examples when we move from the economic non-steady regime to the stable converging regime.

8.2 Future work

Distributed economic MPC: An industrial plant is usually composed of a number of interacting subsystems. In distributed control, the subsystems are controlled independently. Stewart (2010); Stewart, Wright, and Rawlings (2011); Stewart, Venkat, Rawlings, Wright, and Pannocchia (2010) have developed theory and strategies for plantwide distributed control. The results are based on standard tracking objectives and can be extended to handle economic objectives. The theory developed in this thesis can be integrated with the theory of distributed control to optimize economics directly in distributed control systems.

Dial between economic and control performance: Chapter 5 describes ways to enforce convergence in systems where optimizing economics dictates non-steady behavior. As discussed in Section 5.4, adding convex terms and enforcing zero variance constraints are two ways of dialing between economic and control performance in such systems. These methods open a wide range of operation regimes of processes, ranging from maximal economic performance to maximal control performance. The possibility of these wide variety of operations motivates research on ways to dial between the two extremes and study the characteristics of all these regimes. The results will have the potential to offer industrial practitioners to to rethink some of their operational strategies.

Storage function for dissipative systems: The new tools developed in this thesis to address stability theory involves the strict dissipativity assumption. Section 3.4.4 prescribes a terminal cost which depends on the storage function. The approach to remove terminal constraints in Section 3.5 also assumes that the storage function is known. Dissipative systems have been the focus of many research studies in the past (Appendix A). However, there is no generic way to determine the analytical expression for the storage function of dissipative systems. Appendix A discusses some of the fundamental approaches to formulating these functions. These methods address the case of quadratic supply rates and linear systems. However, most of the process systems are nonlinear in nature and hence ways to derive these storage functions for a wider class of systems are required and a subject for future research.

Appendix A

Dissipativity

In this Appendix we review the dissipativity literature and compile some results to get a better understanding of dissipative systems. The notion of dissipativity in the physical sciences, dissipativity is closely related to the notion of energy. A dissipative system is characterized by the property that at any time the amount of energy which the system can conceivably supply to its environment can not exceed the amount of energy that has been supplied to it. Theory of dissipative systems have been extensively studied by Lozano, Brogliato, Egeland, and Maschke (2000) and the references therein. We now briefly review some of these concepts.

A.1 Definitions

Consider a continuous time dynamical system

$$x = f(x(t), u(t)), \qquad x(0) = x_0 \tag{A.1}$$

where $x \in \mathbb{X} \subseteq \mathbb{R}^n$ and $u \in \mathbb{U} \subseteq \mathbb{R}^m$. We also assume $\mathbb{X}$ to be forward invariant.

Definition A.1 (Dissipativity)**.** *A nonlinear dynamical system $x = f(x(t), u(t))$ is said to be dissipative with respect to a real valued function $s(x, u)$, called as the* supply *rate, if there exists a function $\lambda(x) : \mathbb{X} \to \mathbb{R}$, called as the* storage*, such that the following holds:*

$$\lambda(x(t)) - \lambda(x(0)) \leq \int_0^t s(x(t), u(t))dt \tag{A.2}$$

for all $x(0)$, $u(t)$ and $t > 0$.

Definition A.2 (Strict Dissipativity)**.** *A nonlinear dynamical system $x = f(x(t), u(t))$ is said to be strictly dissipative with respect to the supply rate $s(x, u)$, if there exists a storage function $\lambda(x)$ and an $\epsilon > 0$, such that the following holds:*

$$\lambda(x(t)) - \lambda(x(0)) \leq \int_0^t s(x(t), u(t))dt - \epsilon^2 \int_0^t |x(t)|^2 \, dt \tag{A.3}$$

for all $x(0)$, $u(t)$ and $t > 0$.

A.1.1 Storage functions

Consider the system (A.1). Let $x_s \in \mathbb{X}$ be a fixed reference point in the state space. This is usually the optimum steady state minimizing some performance criterion. Contrary to the definition in classical papers (Willems, 1972), we do not require the storage function $\lambda(x)$ to be non-negative. Next we assume that for all $x \in \mathbb{X}$, there exists a $u(t), t \geq 0$, such that $x(t) = x_s$ for t sufficiently large, i.e. each state can be reached from and steered to the equilibrium state. We define two functions, the *available storage*, $\lambda_a(x)$, and the *required* *supply*, $\lambda_r(x)$, as following (Willems, 1972)

$$\lambda_a(x) := \sup\left\{-\int_0^t s(x(t),u(t))dt \mid t \geq 0, \quad x(0) = x, \quad x(t) = x_s\right\}$$
$$\lambda_r(x) := \inf\left\{\int_{-t}^0 s(x(t),u(t))dt \mid t \geq 0, \quad x(0) = x, \quad x(-t) = x_s\right\}$$

$\lambda_a(x)$ is the maximum amount of energy which can be extracted from the system and $\lambda_r(x)$ is the minimum required amount of energy to be injected into the system (Lozano et al., 2000). Without the loss of generality we assume that $\lambda(x_s) = 0$ i.e. x_s is a state of neutral storage. Next we state the necessary and sufficient conditions for dissipativity as established by Willems (1972).

Theorem A.3 (Willems (1972))**.** *The following are equivalent*

1. *There system is dissipative*
2. $\lambda_a(x) < \infty$*, i.e.* $\lambda_a(x)$ *is finite for all* $x \in \mathbb{X}$
3. $-\infty < \lambda_r(x)$*, i.e.* $\lambda_r(x)$ *is finite for all* $x \in \mathbb{X}$

Moreover, if one of these equivalent statements hold, then

1. $\lambda_a(x) \leq \lambda(x) \leq \lambda_r(x)$*, for all* $x \in \mathbb{X}$
2. $\lambda(x) = \alpha\lambda_a(x) + (1-\alpha)\lambda_r(x)$*, for all* $\alpha \in [0,1]$

Proof. Let the system (A.1) be dissipative. Assume that for $t_{-1} \leq 0 \leq t_1$, there exists $u(t) \in \mathbb{U}$ such that for $x(0) = x$, $x(t_{-1}) = x(t_1) = x_s$, i.e. the state x can be reached from and steered to the equilibrium state. From (A.2) we have

$$-\int_0^{t_1} s(x(t),u(t))dt \leq \lambda(x) < \infty \tag{A.4a}$$

$$-\infty < \lambda(x) \leq \int_{t_{-1}}^{0} s(x(t),u(t))dt \tag{A.4b}$$

Taking supremum over all $t_1 \geq 0$ and $u(t) \in \mathbb{U}$ such that $x(t_1) = x_s$, we get $\lambda_a(x) < \infty$ for all $x \in \mathbb{X}$. Similarly taking infimum over all $t_{-1} \leq 0$ and $u(t) \in \mathbb{U}$ such that $x(t_{-1}) = x_s$, we get $-\infty < \lambda_r(x)$ for all $x \in \mathbb{X}$.

To prove the converse, it suffices to show that $\lambda_a(x)$ and $\lambda_r(x)$ are storage functions for the system (A.1). Consider $0 \leq t_1 \leq t_2$, such that $x(t_2) = x_s$. Then

$$\begin{aligned}
\lambda_a(x) &= \sup\left\{-\int_0^{t_2} s(x(t),u(t))dt\right\} \\
&\geq -\int_0^{t_2} s(x(t),u(t))dt, \quad x(t) \in \mathbb{X}, u(t) \in \mathbb{U}, t \geq 0 \\
&= -\int_0^{t_1} s(x(t),u(t))dt - \int_{t_1}^{t_2} s(x(t),u(t))dt \\
&= -\int_0^{t_1} s(x(t),u(t))dt + \lambda_a(x(t_1))
\end{aligned}$$

Hence $\lambda_a(x)$ satisfies (A.2). Similarly we can show $\lambda_r(x)$ also satisfies (A.2).

We now prove the remaining claims.

1. From (A.4) we conclude

$$\lambda_a(x) = \sup\left\{-\int_0^{t_1} s(x(t),u(t))dt\right\} \leq \lambda(x) \leq \inf\left\{\int_{t_{-1}}^{0} s(x(t),u(t))dt\right\} = \lambda_r(x)$$

2. Using the fact that $\lambda_a(x)$ and $\lambda_r(x)$ are storage functions and satisfy (A.2), we can easily see that $\lambda(x) = \alpha\lambda_a(x) + (1-\alpha)\lambda_r(x)$ also satisfies (A.2).

$\square$

Next we state the dicrete time version of dissipativity equation and then formulate storage functions for the standard class of MPC problems: linear systems with a quadratic supply rate.

A.2 Discrete time systems

We consider discrete time systems $x^+ = F(x,u)$, where $F = \phi(x;u;\Delta)$ is the solution to the system (A.1) at time $t = \Delta$ for $x(0) = x \in \mathbb{X}$ and $u(t) = u \in \mathbb{U}, t \in [0,\Delta)$. The supply rate is also considered to be constant over the sample time Δ. $s(x(t),u(t)) = (1/\Delta)s(x,u), \forall t \in [0,\Delta)$

In this scenario, (A.2) reduces to the following inequality

$$\lambda(F(x,u)) - \lambda(x) \leq s(x,u), \quad \forall x \in \mathbb{X}, u \in \mathbb{U} \tag{A.5}$$

For the remainder of the analysis, we will chose our supply rate to be the shifted stage cost $s(x,u) = \ell(x,u) - \ell(x_s,u_s)$. To understand how dissipativity principles agree with our existing control theory, we look at the following cases:

A.2.1 Unconstrained LQR

Consider a stable linear system $x^+ = Ax+Bu$ and a quadratic cost $\ell(x,u) = 0.5(|x|_Q+|u|_R)$. For this problem $x_s = u_s = 0$. Consider the following cases

- **Linear Storage function**: Assume $\lambda(x) = K'x$. (A.5) gives

$$K'(A-I)x + K'Bu \leq (1/2)(x'Qx + u'Ru)$$

For $Q \geq 0$ and $R \geq 0$, the only K that satisfies the above inequality for all $x \in \mathbb{X}$ and $u \in \mathbb{U}$ is $K = 0$. Hence there is no other linear storage function other than the trivial zero function.

- **Quadratic storage function**: Assume $\lambda(x) = (1/2)x'Kx$. (A.5) gives

$$\begin{bmatrix} A'KA - K - Q & A'KB \\ B'KA & B'KB - R \end{bmatrix} \leq 0 \tag{A.6}$$

Next we note that

$$\lambda_a(x) = \max_{\mathbf{u}} \left\{ -\sum_{k=0}^{\infty} \ell(x(k), u(k)), \quad x(0) = x \right\} = -(1/2)x'\Pi x < \infty$$

where Π is the solution to the Riccati equation.

$$\Pi = Q + A'\Pi A - A'\Pi B(B'\Pi B + R)^{-1}B'\Pi A \tag{A.7}$$

We see that $K = -\Pi$ satisfies (A.6), and hence $\lambda_a(x)$ is a storage function for the system.

A.2.2 Inconsistent setpoints (Rawlings et al., 2008)

For this problem $\ell(x,u) = 0.5(|x - x_{sp}|_Q + |u - u_{sp}|_R)$, where x_{sp} and u_{sp} are a pair of inconsistent setpoints i.e. (x_{sp}, u_{sp}) is not a steady state of the system. Hence x_s and u_s are both nonzero.

- **Linear Storage function**: Assume $\lambda(x) = K'x$. (A.5) gives

$$(K'(A-I) - (x_s - x_{sp})'Q)\,(x - x_s) + (K'B - (u_s - u_{sp})'R)\,(u - u_s) \leq$$
$$(1/2)\left(|x - x_s|_Q + |u - u_s|_R\right) \quad \text{(A.8)}$$

Inequality (A.8) is fulfilled if the following is true

$$K'(A-I) - (x_s - x_{sp})'Q = 0 \quad \text{(A.9a)}$$

$$K'B - (u_s - u_{sp})'R = 0 \quad \text{(A.9b)}$$

Note that (A.9) are also the KKT conditions for the steady state optimization problem, with K representing the optimal Langrange multiplier.

- **Quadratic storage function**: Assume $\lambda(x) = (1/2)x'Kx$. (A.5) gives

$$\begin{bmatrix} x - x_s & u - u_s \end{bmatrix}' \begin{bmatrix} A'KA - K - Q & A'KB \\ B'KA & B'KB - R \end{bmatrix} \begin{bmatrix} x - x_s \\ u - u_s \end{bmatrix} \leq$$
$$\begin{bmatrix} (x_s - x_{sp})'Q & (u_s - u_{sp})'R \end{bmatrix} \begin{bmatrix} x - x_s \\ u - u_s \end{bmatrix}$$

The infinite horizon cost to go for this problem can be computed as following (Rawlings and Amrit, 2008)

$$\min \left\{ \sum_{k=0}^{\infty} \ell(x(k), u(k)) - \ell(x_s, u_s) \right\} = (1/2)(x - x_s)'\Pi(x - x_s) + \pi'(x - x_s)$$

in which Π satisfies the usual Lyapunov equation (A.7) and π is given by

$$\pi = (I - \overline{A}')^{-1}\left(Q(x_{sp} - x^*) + K'R(u_{sp} - u^*)\right), \quad \overline{A} = (I - B(B'\Pi B + R)^{-1}B'\Pi)A$$

Hence for this problem $\lambda_a(x) = -(1/2)(x - x_s)'\Pi(x - x_s) - \pi'(x - x_s)$.

Appendix B

NLMPC tool

In Section 6.6, we introduced a software tool: NLMPC tool, which was developed during this thesis to solve nonlinear dynamic regulation problems.

We now present some guidelines to use this tool.

B.1 Installing

NLMPC tool used Ipopt as the NLP solver and ADOL-C for derivative calculations. To be able to use NLMPC, one must first install Ipopt and ADOLC separately. Ipopt is written in C++ and is released as open source code under the Eclipse Public License (EPL). It is available, along with installation instructions, from the COIN-OR initiative website [1]. ADOL-C is an open-source package for the automatic differentiation of C and C++ programs and is released as open source code under the GNU General Public License (GPL). It is also available, along with installation instructions, from the COIN-OR initiative web-

[1] Ipopt: `https://projects.coin-or.org/Ipopt`

site [2].

Once Ipopt and ADOL-C are installed, NLMPC can be checked out from the group repository [3]. After checking out the code, the user must edit the following fields in the Makefile to specify Ipopt and ADOL-C installation paths:

```
IPOPT_BASE = /opt/ipopt/310/install        ## IPOPT's installation path
ADOLC_BASE = /opt/ADOLC/copy/trunk         ## ADOL-C's installation path
```

B.2 Simulation setup

Once the tool has been checked out and its dependencies have been successfully installed and pointed to, the user can setup the dynamic regulation problem using the tool. As pointed in Section 6.6, NLMPC tool has two plugs for interaction with the user. The first one is a C++ file (`problemfuncs.h`), which is used to define the DAE definitions, the stage cost and the constraints (other than hard bounds). The second interface is through GNU Octave, which is used to pass the user parameters to the tool, invoke it and read the results of the simulation.

We will first describe how to provide the DAE definitions, the stage cost and the constraints. The NLMPC installation path contains the two sample files: `problemfuncs.h` and `examplep.m`. The user should copy these to a custom location for simulations.

[2] ADOL-C: `https://projects.coin-or.org/ADOL-C`

[3] For the repository location, contact the author of this thesis

B.2.1 Problem definitions (`problemfuncs.h`)

This file contains the problem definitions in the form of C++ subroutines. Each of these subroutines pass the current state and input vectors in `adouble` data-type. This is to enable NLMPC to use ADOL-C for derivative calculations. `adouble` data-type is identical to the `double` data-type in C++ and all operations can be performed identically. All these subroutines have the following variables common, that pass information for user to define their functions:

1. `params`: Contains all the standard problem parameters and the user passed parameters. Standard parameters include the control horizon/number of finite elements (N), the number of states n, the number of inputs m, the steady state vector x_s, the steady state input vector u_s and the initial state x_0.

2. `x`: Current state vector, dimension n

3. `u`: Current input vector, dimension m

The three subroutines of interest in `problemfuncs.h` are as follows:

1. `void oderhs(adouble* x, adouble* u, adouble* xdot, const double* params)`

   This is the subroutine in which the DAE/ODE's are declared. The vector `xdot` is assigned the right hand side of the differential equations, which is computed using the current values of state (`x`), input (`u`) and any user passed parameters.

2. `adouble stagecost(adouble* x, adouble* u, adouble* slacks, const double* params)`

   The stage cost of the MPC dynamic regulation problem is defined in this subroutine. `ell` is assigned the the value of the stage cost, which is computed using the current values of state (`x`), input (`u`) and any user passed parameters.

3. `void constraints(adouble** x, adouble** u, adouble* h, adouble* slacks,`
   `adouble* residual, const double* params)`

   All user constraints, excluding the hard bounds are defined in this subroutine. The constraints should be of the form $g(x, u, p) \leq 0$, where p are the user-passed parameters, if any. Unlike the previous subroutines, `constraints` passes `x` and `u` as two dimentional arrays instead of single dimentional vectors. The dimentions of these arrays are $(N + 1) \times n$ and $N \times m$ respectively, and hence allows user to define constraints in terms of all the states at each time point in the prediction horizon and all inputs at all time points in the control horizon. `residual` is asigned the values of $g(x, u, p)$.

B.2.2 Problem parameters and results using GNU Octave (`examplep.m`)

Once the problem definitions have been provided in `problemfunc.h`, GNU Octave's `.oct` interface allows us to compile the NLMPC tool along with the problem function provided by the user and Ipopt and ADOL-C libraries, and call it from Octave's interpretter. To call this NLMPC interface, we set up the problem's parameters using structures in Octave. The following Octave stuctures are initialized

1. `bounds`: Bounds for the variables

   `bounds.ulb, bounds.uub`: Input lower and upper bounds

   `bounds.xlb, bounds.xub`: State lower and upper bounds

2. `data`: Problem parameters:

   `data.N`: Control horizon/Number of finite elements

   `data.m`: Number of inputs

   `data.n`: Number of states

   `data.T`: Final time

   `data.numslacks`: Number of slack variables (for soft constraints)

   `data.xs`: Refference steady state values

   `data.us`: Refference input values

   `data.params`: Parameter vector (which includes the intial state)

Once the problem parameters are defined in the structures above, we are ready to call the NLMPC tool to solve our optimal control problem. The NLP solver, and hence NLMPC tool requires an initial guess to start. Once the user defines an initial input sequence, NLMPC package provides an Octave routine, `gen_ic`, that generates the intial values of all the variables in the direct collocation NLP problem. Hence this routine is called and the return values are stored in the data structure defined above. Then the main solver is called using the following syntax

```
[outstat, u, x,t,tc,h,xc,xdot,eta] = nlmpc(x0,u0,bounds,data,options);
```

The following values are returned

1. `outstat`: Return status of Ipopt
2. `u`: Optimal input sequence
3. `x`: Optimal state sequence, values at the end of each finite element
4. `t`: time vector
5. `tc`: time values at all the collocation points in each of the finite elements
6. `h`: Length of each finite element (= sample time)
7. `xc`: Optimal state values at all the collocation points in each of the finite elements
8. `xdot`: Optimal values of dx/dt at all the collocation points in each of the finite elements
9. `eta`: Optimal value of the slack variables

B.3 Example

To aid the user manual in this appendix, we provide example code for the CSTR example with consecutive competitve reactions discussed in Section 7.4. As discussed above the problem definition is declared in the file

```
void oderhs(adouble* x, adouble* u, adouble* xdot, const double* params)
{

  int N = (int)params[0]; // Control horizon = Number of finite elements
  int n = (int)params[1]; // Number of states
  int m = (int)params[2]; // Number of inputs

  int pcount = 6+n+m+n; // This the fixed number of required
                        // parameters. Counter starts from here for user
                        // passed parameters

  /********** Begin user definintion ***********/

  /*******************/
  /* ODE definitions */
  /*******************/
  double sig41 = 1.0;
  double sig42 = 0.4;
  xdot[0] = (u[0]-x[0] - sig41*x[0]*x[1]);
  xdot[1] = (u[1]-x[1]-sig41*x[0]*x[1]-sig42*x[1]*x[2]);
  xdot[2] = (-x[2] + sig41*x[0]*x[1]-sig42*x[1]*x[2]);
  xdot[3] = -x[3] + sig42*x[1]*x[2];

  /********** End user definition ***********/
```

```
}
```

```
adouble stagecost(adouble* x, adouble* u, adouble* slacks,
                  const double* params)
{

  adouble ell = 0.0;
  int i;

  int N = (int)params[0]; // Control horizon = Number of finite elements
  int n = (int)params[1]; // Number of states
  int m = (int)params[2]; // Number of inputs
  double xc[n];
  double uc[m];
  double uprev;

  /* Extract reference states */
  for(i = 0; i<n; i++) // Extract x_s
    xc[i] = params[6+n+m+i];

  for(i = 0; i<m; i++) // Extract u_s
    uc[i] = params[6+n+i];

  int pcount = 6+n+m+n; // This the fixed number of required
                        // parameters. Counter starts from here for user
                        // passed parameters
```

```
  /********** Begin user definintion ***********/

  ell = -x[2];

  /********** End user definition ***********/


  return ell;
}
```

```
void constraints(adouble** x, adouble** u, adouble* h, adouble* slacks,
                 adouble* residual, const double* params)
{
  int N = (int)params[0]; // Control horizon = Number of finite elements
  int n = (int)params[1]; // Number of states
  int m = (int)params[2]; // Number of inputs
  int count = 0;
  number_of_constraints = 9;
  int i, j, k;
  adouble sum = 0;

  // Extract the refference steady states
  double xs[n];
  for(i = 0; i<n; i++)
    xs[i] = params[6+n+m+i];

  double u1s = params[6+n];

  // Average constraint
  for(i = 0; i<N; i++)       /* For all finite elements */
      for(j = 0; j<nce; j++)   /* For all collocation points */
        sum += h[i]*a[j][2]*u[i][0];

  residual[count++] = sum - u1s; // Averaging constraint
```

```
  // Terminal Constraint //
  residual[count++] = -x[N][0] + xs[0];
  residual[count++] = -x[N][1] + xs[1];
  residual[count++] = -x[N][2] + xs[2];
  residual[count++] = -x[N][3] + xs[3];


  residual[count++] = x[N][0] - xs[0];
  residual[count++] = x[N][1] - xs[1];
  residual[count++] = x[N][2] - xs[2];
  residual[count++] = x[N][3] - xs[3];
}
```

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