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Nonlinear Process Control Using Contraction Theory

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Abstract

Contraction theory is a recently developed nonlinear control system tool based on an exact differential analysis of convergence. This paper applies contraction theory to stability analysis and control system design for nonlinear chemical processes. Simple designs with explicit stability and convergence guarantees are obtained by taking advantage of the monotonicity of the reaction rates and the linear ambiguity in the choice of the chemical state.

Introduction

Nonlinear control system design has been very successfully applied to particular classes of systems and problems (Isidori, 1995a; Marino and Tomei, 1995; Khalil, 1995; Vidyasagar, 1992; Slotine and Li, 1991; Nijmeijer and van der Schaft, 1990). In an attempt to systematically generalize its range of application, (Lohmiller and Slotine, 1998) derived a body of new results, referred to as *contraction analysis*, using elementary tools from continuum mechanics and differential geometry. This paper exploits these results to derive new controller and observer designs for nonlinear process control systems.

Many approaches to nonlinear process control have been developed, either as direct applications of general nonlinear control techniques, or as more tailored approaches to the system physics. These include linear approximation, feedback linearization, nonlinear model predictive control, Lyapunov-based and physically-based designs, intelligent systems, and adaptive control. Recent overviews of these approaches and their practical applications can be found e.g. in (Henson and Seborg, 1997; Bemporad, et al., 1999; Hangos, et al., 1999; Stephanopoulos and Han, 1996; Astrom and Wittenmark, 1995).

In this paper, we show that the general tools of contraction theory can be specifically tailored to important classes of nonlinear process control problems, and lead to systematic design techniques with explicit guarantees of local or global exponential convergence. The relative simplicity of these designs stems from their effective exploitation of the systems' structural specificities and physical properties. The extent of convergence, typically conditioned by input constraints and desired nominal performance, can be explicitly quantified.

The layout of the paper is as follows. After a brief review of the basic results of (Lohmiller and Slotine, 1998), switching systems and systems with convex constraints are studied, and a separation principle for nonlinear systems is derived. The contraction behavior of general nonlinear reaction dynamics is then analyzed. The monotonicity of the chemical reaction rates and the linear ambiguity in the choice of the chemical state allow one to reduce the discussion to a set of constant linear matrix inequalities. Corresponding nonlinear chemical controller and observer designs are then detailed. The last section offers brief concluding remarks.

Contraction Analysis

Stability analysis using differential approximation is the basis of all linear control system design. What is new in contraction analysis is that differential stability analysis can be made *exact*, and in turn yield global results on the nonlinear system. In this section, we summarize the basic results of (Lohmiller and Slotine, 1998a), to which the reader is referred for more details.

We consider general deterministic systems of the form

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, t) \tag{1}$$

where $\mathbf{f}$ is an $n \times 1$ nonlinear vector function and $\mathbf{x}$ is the $n \times 1$ state vector. The above equation may also represent the closed-loop dynamics of a controlled system with state feedback $\mathbf{u}(\mathbf{x}, t)$. All quantities are assumed to be real and smooth, by which it is meant that any required derivative or partial derivative exists and is continuous.

The plant equation (1) can be thought of as an n-dimensional fluid flow, where $\dot{\mathbf{x}}$ is the n-dimensional "velocity" vector at the n-dimensional position $\mathbf{x}$ and time t. Assuming as we do that $\mathbf{f}(\mathbf{x}, t)$ is continuously differentiable, (1) yields the exact differential relation

$$\delta\dot{\mathbf{x}} = \frac{\partial \mathbf{f}}{\partial \mathbf{x}}(\mathbf{x}, t)\ \delta\mathbf{x} \tag{2}$$

where $\delta\mathbf{x}$ is a virtual displacement $-$ recall that a virtual displacement is an infinitesimal displacement *at fixed time* (Figure 1). Note that virtual displacements, pervasive in physics and in the calculus of variations, are also well-defined mathematical objects (Arnold, 1978; Schwartz, 1993). In particular, if we view the position of the system at time t as a smooth function of the initial condition $\mathbf{x}_o$ and of time, $\mathbf{x} = \mathbf{x}(\mathbf{x}_o, t)$, then one simply has $\delta\mathbf{x} = \frac{\partial \mathbf{x}}{\partial \mathbf{x}_o}\ d\mathbf{x}_o$.

The line vector $\delta\mathbf{x}$ can also be expressed using the differential coordinate transformation

$$\delta\mathbf{z} = \mathbf{\Theta}\delta\mathbf{x} \tag{3}$$

where $\mathbf{\Theta}(\mathbf{x}, t)$ is a square matrix. This leads to

$$\delta\mathbf{z}^T\delta\mathbf{z} = \delta\mathbf{x}^T\mathbf{M}\ \delta\mathbf{x} \tag{4}$$

where $\mathbf{M}(\mathbf{x}, t) = \mathbf{\Theta}^T\mathbf{\Theta}$ represents a symmetric and continuously differentiable *metric* $-$ formally, equation (4) defines a Riemann space (Lovelock and Rund, 1989). Since (3) is

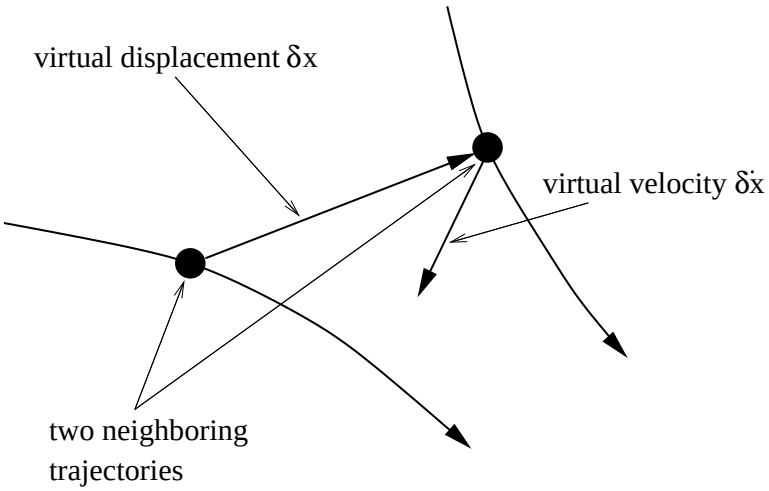

Figure 1: Virtual dynamics of two neighboring trajectories

in general not integrable, we cannot expect to find explicit new coordinates $\mathbf{z}(\mathbf{x},t)$, but $\delta\mathbf{z}$ and $\delta\mathbf{z}^T\delta\mathbf{z}$ can always be defined, which is all we need. We shall require $\mathbf{M}$ to be uniformly positive definite, so that exponential convergence of $\delta\mathbf{z}$ to $\mathbf{0}$ also implies exponential convergence of $\delta\mathbf{x}$ to $\mathbf{0}$. Distance between two points P_1 and P_2 with respect to the metric $\mathbf{M}$ is defined as the shortest path length (i.e., the smallest path integral $\int_{P_1}^{P_2} \|\delta\mathbf{z}\|$) between these two points. Accordingly, a ball of center $\mathbf{c}$ and radius R is defined as the set of all points whose distance to $\mathbf{c}$ with respect to $\mathbf{M}$ is strictly less than R.

Computing

$$\frac{d}{dt}\,\delta\mathbf{z} \;=\; \mathbf{F}\;\delta\mathbf{z} \qquad \text{where} \qquad \mathbf{F} = \left(\dot{\mathbf{\Theta}} + \mathbf{\Theta}\frac{\partial \mathbf{f}}{\partial \mathbf{x}}\right)\mathbf{\Theta}^{-1} \tag{5}$$

we can state the following definition and main result (Lohmiller and Slotine, 1998)

Definition 1 *Given the system equations $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x},t)$, a region of the state space is called a contraction region with respect to a uniformly positive definite metric $\mathbf{M}(\mathbf{x},t) = \mathbf{\Theta}^T\mathbf{\Theta}$ if $\mathbf{F}$ in (5) is uniformly negative definite in that region.*

Regions where $\mathbf{F}$ is negative semi-definite are called semi-contracting, and regions where $\mathbf{F}$ is skew-symmetric are called indifferent.

Theorem 1 *Given the system equations $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x},t)$, any trajectory, which starts in a ball of constant radius with respect to the metric $\mathbf{M}(\mathbf{x},t)$, centered at a given trajectory and contained at all times in a contraction region with respect to $\mathbf{M}(\mathbf{x},t)$, remains in that ball and converges exponentially to this trajectory.*

Furthermore global exponential convergence to the given trajectory is guaranteed if the whole state space is a contraction region with respect to the metric $\mathbf{M}(\mathbf{x},t)$.

The generality of contraction analysis, as compared to related classical results on autonomous systems (Krasovskii, 1959; Hahn, 1967; Hartmann, 1982), stems from its use of pure differential analysis, and specifically of a pure *differential coordinate transformation*, leading to a necessary and sufficient characterization of exponential convergence for nonlinear non-autonomous systems. Indeed, it can be shown conversely that the existence of a uniformly positive definite metric with respect to which the whole state space is a contraction region is actually a necessary condition for global exponential convergence. Furthermore, the exponential convergence rate can be evaluated explicitly as an upper bound on the absolute value of the largest eigenvalue of the symmetric part of $\mathbf{F}$. In the linear time-invariant case, a system is globally contracting if and only if it is strictly stable, with $\mathbf{F}$ simply being a normal Jordan form of the system and $\mathbf{\Theta}$ the coordinate transformation to that form.

Example 1: Consider a generalized Van-der-Pol oscillator, of the form

$$\ddot{x} + (x^2 - 1)\dot{x} + f(x,t) = 0$$

where $f(x,t)$ can be any smooth function, and assume that x is measured and $v = \dot{x}$ is to be estimated.

Define a reduced-order observer for this system by

$$\dot{\bar{v}} + (x^2 + k - 1)\hat{v} + f(x,t) = 0$$

$$\hat{v} = \bar{v} + kx$$

where $k > 1$ is a constant and the intermediate variable $\bar{v}$ can be initialized arbitrarily. This choice implies that

$$\dot{\hat{v}} + (x^2 - 1)\hat{v} + k(\hat{v} - v) + f(x,t) = 0$$

so that the observer contains the actual v as a particular solution, and furthermore the Jacobian $-(x^2 + k - 1)$ is uniformly negative definite. Thus, the estimate $\hat{v}$ converges globally and exponentially to the actual v. □

Note that the conditioning of the coordinate tranformation $\mathbf{\Theta}$ determines the transitory overshoot in the exponential convergence. Indeed

$$\frac{d}{dt}\ \delta\mathbf{z}^T\delta\mathbf{z}\ \leq\ 2\ \lambda_{\mathbf{F}}\ \delta\mathbf{z}^T\delta\mathbf{z}$$

where $\lambda_{\mathbf{F}}(\mathbf{x},t)$ denotes the largest eigenvalue of the symmetric part of the generalized Jacobian $\mathbf{F}$. This implies that

$$\sigma_{min}^2\ \delta\mathbf{x}^T\delta\mathbf{x}\ \leq\ \delta\mathbf{z}^T\delta\mathbf{z}\ \leq\ \ e^{-2\ |\lambda_{\mathbf{F}}|\ t}\ (\delta\mathbf{z}^T\delta\mathbf{z})_{t=0}\ \leq\ \ e^{-2\ |\lambda_{\mathbf{F}}|\ t}\ (\sigma_{max}^2\ \delta\mathbf{x}^T\delta\mathbf{x})_{t=0}$$

where the σ's denote the singular values of $\mathbf{\Theta}$. Also note that the metric is unchanged by an additional (perhaps time-varying or state-dependent) orthonormal transformation, i.e., by left-multiplying $\mathbf{\Theta}$ by an orthonormal matrix.

Further results on contraction analysis

After recalling a basic combination property of contracting systems, this section derives a new separation principle for nonlinear systems, analyzes hybrid and switched systems, discusses contracting systems under convex constraints, and further studies semi-contracting systems. These results will be exploited in the next two sections.

Hierarchies

Combinations of contraction systems enjoy some useful closure properties (Lohmiller and Slotine, 1998). In particular, consider a smooth virtual dynamics of the form

$$\frac{d}{dt}\begin{pmatrix} \delta \mathbf{z}_1 \\ \delta \mathbf{z}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{F}_{11} & \mathbf{0} \\ \mathbf{F}_{21} & \mathbf{F}_{22} \end{pmatrix} \begin{pmatrix} \delta \mathbf{z}_1 \\ \delta \mathbf{z}_2 \end{pmatrix}$$

The first equation does not depend on the second, so that exponential convergence of $\delta \mathbf{z}_1$ to zero can be concluded for uniformly negative definite $\mathbf{F}_{11}$. In turn, for *bounded* $\mathbf{F}_{21}$, $\mathbf{F}_{21}\delta \mathbf{z}_1$ represents an exponentially decaying disturbance in the second equation. Thus, uniform negative definitiveness of $\mathbf{F}_{22}$ implies exponential convergence of $\delta \mathbf{z}_2$ to zero, so that the augmented system is contracting as well. By recursion, the result can be extended to systems similarly partitioned in more than two equations.

An example of such dynamical hierarchies are polymerisation processes, as illustrated in (Lohmiller and Slotine, 1998). Another illustration of this important property is offered by the following classical problem.

Example 2: Consider a stirred tank fed with two incoming flows with controllable flow rate q_1 and constant flow rate $q_2 = 1$ (Kwakernaak and Sivan, 1972). Both flows contain dissolved material with constant concentrations c_1 and c_2. The outgoing flow has a flow rate $q = k\sqrt{V}$, with V the fluid volume in the tank and k an outflow constant. Denoting by V_c the partial volume of the dissolved material in the tank, the corresponding dynamics

$$\begin{aligned} \dot{V} &= q_1 + q_2 - k\sqrt{V} \\ \dot{V}_c &= c_1 q_1 + c_2 q_2 - k V_c \frac{1}{\sqrt{V}} \end{aligned}$$

is a hierarchy from V to V_c , and it is contracting since $\frac{\partial \dot{V}}{\partial V} = -\frac{k}{2\sqrt{V}}$ and $\frac{\partial \dot{V}_c}{\partial V_c} = -\frac{k}{\sqrt{V}}$ are both uniformly negative. A tracking controller of the form

$$q_1 = V_d - V - q_2 + k\sqrt{V_d} + \dot{V}_d$$

preserves the hierarchy from V to V_c. □

Separation Principle

Consider a plant dynamics in terms of an explicit state vector $\mathbf{z}$,

$$\dot{\mathbf{z}} = \mathbf{f}(\mathbf{z}, t) + \mathbf{G}(\mathbf{z}, t)\mathbf{u}(\hat{\mathbf{z}}, t)$$

combined with the observer

$$\dot{\hat{\mathbf{z}}} = \mathbf{f}(\hat{\mathbf{z}}, t) - (\mathbf{e}(\hat{\mathbf{z}}) - \mathbf{e}(\mathbf{z})) + \mathbf{G}(\mathbf{z}, t)\mathbf{u}(\hat{\mathbf{z}}, t)$$

where $\hat{\mathbf{z}}$ is the state estimate, and $\mathbf{u}(\hat{\mathbf{z}}, t)$ the control input. Letting $\tilde{\mathbf{z}} = \hat{\mathbf{z}} - \mathbf{z}$, the Lyapunov-like analysis

$$\frac{d}{dt}\left(\tilde{\mathbf{z}}^T \tilde{\mathbf{z}}\right) = 2\ \tilde{\mathbf{z}}^T \int_o^1 \frac{\partial (\mathbf{f} - \mathbf{e})}{\partial \mathbf{z}}(\mathbf{z} + \lambda \tilde{\mathbf{z}})\ d\lambda\ \ \tilde{\mathbf{z}}$$

then shows that the convergence rate of $\hat{\mathbf{z}}$ to $\mathbf{z}$ is specified by $\frac{\partial(\mathbf{f}-\mathbf{e})}{\partial\hat{\mathbf{z}}}$. For bounded $\mathbf{G}$ this system is a hierarchy, and thus the convergence rate of the plant dynamics is given by $\frac{\partial(\mathbf{f}-\mathbf{G}\mathbf{u})}{\partial\mathbf{z}}$. This result may be viewed as an extension of the standard linear separation principle in (Luenberger, 1979).

Hybrid systems

Hybrid dynamics, i.e., dynamics which combine continuous-time and discrete-time elements (Branicky, 1994), occur in many systems of practical importance, as e.g. in a continuous observer problem with discrete measurements. Sufficient conditions for contraction can be easily derived for such systems.

Specifically, consider a continuous system

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, t)$$

which is switched to a discrete system

$$\mathbf{x}_{i+1} = \mathbf{f}_i(\mathbf{x}_i, i)$$

every Δt_i for one discrete step. Letting, in the *same coordinate system* $\mathbf{\Theta}$, $\bar{\lambda}$ be the largest eigenvalue of the symmetric part of $\mathbf{F}$, and $\bar{\lambda}_i$ be the largest eigenvalue of $\mathbf{F}_i^T\mathbf{F}_i$ (which is the corresponding discrete-time quantity, as detailed in (Lohmiller and Slotine, 1998)), the length dynamics over Δt_i for one discrete step i is bounded by

$$\delta\mathbf{z}_{i+1}^T\delta\mathbf{z}_{i+1} \leq \bar{\lambda}_i e^{\bar{\lambda}\Delta t_i}\delta\mathbf{z}_i^T\delta\mathbf{z}_i$$

Thus, the hybrid system is contracting if

$$\exists\ \alpha < 1, \forall i, \qquad 0 \leq \bar{\lambda}_i e^{\bar{\lambda}\Delta t_i} \leq \alpha \tag{6}$$

Example 3: Consider a hybrid observer

$$\dot{\hat{\mathbf{x}}} = \mathbf{f}(\hat{\mathbf{x}}, t)$$

which incorporates a discrete measurement every Δt_i, with

$$\hat{\mathbf{x}}_{i+1} = \mathbf{f}_i(\hat{\mathbf{x}}_i, i)$$

and verifies (6). Assume that there is a bounded model uncertainty $\mathbf{d}$ in the prediction part and a bounded measurement uncertainty $\mathbf{d}_i$. The observer error $R_i = \int_x^{\hat{x}} ||\delta\mathbf{z}_i||$ then verifies, similarly to the basic robustness result in (Lohmiller and Slotine, 1998)

$$R_{i+1} + \alpha R_i \leq ||\mathbf{d}\Delta t_i + \mathbf{d}_i||_M$$

and any observer trajectory converges exponentially to a ball of radius R_i around the actual trajectory. □

Switched systems

Consider an arbitrary number of continuously differentiable dynamics

$$\dot{\mathbf{x}} = \mathbf{f}_i(\mathbf{x}, t)$$

defined in separate regions V_i of the state space and t under the requirement that the resulting combined dynamics is *continuous in space*. Typical examples of such continuous switching are the min and max operators on components of $\mathbf{f}$, or switching $\mathbf{f}_i$ as a function of time t only.

Now assume that all $\mathbf{f}_i$ are contracting with respect to the *same* continuous metric $\mathbf{M}(\mathbf{x}, t)$, then any such continuous switching of contracting systems is itself contracting, as we now show.

Indeed, consider the distance $\int_{P_1}^{P_2} \|\delta\mathbf{z}\|$ between two trajectories P_1 and P_2, which is simply the sum of the distances $\int_i \|\delta\mathbf{z}_i\|$ in the regions V_i. Since any $\|\delta\mathbf{z}_i\|$ converges exponentially to zero and no jump in $\dot{\mathbf{x}}$ and $\mathbf{M}(\mathbf{x}, t)$ can occur, the trajectories P_1 and P_2 converge exponentially to each other. This result may be regarded as a generalization of the stability analysis of linear switching systems in (Shorten and Narendra, 1998).

Example 4: Consider an arbitrary number of continuously differentiable dynamics

$$\dot{\mathbf{x}} = \mathbf{f}_i(\mathbf{x}, t)$$

that are all locally contracting around different operating points $\mathbf{x}_i$ with respect to possibly different $\mathbf{\Theta}_i$. Typical examples of such systems are gain-scheduled designs (Lawrence and Rugh, 1995).

Consider a particular trajectory $\mathbf{x}(t)$ which belongs at the same time to a contracting ball around each $\mathbf{x}_i$. Then, according to Theorem 1, each single dynamic $\dot{\mathbf{x}} = \mathbf{f}_i(\mathbf{x}, t)$ leads to exponential convergence to $\mathbf{x}_i$, i.e., any switching from one dynamics to another dynamics is contracting. □

Extension to more general hybrid and switched systems (Isidori, 1995b) are a subject of current research. Consider for instance a general, possibly discontinuous dynamics

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, t)$$

and assume that unique solutions exist in the sense of (Filippov, 1960), and that the Jacobian $\frac{\partial \mathbf{f}}{\partial \mathbf{x}}$ can be computed in the sense of distributions (Schwartz, 1993). Then, generalized Jacobians $\mathbf{F}(\mathbf{x}, t)$ and their negative definiteness can be evaluated in the sense of distributions, and the argumentation of Theorem 1 can be extended formally to such systems. Recall that a generalized Jacobian $\mathbf{F}(\mathbf{x}, t)$, computed in the sense of distributions, is uniformly negative definite, if $\exists\ \alpha > 0$ such that for any time $t \geq 0$, and any C^∞ vector field $\mathbf{g}(\mathbf{x})$ with compact support,

$$\int_{\mathbf{R}^n} \mathbf{g}^T(\mathbf{x})\ \mathbf{F}(\mathbf{x}, t)\ \mathbf{g}(\mathbf{x})\ d\mathbf{x}\ \leq\ -\ \alpha$$

Example 5: Consider a inertia-damping system with discontinuous damping

$$\dot{v} = -\mathrm{sgn}v - v + u(t)$$

Denoting by $\dot{h}$ the unit Dirac impulse, the Jacobian $(-1 - \dot{h}(v))$ is uniformly negative definite, and hence any δv converges exponentially to zero. □

Contraction analysis on convex regions

In some control contexts, it is common to have to enforce convex constraints on the states or inputs. In process control, this occurs for instance when the control input or state estimate is a chemical concentration (which must lie between 0 and 1) or a temperature (which must be positive). This section discusses the incorporation of convex constraints in contraction analysis.

Consider a contracting system

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, t)$$

which, assuming the explicit existence of $\mathbf{z}$, can be transformed into

$$\dot{\mathbf{z}} = \mathbf{\Theta f}(\mathbf{x}, t)$$

on a convex region $\mathbf{\Omega}$ (i.e. a region $\mathbf{\Omega}$ in which any shortest connecting line (geodesic) $\int_{\mathbf{x}_1}^{\mathbf{x}_2} \|\delta \mathbf{z}\|$ between two arbitrary points $\mathbf{x}_1$ and $\mathbf{x}_2$ in $\mathbf{\Omega}$ is completely contained in $\mathbf{\Omega}$). Using the argumentation of the previous section implies that the distance $\int_{\mathbf{x}_1}^{\mathbf{x}_2} \|\delta \mathbf{z}\|$ between two arbitrary trajectories $\mathbf{x}_1$ and $\mathbf{x}_2$ in $\mathbf{\Omega}$ which stay in $\mathbf{\Omega}$ converges exponentially to zero. Now maintain all trajectories in $\mathbf{\Omega}$ with an extra term

$$\dot{\mathbf{x}} = \mathbf{f} - \frac{1}{\frac{\partial h}{\partial \mathbf{z}} \frac{\partial h}{\partial \mathbf{z}}^T} \mathbf{\Theta}^{-1} \frac{\partial h}{\partial \mathbf{z}}^T \frac{\partial h}{\partial \mathbf{z}} \mathbf{\Theta f}$$

that is, in $\mathbf{z}$ coordinates

$$\dot{\mathbf{z}} = \mathbf{\Theta f} - \frac{1}{\frac{\partial h}{\partial \mathbf{z}} \frac{\partial h}{\partial \mathbf{z}}^T} \frac{\partial h}{\partial \mathbf{z}}^T \frac{\partial h}{\partial \mathbf{z}} \mathbf{\Theta f}$$

at outflowing boundaries $0 = h(\mathbf{z}(\mathbf{x}))$ (recall that by convention $\frac{\partial h}{\partial \mathbf{z}}$ is a row-vector, to be consistent with the notation of Jacobians). Since the projection of the superimposed flow on any interior geodesic is positive, it can only speed up the convergence rate of $\int_{\mathbf{x}_1}^{\mathbf{x}_2} \|\delta \mathbf{z}\|$ to zero. As a result all trajectories in $\mathbf{\Omega}$ converge exponentially to a single trajectory.

Semi-contracting systems

Finally, let us discuss some technical extensions which may be useful in particular cases. Consider the rate of change of length (Lohmiller and Slotine, 1998)

$$\frac{d}{dt}\left(\delta \mathbf{x}^T \mathbf{M}\ \delta \mathbf{x}\right) = \delta \mathbf{x}^T \left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}}^T \mathbf{M} + \dot{\mathbf{M}} + \mathbf{M} \frac{\partial \mathbf{f}}{\partial \mathbf{x}} \right) \delta \mathbf{x}$$

and assume that $\left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}}^T \mathbf{M} + \mathbf{M} \frac{\partial \mathbf{f}}{\partial \mathbf{x}} + \dot{\mathbf{M}} \right)$ is only negative semi-definite. Assuming $\frac{d^2}{dt^2}\left(\delta \mathbf{x}^T \mathbf{M}\ \delta \mathbf{x}\right)$ to be bounded, the use of Barbalat's lemma (Slotine and Li, 1991) shows asymptotic convergence of

$$\delta \mathbf{x}^T \left(\frac{\partial \mathbf{f}}{\partial \mathbf{x}}^T \mathbf{M} + \dot{\mathbf{M}} + \mathbf{M} \frac{\partial \mathbf{f}}{\partial \mathbf{x}} \right) \delta \mathbf{x}$$

to zero. This means that only a subset of the state $\mathbf{x}$ converges asymptotically to a single trajectory. Furthermore, any distance in the complementary subset does not increase. This result is of practical use for nonlinear parameter adaptation, as we shall see when we study process observers. A more general discussion of semi-contracting systems can be found in (Lohmiller and Slotine, 1999).

Finally, note that if the metric itself $\mathbf{M}$ in 8 can only be shown to be negative semi-definite, then $\mathbf{M}$ defines an exponentially convergent subspace.

Nonlinear Chemical Processes

This section analyzes the contraction behavior of nonlinear chemical reactions. We first analyze general nonlinear chemical reactions, and then discuss the specific properties of chemical chain reactions. Choosing a constant metric $\mathbf{M}$ from Theorem 1 corresponds to resolving the linear ambiguity left when choosing the chemical state with respect to element and energy conservation laws.

Contraction analysis of chemical reactions

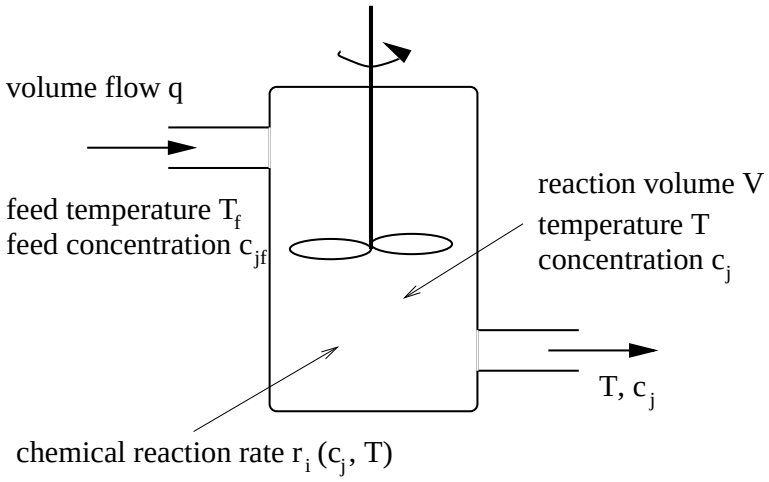

Figure 2: Open stirred tank

Figure 2 describes a general smooth n-dimensional reaction dynamics in an open stirred tank (Henson and Seborg, 1997)

$$\dot{\mathbf{x}} = q(t)\,(\mathbf{x}_f - \mathbf{x}) + \mathbf{N}\mathbf{r} \tag{7}$$

with $\mathbf{N}$ the reaction rate coefficients, $\mathbf{x} = (c_1 \ \ldots \ c_{n-1} \ \ T)^T$ the state vector consisting of the chemical concentrations $c_i \geq 0$ and the temperature $T \geq 0$, $\mathbf{x}_f(t)$ the corresponding feed vector and $q(t) \geq 0$ the specific volume flow. The normalized reaction rates $r_i =$

$e^{-\frac{E_i}{T}} \prod_j c_j^{\nu_{ij}}, i = 1, ..., p$ contain the specific activation energies $E_i \geq 0$ and the stoichiometric coefficients ν_{ij}. The Jacobian of (7) can be written as

$$-q(t)\mathbf{I} + \sum_{i=1}^{p} \sum_{j=1}^{n} \mathbf{N}_{ij} \frac{\partial r_i}{\partial x_j}(\mathbf{x})$$

where $\mathbf{N}_{ij}$ is a matrix of zeroes except for the j'th column, which is taken equal to the i'th column of $\mathbf{N}$. In the particular case of common terms, $\frac{\partial r_{i_1}}{\partial x_{j_1}} = \frac{\partial r_{i_2}}{\partial x_{j_1}}$ for $i_1 \neq i_2$ or $j_1 \neq j_2$, by convention the corresponding matrices are added and combined in a single matrix $\mathbf{N}_{i_1 j_1}$.

In the physical modelling of the reaction dynamics (7), one has to choose a linear state $\mathbf{x}$ under linear energy and element conservation. In order to resolve this linear ambiguity in $\mathbf{x}$, we analyze (7) with a general constant metric $\mathbf{M}$, corresponding to a general linear coordinate transformation.

In addition, the monotonic behavior of the reaction rates implies that all $\frac{\partial r_i}{\partial x_j}$ are positive, for all $c_i \geq 0$ and $T > 0$. As a result we can conclude on contraction behavior with Theorem 1 if there exists a constant metric

$$\mathbf{M} > \mathbf{0} \tag{8}$$

such that

$$\forall i, j \qquad \mathbf{N}_{ij}^T \mathbf{M} + \mathbf{M} \mathbf{N}_{ij} \ \leq \ \mathbf{0} \tag{9}$$

These linear matrix inequalities are equivalent to the stability problem of linear switching systems (Shorten and Narendra, 1998). (Boyd, et al., 1994) provide general numerical schemes to solve (8) and (9) for $\mathbf{M}$ if feasible.

Finally, note that the reaction rate vector $\mathbf{r}$ can be augmented with other monotonic functions such as radiation or heat convection. Furthermore, if a non-monotonic function is included in $\mathbf{r}$, then the linear matrix inequality (9) has to be replaced with a more stringent linear matrix equality – the system may still be solvable for an adequate metric since the coefficient matrices are rather sparse.

Also, an alternative to the above derivation is to first augment the reaction rate vector $\mathbf{r}$ with $q\mathbf{x}$. Exponential convergence can then still be guaranteed if at least one strict inequality in (9) holds for a strictly positive $\frac{\partial r_i}{\partial x_j}$. If this is not the case, the results of the section on semi-contracting systems may still be applied. This more technical alternative will be of practical importance in the section on observer design, where it will allow nonlinear parameter adaptation.

Contraction analysis of chemical chain reactions

The analysis can be simplified in the case that the dynamics is in a specific form of (7), which we shall refer to as a chemical chain reaction

$$\begin{aligned} \dot{x}_1 &= q\,(x_{1f} - x_1) + f_1(x_1) \\ \dot{x}_2 &= q\,(x_{2f} - x_2) + f_2(x_1, x_2) \\ &\vdots \end{aligned}$$

This dynamics represents a hierarchy for bounded $\frac{\partial \mathbf{f}}{\partial \mathbf{x}}$. As a result the system is exponentially convergent if $-q + \frac{\partial f_i}{\partial x_i}$ is uniformly strictly negative $\forall i, 1 \leq i \leq n$. Corresponding robustness guarantees are given in (Lohmiller and Slotine, 1998).

Example 6: Consider a temperature independent set of chain reactions similar to (Henson and Seborg, 1997), composed of a primary reaction of the reactant A, a further reaction of the desired product B into a side product C, and an additional reaction of A into the side product D:

$$\begin{aligned} A &\rightarrow B \rightarrow \frac{1}{2}C \\ 2A &\rightarrow D \end{aligned}$$

The reaction dynamics can be written as

$$\begin{aligned} \dot{c}_A &= q(c_{Af} - c_A) - n_1 c_A - n_3 c_A^2 \\ \dot{c}_B &= -q c_B + n_1 c_A - n_2 c_B^2 \end{aligned}$$

with c_A and c_B the concentrations of A and B, c_{Af} the inlet concentration of A, $q > 0$ the specific inlet flow rate, and n_1, n_2, and n_3 positive reaction rate constants. The Jacobian of this dynamics is a bounded lower triangular matrix with uniformly negative definite main diagonal: this chain reaction is an exponentially convergent hierarchy.

Note that choosing instead c_C and c_D as state variables simply corresponds to a linear coordinate transformation $\mathbf{z} = \mathbf{\Theta x}$, i.e. to choosing a constant metric $\mathbf{M} = \mathbf{\Theta}^T \mathbf{\Theta}$. However, this particular choice does not preserve the hierarchy. □

Chemical Controller and Observer Designs

This section studies nonlinear chemical controller and observer designs suggested by the previous section. It also incorporates explicitly some of the general tools developed in the section on system combinations, such as hierarchical analysis and the possibility to include input constraints.

Chemical controller design

Consider again the reaction dynamics (7)

$$\dot{\mathbf{x}} = q\,(\mathbf{x}_f - \mathbf{x}) + \mathbf{N}\mathbf{r} + \mathbf{G}\mathbf{u} \tag{10}$$

now controlled with $\mathbf{u} = \mathbf{K} \int \frac{\partial \mathbf{r}}{\partial \mathbf{x}}(\mathbf{x}) d\mathbf{x} + \mathbf{u}_d(t)$, where $\int \frac{\partial \mathbf{r}}{\partial \mathbf{x}} d\mathbf{x}$ is any function whose partial derivatives are within the set spanned by $\frac{\partial r_i}{\partial x_j}$, and $\mathbf{K}$ is a constant gain matrix to be specified. The Jacobian of (10) can be written as

$$-q(t)\mathbf{I} + \sum_{i=1}^{p} \sum_{j=1}^{n} (\mathbf{N} + \mathbf{G}\mathbf{K})_{ij} \frac{\partial r_i}{\partial x_j}(\mathbf{x})$$

where the j'th column of $(\mathbf{N}+\mathbf{GK})_{ij}$ is the i'th column of $(\mathbf{N}+\mathbf{GK})$ and the remaining elements are zero. Similarly to the analysis section, identical $\frac{\partial r_i}{\partial x_j}$ can be combined in a single term. Using a constant metric $\mathbf{M} > \mathbf{0}$, the system is contracting if

$$\forall i,j \;\exists\, \mathbf{K}, \qquad (\mathbf{N}+\mathbf{GK})_{ij}^T \mathbf{M} + \mathbf{M}\,(\mathbf{N}+\mathbf{GK})_{ij} \;\leq\; \mathbf{0} \tag{11}$$

This problem is formally equivalent to the stabilization problem of linear switching systems (Shorten and Narendra, 1998). Again, (Boyd, et al., 1994) provide general numerical schemes to solve (11) for $\mathbf{M} > \mathbf{0}$ and $\mathbf{K}$ if feasible.

Example 7: Consider again the chain reaction in Example 6

$$\begin{aligned} \dot{c}_A &= q(u-c_A) - n_1 c_A - n_3 c_A^2 \\ \dot{c}_B &= -q c_B + n_1 c_A - n_2 c_B^2 \end{aligned} \tag{12}$$

with constant $q > 0$, which now includes a control input u. According to the previous discussion, any controller consisting of the nonlinearities in (12)

$$u = k_1 c_A + k_2 c_A^2 + k_3 c_B + u_d(t)$$

with $qk_1 - q - n_1 < 0$, $qk_2 - n_3 < 0$, $k_3 < 0$ and the metric

$$\mathbf{M} = \begin{pmatrix} n_1 & 0 \\ 0 & -qk_3 \end{pmatrix}$$

can be used to increase the exponential convergence rate of the system.

Finally, an appropriate open-loop term $u_d(t)$ can be immediately computed from the system dynamics so as to converge to a specified $c_{Ad}(t)$ or $c_{Bd}(t)$. □

Note that, while for this low dimensional system the design is almost trivial once the basic principle is understood, it can be extended numerically (Boyd, et al., 1994) to chemical systems of any order.

The above design by itself does not account for input constraints. Depending on the required nominal performance, such constraints may have to be made explicit. This will typically replace global exponential convergence results by exponential convergence in a known finite region around the desired trajectory.

Example 8: Consider again the reaction above. The control input u is the inlet concentration of A, and thus must verify

$$0 \leq u \leq 1$$

We can use Theorem 1 to quantify the corresponding extent of convergence: any trajectory within the largest ball around the desired trajectory that does not violate the constraints

$$0 \leq k_1 c_A + k_2 c_A^2 + k_3 c_B + u_d(t) \leq 1$$

will converge exponentially to the desired trajectory. Of course, the desired trajectory itself must satisfy the above constraints. □

Alternatively, the earlier results on switching systems may be applied to such cases. For instance, assume that the system is naturally contracting with respect to a metric $\mathbf{M}$, and controlled with $\mathbf{u} = \mathbf{K} \int \frac{\partial \mathbf{r}}{\partial \mathbf{x}} d\mathbf{x} + \mathbf{u}_d(t)$ using the same metric. Additional input constraints of the form

$$u_{min} \leq u \leq u_{max}$$

lead to a switching between the natural contraction behavior and the stabilized contraction behavior in the same metric. Based on the results on switching systems, the resulting dynamics is still contracting.

Example 9: Consider again the chain reaction above. Since the reaction is exponentially convergent in open-loop, letting

$$u = k_1 c_A + k_2 c_A^2 + u_d(t)$$

with $qk_1 - q - n_1 < 0$, $qk_2 - n_3 < 0$, and bounding u with the constraints $0 \leq u \leq 1$, leads to global exponential convergence. □

Chemical observer design

Similarly, consider again the chemical reaction dynamics (7)

$$\dot{\mathbf{x}} = q\,(\mathbf{x}_f - \mathbf{x}) + \mathbf{N}\mathbf{r}(\mathbf{x})$$

with a linear measurement $\mathbf{y} = \mathbf{H}\mathbf{x}$, where $\mathbf{H}$ is constant. Since only $\mathbf{y}$ is available for feedback, we will denote by $\int_{\mathbf{y}}^{\hat{\mathbf{y}}} \frac{\partial \mathbf{r}}{\partial \mathbf{x}}(\mathbf{x}) d\mathbf{x}$ any function of $\hat{\mathbf{y}}$ whose partial derivatives are within the set spanned by $\frac{\partial r_i}{\partial x_j}(\hat{\mathbf{x}})$, and which equals zero for $\hat{\mathbf{y}} = \mathbf{y}$ − such a function, if it exists, generalizes the usual linear feedback term in $(\hat{\mathbf{y}} - \mathbf{y})$. With the help of a coordinate error feedback (Lohmiller and Slotine, 1998) we can design the observer

$$\begin{aligned} \dot{\bar{\mathbf{x}}} &= q\,(\mathbf{x}_f - \hat{\mathbf{x}}) + \mathbf{N}\mathbf{r}(\hat{\mathbf{x}}) + \mathbf{L}\mathbf{H}\,(\mathbf{N}\mathbf{r}(\hat{\mathbf{x}}) + q\,(\mathbf{x}_f - \mathbf{x})) + \mathbf{K} \int_{\mathbf{y}}^{\hat{\mathbf{y}}} \frac{\partial \mathbf{r}}{\partial \mathbf{x}}(\mathbf{x}) d\mathbf{x} \\ \hat{\mathbf{x}} &= \bar{\mathbf{x}} - \mathbf{L}\mathbf{y} \end{aligned}$$

leading to the observer dynamics

$$\dot{\hat{\mathbf{x}}} = q\,(\mathbf{x}_f - \hat{\mathbf{x}}) + \mathbf{N}\mathbf{r}(\hat{\mathbf{x}}) + \mathbf{L}\mathbf{H}\mathbf{N}\,(\mathbf{r}(\hat{\mathbf{x}}) - \mathbf{r}(\mathbf{x})) + \mathbf{K} \int_{\mathbf{y}}^{\hat{\mathbf{y}}} \frac{\partial \mathbf{r}}{\partial \mathbf{x}}(\mathbf{x}) d\mathbf{x} \tag{13}$$

The Jacobian of (13) can be rewritten as

$$-q\mathbf{I} + \sum_{i=1}^{p} \sum_{j=1}^{n} (\mathbf{N} + \mathbf{L}\mathbf{H}\mathbf{N} + \mathbf{K})_{ij} \frac{\partial r_i}{\partial x_j}(\hat{\mathbf{x}})$$

where the j'th column of $(\mathbf{N} + \mathbf{L}\mathbf{H}\mathbf{N} + \mathbf{K})_{ij}$ is the i'th column of $(\mathbf{N} + \mathbf{L}\mathbf{H}\mathbf{N} + \mathbf{K})$ and the remaining elements are zero. Again, identical $\frac{\partial r_i}{\partial x_j}$ can be combined. Assuming as earlier a constant metric $\mathbf{M} > \mathbf{0}$, the system is contracting if

$$\forall i, j \quad \exists\, \mathbf{L}, \mathbf{K} \qquad (\mathbf{N} + \mathbf{L}\mathbf{H}\mathbf{N} + \mathbf{K})_{ij}^T \mathbf{M} + \mathbf{M}\,(\mathbf{N} + \mathbf{L}\mathbf{H}\mathbf{N} + \mathbf{K})_{ij} \;\leq\; \mathbf{0} \tag{14}$$

Again, (Boyd, et al., 1994) provide general numerical schemes to solve (14) for $\mathbf{M} > \mathbf{0}$, $\mathbf{K}$ and $\mathbf{L}$ if feasible.

Example 10: Consider the temperature-dependent reaction $A \to B$ in an open stirred tank

$$\frac{d}{dt}\begin{pmatrix} c_A \\ T \end{pmatrix} = q\begin{pmatrix} c_{Af} - c_A \\ T_f - T \end{pmatrix} + \begin{pmatrix} -1 \\ -1 \end{pmatrix} e^{-\frac{E}{T}} c_A$$

with c_A the concentration of A, c_{Af} the inlet concentration of A, T the measured temperature, T_f the inlet temperature, q the specific inlet flow rate, and E the specific activation energy. Define the observer

$$\frac{d}{dt}\begin{pmatrix} \hat{c}_A \\ \hat{T} \end{pmatrix} = q\begin{pmatrix} c_{Af} - \hat{c}_A \\ T_f - \hat{T} \end{pmatrix} + \begin{pmatrix} -1 \\ -1 \end{pmatrix} e^{-\frac{E}{T}} \hat{c}_A + \begin{pmatrix} k_1 \\ k_2 \end{pmatrix} \int_T^{\hat{T}} e^{-\frac{E}{T}} dT$$

This observer design is contracting if $\exists k_1, k_2, \mathbf{M}$ such that

$$\begin{aligned} \mathbf{0} &< \mathbf{M} = \begin{pmatrix} M_{11} & M_{12} \\ M_{12} & M_{22} \end{pmatrix} \\ \mathbf{0} &\geq \begin{pmatrix} 0 & -M_{11} - M_{12} \\ -M_{11} - M_{12} & -2M_{12} - 2M_{22} \end{pmatrix} \\ \mathbf{0} &\geq \begin{pmatrix} -2M_{11} - 2M_{12} & k_1 M_{11} + (k_2 - 1)M_{12} - M_{22} \\ k_1 M_{11} + (k_2 - 1)M_{12} - M_{22} & 2k_1 M_{12} + 2k_2 M_{22} \end{pmatrix} \end{aligned}$$

One can easily verify that these conditions are met, and thus the observer design is contracting, for $k_1 \geq k_2$ and $k_2 \leq 0$.

System responses to the input $c_{Af} = 0.2 \sin t + 0.5$ and $T_f = 50 \sin t + 300$, volume flow $q = 0$, activation energy $E = 500$ and initial conditions $c_A(0) = 0.5$, $T(0) = 300$, $\hat{c}_A(0) = 1.0$, $\hat{T}(0) = 400$ are illustrated in Figure 3 and Figure 4. The solid line represents the actual plant, the dashed line represents an observer design with $k_1 = -0.04$ and $k_2 = -10.0$ and the dotted line represents an identity observer ($k_1 = 0$ and $k_2 = 0$). Both observer designs are contracting, however the feedback observer has an increased convergence rate. Note that a coordinate error feedback would allow to augment the natural reaction rate coefficients -1.

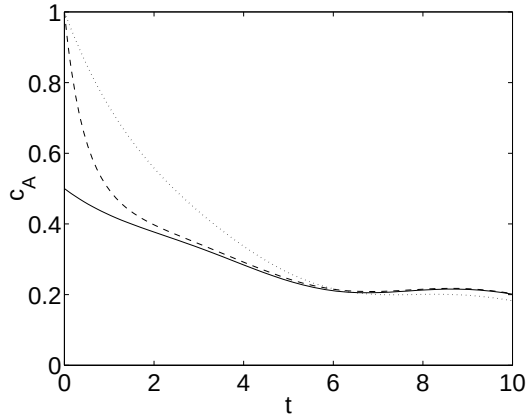

Figure 3: Observer and plant dynamics: concentration c_A

Figure 5 and Figure 6 describe the same responses under temperature measurement "noise" $\sin 10t + 3 \cos t$. The identity observer is unaffected whereas the feedback observer converges according to (Lohmiller and Slotine, 1998) to a bounded ball around the actual plant trajectory. □

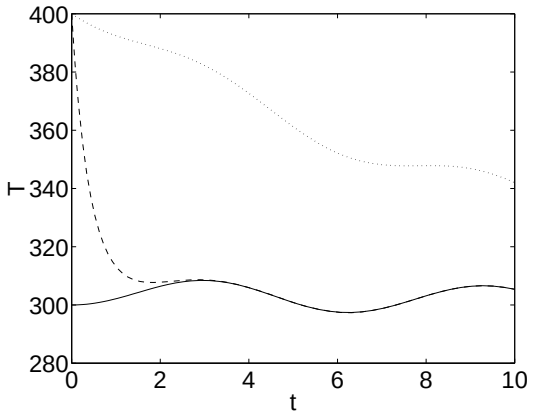

Figure 4: Observer and plant dynamics: temperature T

Since observer trajectories do not necessarily remain in the convex region $\hat{c}_i \geq 0, \hat{T} > 0$, if needed they can be restricted to that region with the means of the section on convex constraints.

Finally, in the case that the activation energies $E_i > 0$ are unknown, but constant, the above procedure can still be applied, by augmenting the system dynamics (7) with $\dot{E}_i = 0$ and the reaction rate vector $\mathbf{r}$ with $q\mathbf{x}$. Indeed, this preserves the monotonicity of the augmented $\mathbf{r}$ with respect to the augmented state. The convex condition $\hat{E}_i > 0$ can be enforced similarly. However, we can in general only expect semi-contraction behavior, the implications of which are detailed earlier in the section on semi-contracting systems.

Concluding Remarks

This paper exploits the monotonicity of chemical reaction rates and the linear ambiguity in the choice of state to analyze the stability of nonlinear chemical reaction processes. A corresponding nonlinear controller and observer design directly results from this physical interpretation. Extensions to distributed nonlinear reaction-diffusion-convection processes are the subject of a separate publication.

From a general control perspective, one can easily see that, conversely, the technique can be applied to any nonlinear dynamics with constant linear ambiguities in the choice of state. Extending further the work above to a state dependent metric $\mathbf{M}(\mathbf{x})$ is a topic of current research.

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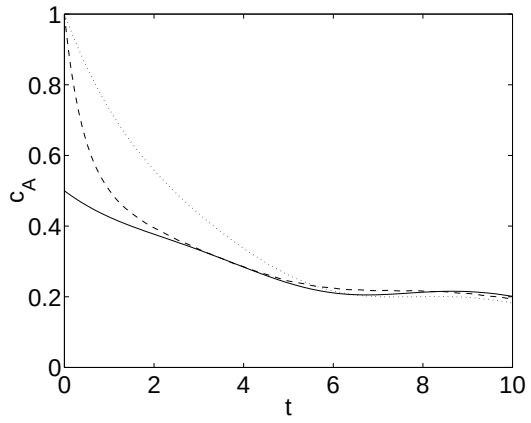

Figure 5: Observer and plant dynamics with measurement noise: c_A

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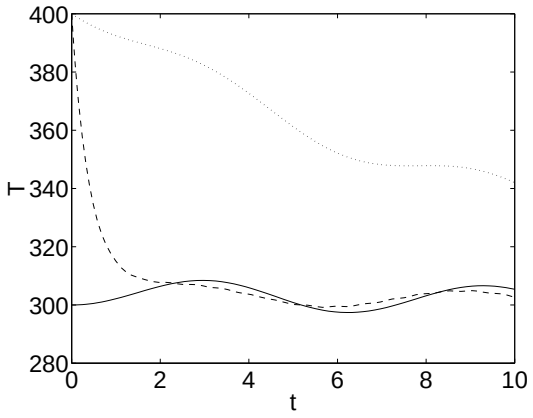

Figure 6: Observer and plant dynamics with measurement noise: T

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