OPTIMAL FEEDBACK CONTROL OF BATCH REACTORS WITH A STATE INEQUALITY CONSTRAINT AND FREE TERMINAL TIME

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Abstract—In this paper we derive optimal state feedback laws for end-point optimization of a dynamic system where the final time is free and the system has a scalar inequality constraint. The existence of a singular region as well as the *nature* of the state feedback law (static or dynamic) is completely characterized in terms of the system dynamics. Explicit synthesis formulae for the state feedback laws are presented. Once the state feedback laws for end-point optimization have been derived, issues on how these laws can be implemented as part of a closed-loop scheme are discussed. As illustrative examples of application of the proposed methodology, several end-point optimization problems in batch chemical reactors are considered.

INTRODUCTION

Batch and semi-batch processes are of great importance to the chemical industry. A wide variety of speciality chemicals such as antibiotics and polymers are produced in batch reactors. Since batch reactors produce low-volume, high value products, optimal operation is very important. In a previous paper (Palanki *et al.*, 1993), we had synthesized optimal feedback laws for end-point optimization of batch processes with fixed final time. In this paper we will study the general problem of synthesizing optimal state feedback laws which guarantee optimality when the system has a *state inequality constraint* and the final time of the batch is left *free*.

State inequality constraints are usually physical constraints to the system. For example, in a semi-batch reactor one can feed only a finite amount of substrate due to a volume constraint on the reactor. Similarly, one may not want to operate a reactor beyond a certain maximum temperature for safety reasons. In a fed-batch bioreactor there could be constraints on the cell mass concentration (beyond which oxygen transfer is limited) or the substrate concentration (beyond which undesirable side reactions occur). Due to batch-to-batch variation in yield, the final time may not be fixed *a priori*. The reactor operation is stopped when the optimum yield is achieved. Thus, it is important to consider yield optimization problems with state inequality constraints and free terminal time. The purpose of this paper is to develop state feedback laws for such optimization problems.

FORMULATION OF THE END-POINT OPTIMIZATION PROBLEM: THE CLASSICAL OPTIMAL CONTROL PERSPECTIVE

The end-point optimization problem can be mathematically formulated as follows:

Minimize the performance index,

$$J = \phi(x(t_f), t_f) \tag{1}$$

subject to the dynamics

$$\dot{x} = f(x) + g(x)u, \quad 0 \leqslant t \leqslant t_f \quad u_{\min} \leqslant u \leqslant u_{\max}$$

$$x(0) = x_0 \tag{2}$$

and the scalar state inequality constraint:

$$C(x) \leqslant 0. \tag{3}$$

In this formulation u is the scalar manipulated input bounded by $u_{\min}$ and $u_{\max}$, x is the n-vector of states, t_f is the free final time, $f(x)$ and $g(x)$ are smooth vector functions and $\phi(x)$ is a smooth scalar function such that

$$g(x) \neq [0\ 0 \ldots 0]$$

$$\frac{\partial \phi}{\partial x} \neq [0\ 0 \ldots 0] \tag{4}$$

for all x.

The part of the optimal solution where the state constraint is hit ($C(x) = 0$) is called the *constrained arc* or the *boundary arc*. The part of the solution where $C(x) < 0$ is called the *unconstrained arc* or the *interior arc*.

Necessary conditions for optimality on an unconstrained arc

By Pontryagin's Principle, the minimization problem (1) is equivalent to minimizing the Hamiltonian:

$$H(x, \lambda, u) = \lambda^T f(x) + \lambda^T g(x)u \tag{5}$$

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where λ is the solution of

$$\lambda^T = -\lambda^T \frac{\partial f}{\partial x}(x) - \lambda^T \frac{\partial g}{\partial x}(x)u$$

$$\lambda(t_f) = \frac{\partial \phi(x, t_f)}{\partial x}\bigg|_{t=t_f}. \tag{6}$$

The coefficient of u in eq. (5), $\lambda^T g(x)$, is called the *switching function*. When the switching function is negative, $u = u_{max}$ and when the switching function is positive, $u = u_{min}$. The region where the switching function vanishes is called the *singular region*. In the singular region,

$$\lambda^T g(x) = 0. \tag{7}$$

Therefore its successive time derivatives are also zero. Thus, we have:

$$\frac{d}{dt}(\lambda^T g(x)) = 0$$

$$\frac{d^2}{dt^2}(\lambda^T g(x)) = 0. \tag{8}$$

$$\vdots$$

This sequence of differentiations is performed until u appears explicitly. The resulting expression can then be solved for u in terms of x and λ. Furthermore, since the final time is free (Bryson and Ho, 1975)

$$\left(\frac{\partial \phi}{\partial t} + H\right)_{t=t_f} = 0. \tag{9}$$

When the objective function ϕ is not an explicit function of the final time t_f, we obtain

$$(H)_{t=t_f} = 0. \tag{10}$$

Furthermore, since the functions f and g are not explicit functions of time, the Hamiltonian H is constant on the optimal trajectory (Bryson and Ho, 1975). Thus,

$$H = (H)_{t=t_f} = 0. \tag{11}$$

Since, $\lambda^T g(x) = 0$ in the singular region, we have, from equation (11),

$$\lambda^T f(x) = 0 \tag{12}$$

in the *singular* region. This can be used as an extra first-order necessary condition for optimality when the objective function ϕ is not an *explicit* function of the final time t_f.

Necessary conditions for optimality on a constrained arc

On the constrained arc

$$C(x) = 0. \tag{13}$$

The Hamiltonian H is defined as

$$H = \lambda^T f(x) + \lambda^T g(x)u + \mu(t)C(x) \tag{14}$$

where

$$\mu(t) \geqslant 0 \tag{15}$$

and the adjoint states are defined as (Bryson *et al.*, 1963)

$$\frac{d\lambda^T}{dt} = -\lambda^T \frac{\partial f(x)}{\partial x} - \lambda^T \frac{\partial g(x)}{\partial x}u - \mu(t)\left[\frac{\partial C(x)}{\partial x}\right]. \tag{16}$$

On the constraint boundary, $\mu(t)$ is so chosen that

$$\frac{\partial H}{\partial u} = \lambda^T g(x) = 0. \tag{17}$$

Thus, the boundary arc is a *singular arc* in the sense of the minimum principle (Maurer, 1977).

Solution of optimization problem

There are $2n + 2$ equations [n state equations, n adjoint equations, eq. (9), and eq. (17)] and $2n + 2$ variables [n state variables, n adjoint variables, the final time t_f and the parameter $\mu(t)$]. However, the boundary conditions for the state and adjoint equations are split, i.e. the initial conditions of the state equations and the terminal conditions of the adjoint equations are known. Thus, we have a two point boundary value problem which can be computationally quite expensive to solve. Furthermore, in this formulation, the numerical problem has to be solved separately every time there is a change in initial conditions or model parameters. The optimal solution has to be implemented in an *open-loop* fashion and so uncertainties and disturbances to the process are not attenuated. These problems can be alleviated if the optimal solution is derived as a state feedback law.

END-POINT OPTIMIZATION OF FREE TIME PROBLEMS: A GEOMETRIC PERSPECTIVE

The previous sub-section gave an overview of the classical optimal control formulation. In the present subsection it will be seen that geometric tools can be used to obtain a more concrete and transparent representation of the necessary conditions for optimality. These results will be used to develop a general framework for end-point optimal state feedback synthesis.

Throughout this section, we will make the standing assumption that $g(x), ad_f^1 g(x), \ldots, ad_f^{n-1} g(x)$ are linearly independent *almost everywhere in x*, where $ad_f^k g(x)$ is the system Lie bracket of order k. This assumption guarantees local controllability of the system almost everywhere (Hunt, 1982) and is equivalent to

$$\det [g(x) \vdots ad_f^1 g(x) \vdots \ldots \vdots ad_f^{n-1} g(x)] \neq 0. \tag{18}$$

Optimal state feedback laws on unconstrained arcs

Definition 1 (*Krener, 1977; Palanki* et al., *1993*): *The system governed by eq. (2) has a finite* **degree of singularity** s *if*

$$[g, ad_f^v g](x) \in \text{span}\{g(x), ad_f^1 g(x), \ldots, ad_f^v g(x)\}$$

$$\textit{for all } v \leqslant s - 1 \tag{19}$$

$$[g, ad_f^s g](x) \notin \text{span}\{g(x), ad_f^1 g(x), \ldots, ad_f^s g(x)\}. \tag{20}$$

The system governed by equation (2) has an **infinite degree of singularity** (s = ∞) if

$$[g, ad_f^v g](x) \in \text{span}\{g(x), ad_f^1 g(x), \ldots, ad_f^v g(x)\}$$

$$\text{for all } v \geqslant 0. \quad (21)$$

Since $g(x), ad_f^1 g(x), \ldots, ad_f^{n-1} g(x)$ are assumed to be linearly independent, it follows from the definition that $1 \leqslant s \leqslant (n-2)$ or $s = \infty$.

The following proposition is a rather straightforward consequence of known results (see Gabasov and Kirillova, 1972).

Proposition 1: *Consider a system governed by eq. (2) with finite degree of singularity s. Then s is odd and the first-order necessary conditions for optimality for a singular extremal can be written as follows:*

$$\lambda^T ad_f^k g(x) = 0 \quad k = 0, 1, 2, \ldots, s$$

$$\lambda^T ad_f^{s+1} g(x) + \lambda^T [g, ad_f^s g](x) u = 0. \quad (22)$$

Furthermore, the second-order necessary condition for optimality in the singular region takes the form

$$(-1)^{\frac{s+1}{2}} \lambda^T [g, ad_f^s g](x) \geqslant 0. \quad (23)$$

If eq. (2) has an infinite degree of singularity, then the first-order necessary conditions for optimality take the form $\lambda^T ad_f^v g(x) = 0$ for all $v \geqslant 0$.

If ϕ is independent of the final time t_f, then an additional necessary condition for optimality in the singular region is

$$\lambda^T f(x) = 0.$$

Theorem 1: *Consider a system of the form of eq. (2) with degree of singularity s = ∞. If f(x) is linearly dependent on g(x), ad_f^1 g(x), \ldots, ad_f^{n-2} g(x) almost everywhere or the performance index depends explicitly on the free final time, then the state trajectories corresponding to a singular extremal evolve on the following surface:*

$$S(x) = \det [g(x) \vdots ad_f^1 g(x) \vdots \ldots \vdots ad_f^{n-1} g(x)] = 0. \quad (24)$$

Proof: See Appendix A.   □

Theorem 2: *Consider a system of the form of eq. (2) with degree of singularity s = n − 2. (i) If f(x) is linearly independent of g(x), ad_f^1 g(x), \ldots, ad_f^{n-2} g(x) almost everywhere and the performance index does not depend explicitly on the free final time, then the state trajecto-*

ries corresponding to a singular extremal evolve on the surface given by

$$S(x) =$$

$$\det [f(x) \vdots g(x) \vdots ad_f^1 g(x) \vdots \ldots \vdots ad_f^{n-2} g(x)] = 0. \quad (25)$$

(ii) *If f(x) is linearly dependent on g(x), ad_f^1 g(x), \ldots, ad_f^{n-2} g(x) or the performance index depends explicitly on the free final time, then the optimal static state feedback is given by*

$$u = -\frac{\det [g(x) \vdots ad_f^1 g(x) \vdots \ldots \vdots ad_f^{n-1} g(x)]}{\det [g(x) \vdots ad_f^1 g(x) \vdots \ldots \vdots ad_f^{n-2} g(x) \vdots [g, ad_f^{n-2} g](x)]}. \quad (26)$$

Proof: See Appendix B.   □

Theorem 3: *Consider a system of the form of eq. (2) with degree of singularity s = n − 3. (i) If f(x) is linearly independent of g(x), ad_f^1 g(x), \ldots, ad_f^{n-2} g(x) and the performance index does not depend explicitly on the free final time, then the optimal static state feedback is given by*

$$u = -\frac{\det [f(x) \vdots g(x) \vdots ad_f^1 g(x) \vdots \ldots \vdots ad_f^{n-2} g(x)]}{\det [f(x) \vdots g(x) \vdots ad_f^1 g(x) \vdots \ldots \vdots ad_f^{n-3} g(x) \vdots [g, ad_f^{n-3} g](x)]}. \quad (27)$$

(ii) *If f(x) is linearly dependent on g(x), ad_f^1 g(x), \ldots, ad_f^{n-2} g(x) or the performance index depends explicitly on the free final time, then the optimal dynamic state feedback is given by*

$$\Phi\left(x, u, \frac{du}{dt}\right) = 0 \quad (28)$$

where Φ is an algebraic function. This is obtained by setting the determinant of

$$g(x)$$

$$ad_f^1 g(x)$$

$$\vdots$$

$$ad_f^{n-3} g(x)$$

$$ad_f^{n-2} g(x) + [g, ad_f^{n-3} g](x) u(t) \quad (29)$$

$$ad_f^{n-1} g(x) + [g, ad_f^{n-2} g](x) u(t)$$

$$+ \left(I \frac{d}{dt} - \frac{\partial f(x)}{\partial x} - \frac{\partial g(x)}{\partial x} u(t)\right)([g, ad_f^{n-3} g](x) u(t))$$

equal to zero.

In the above equations, I is the identity matrix and $\frac{d(.)}{dt}$ is the total time derivative operator,

$$\frac{d(.)}{dt} = [f(x) + g(x) u(t)] \frac{\partial(.)}{\partial x} + \frac{\partial(.)}{\partial t}.$$

Theorem 4: *Consider a system of the form of eq. (2) with degree of singularity s ⩽ n − 4. (i) If f(x) is linearly*

independent of $g(x)$, $ad_f^1 g(x)$, ..., $ad_f^{n-2} g(x)$ *and the performance index does not depend explicitly on the free final time, then the optimal dynamic state feedback is given by*

$$\Phi\left(x, u, \frac{du}{dt}, \ldots, \frac{d^{n-s-3}u}{dt^{n-s-3}}\right) = 0$$

where Φ is an algebraic function. This is obtained by setting the determinant of

$$f(x)$$
$$g(x)$$
$$ad_f^1 g(x)$$
$$\vdots$$
$$ad_f^{s-1} g(x)$$
$$ad_f^s g(x) + [g, ad_f^{s-1}g](x) u(t) \qquad (30)$$
$$ad_f^{s+1} g(x) + [g, ad_f^s g](x) u(t)$$
$$+ \left(I\frac{d}{dt} - \frac{\partial f(x)}{\partial x} - \frac{\partial g(x)}{\partial x} u(t)\right)([g, ad_f^{s-1}g](x) u(t))$$
$$\vdots$$
$$ad_f^{n-2} g(x) + \sum_{k=0}^{n-s-3}\left(I\frac{d}{dt} - \frac{\partial f(x)}{\partial x}\right.$$
$$\left. - \frac{\partial g(x)}{\partial x} u(t)\right)^k ([g, ad_f^{n-k-3}g](x) u(t))$$

equal to zero.

(ii) *If* $f(x)$ *is linearly dependent on* $g(x)$, $ad_f^1 g(x)$, ..., $ad_f^{n-2} g(x)$ *or the performance index depends explicitly on the free final time, then the optimal dynamic state feedback is given by*

$$\Phi\left(x, u, \frac{du}{dt}, \ldots, \frac{d^{n-s-2}u}{dt^{n-s-2}}\right) = 0$$

where Φ is an algebraic function. This is obtained by setting the determinant of

$$g(x)$$
$$ad_f^1 g(x)$$
$$\vdots$$
$$ad_f^s g(x)$$
$$ad_f^{s+1} g(x) + [g, ad_f^s g](x) u(t) \qquad (31)$$
$$ad_f^{s+2} g(x) + [g, ad_f^{s+1}g](x) u(t)$$
$$+ \left(I\frac{d}{dt} - \frac{\partial f(x)}{\partial x} - \frac{\partial g(x)}{\partial x} u(t)\right)([g, ad_f^s g](x) u(t))$$
$$\vdots$$
$$ad_f^{n-1} g(x) + \sum_{k=0}^{n-s-2}\left(I\frac{d}{dt} - \frac{\partial f(x)}{\partial x}\right.$$
$$\left. - \frac{\partial g(x)}{\partial x} u(t)\right)^k ([g, ad_f^{n-k-2}g](x) u(t))$$

equal to zero.

Proof: See Appendix D. □

Optimal state feedback laws on constrained arcs

On the constrained arc, the optimization problem is reduced to the following regulation problem:

Regulate the output

$$y = C(x) \qquad (32)$$

with zero set point subject to dynamics:

$$\dot{x} = f(x) + g(x)u. \qquad (33)$$

At the point where the system enters or leaves a constrained arc, a feasible *unconstrained arc* passing through this point must satisfy certain tangency conditions, namely, this arc must have zero values of the state variable constraint and all its time derivatives that *do not* involve the control variable (Speyer and Bryson, 1968). Thus, if the relative order of the system (33) is r, then at the entry point, exit point and on the constrained arc, the following tangency conditions must be satisfied:

$$C(x) = L_f^0 C(x) = 0$$
$$\frac{dC(x)}{dt} = L_f^1 C(x) = 0$$
$$\vdots \qquad (34)$$
$$\frac{d^{r-1}C(x)}{dt^{r-1}} = L_f^{r-1} C(x) = 0.$$

If the system possesses a finite relative order, a state feedback for this regulation problem can be found by standard techniques. For instance (Kravaris and Chung, 1987) the state transformation,

$$u = \psi(x, v) = \frac{v - \sum_{k=0}^{r} \beta_k L_f^k C(x)}{\beta_r L_g L_f^{r-1} C(x)} \qquad (35)$$

transforms the system (33) into an input/output linear system of the form

$$\sum_{k=0}^{r} \beta_k \frac{d^k y}{dt^k} = v \qquad (36)$$

where $\beta_0, \beta_1, \ldots, \beta_r$ are completely arbitrary. When the poles of the v–y system are appropriately placed "far left" in the complex plane, one can use an external linear controller to force the system output $y(t)$ to zero.

Implementation

In the previous section, state feedback laws have been derived for the unconstrained as well as the constrained regions. To implement the optimal state feedback laws as a closed-loop scheme, the sequence in which singular, nonsingular and constrained arcs appear should be known *a priori*. Furthermore, the switching times between singular, non-singular and constrained arcs is required. The switch to a constrained arc from an unconstrained arc occurs when the system reaches the constraint boundary. The switch to a singular arc can be calculated analytically

for a restricted class of systems [for example, for systems where a switching surface such as eqs (24) and (25) can be calculated]. In most practical situations, these have to be computed numerically. From the off-line solution of the first-order necessary conditions of optimality, the switching times and the values of the system states at the junctions between singular and non-singular regions are known. This information can be used to set up on-line criteria for the onset of the singular region in terms of the system states (Modak, 1988). Alternatively, one can use the *a priori* calculated switching times determined from the off-line analysis. When the state feedback law is dynamic, we

The forward reaction is second order with respect to the concentration of species A while the reverse reaction is first order with respect to the concentration of species B. It is desired to find the optimal temperature profile to minimize the following objective function:

$$J = -(C_B - \varepsilon t_f). \tag{38}$$

There is a constraint on the maximum allowable reactor temperature

$$T - T_{\max} \leqslant 0. \tag{39}$$

The manipulated input is the cooling rate of the reactor. The mass and energy balance for this system are as follows.

$$\frac{d}{dt}\begin{bmatrix} C_A \\ T \end{bmatrix} = \begin{bmatrix} -k_1(T)C_A^2 + k_2(T)(C_{A0} - C_A) \\ \left(\dfrac{-\Delta H}{\rho C_p}\right)(k_1(T)C_A^2 - k_2(T)C_{A0} + k_2(T)C_A) \end{bmatrix} + \begin{bmatrix} 0 \\ \dfrac{T_c - T}{\rho C_p} \end{bmatrix} u \tag{40}$$

also need initial conditions for the dynamic state feedback law. These initial conditions have to be set up in a similar fashion as the switching times. If the model parameters are known *a priori*, the feedback laws derived in the previous sections can be used in conjunction with state estimators. Such an implementation can attenuate errors in the initial conditions

where

$$k_1 = k_{10} \exp\left[\frac{-E_1}{RT}\right]$$

$$k_2 = k_{20} \exp\left[\frac{-E_2}{RT}\right]. \tag{41}$$

This system is of the form (2) with

$$x = \begin{bmatrix} C_A \\ T \end{bmatrix}, \quad f(x) = \begin{bmatrix} -k_1(T)C_A^2 + k_2(T)(C_{A0} - C_A) \\ \left(\dfrac{-\Delta H}{\rho C_p}\right)(k_1(T)C_A^2 - k_2(T)C_{A0} + k_2(T)C_A) \end{bmatrix}, \quad g(x) = \begin{bmatrix} 0 \\ \dfrac{T_c - T}{\rho C_p} \end{bmatrix}. \tag{42}$$

and process disturbances. If some of the model parameters are not accurately known *a priori*, these need to be estimated on-line. In this situation, a parameter estimation algorithm is also required.

If one uses *a priori* determined switching times and model parameters, a successful feedback implementation of the optimal feedback law depends on how sensitive the final performance index is to errors in the switching times. In the absence of rigorous robustness proofs, one resorts to numerical simulations to define a region in the parameter space where the feedback implementation is successful.

The final time can be calculated on-line as follows. Using eqs (5) and (6), it can be shown that

$$(H)_{t=t_f} = \left(\frac{\partial \phi}{\partial x}f(x) + \frac{\partial \phi}{\partial x}g(x)u\right)_{t=t_f} = \left(\frac{\partial \phi}{\partial x}\dot{x}\right)_{t=t_f}.$$

Substituting the right-hand side of the above equation in (9), we obtain

$$\left(\frac{\partial \phi}{\partial t} + H\right)_{t=t_f} = \left(\frac{\partial \phi}{\partial t} + \frac{\partial \phi}{\partial x}\dot{x}\right)_{t=t_f} = \left(\frac{d\phi}{dt}\right)_{t=t_f} = 0. \tag{37}$$

The stopping condition is obtained at the point where the performance index reaches its optimum value.

ILLUSTRATIVE EXAMPLES

Example 1: The following exothermic reversible reaction is taking place in a batch reactor:

$$A \rightleftharpoons B.$$

It can be easily shown that $n = 2$, $s = \infty$ and $g(x)$ and $ad_f^1 g(x)$ are linearly independent almost everywhere in x.

Unconstrained arc

Equation (38) depends explicitly on the final time and so eq. (24) is valid in the singular region. Using eq. (24) we obtain

$$S(C_A, T) = \det[g(x) \vdots ad_f^1 g(x)] = E_1 k_1(T)C_A^2 + E_2 k_2(T)C_A - E_2 k_2(T)C_{A0} = 0. \tag{43}$$

Thus, the optimization problem reduces to regulating the function $S(C_A, T)$ to zero where the system states C_A and T are described by eq. (40). It can be easily verified that the relative order for this regulation problem is unity. Thus, an appropriate nonlinear feedback law for this problem is (see Kravaris and Chung, 1987)

$$u = -\frac{\left[\dfrac{\partial S}{\partial x}f(x) + \beta_1 S\right]}{\dfrac{\partial S}{\partial x}g(x)} \tag{44}$$

where x, $f(x)$ and $g(x)$ are given by eq. (42), the expression for S is given by eq. (43) and β_1 is an adjustable parameter. Substituting for x, $f(x)$, $g(x)$ and

S, we obtain

$$u = -\frac{\frac{\partial S}{\partial C_A}(-k_1 C_A^2 + k_2(C_{A0} - C_A)) + \frac{\partial S}{\partial T}\left(\left(\frac{-\Delta H}{\rho C_p}\right)(k_1 C_A^2 - k_2 C_{A0} + k_2 C_A)\right) + \beta_1 S}{\frac{\partial S}{\partial T}\left(\frac{T_c - T}{\rho C_p}\right)}. \quad (45)$$

Constrained arc

On the constraint boundary the control objective is to keep the system at $C(T) = T - T_{max} = 0$. It can be easily verified that for this system the relative order is unity. Thus, we derive a nonlinear feedback law similar to eq. (44) to obtain

$$u = -\frac{\frac{\partial C}{\partial T}\left(\left(\frac{-\Delta H}{\rho C_p}\right)(k_1 C_A^2 - k_2 C_{A0} + k_2 C_A)\right) + \beta_2 C}{\frac{\partial C}{\partial T}\left(\frac{T_c - T}{\rho C_p}\right)} \quad (46)$$

where β_2 is an adjustable parameter.

Figure 1 shows the optimal temperature profile for the system parameters given in Table 1 and the initial conditions given in Table 2. It was found through numerical simulations that $\beta_1 = 1$ and $\beta_2 = 1$ were appropriate for this system. Figure 2 shows the optimal cooling rate of the reactor. Since the reactant is cold at $t = 0$, there is an initial nonsingular region where $u = 0$. Since the reaction is exothermic, the temperature rises till it hits the constraint T_{max} at time $t = t_b$. In the constraint boundary eq. (46) is used. At $t = t_s$, the singular region is hit and eq. (45) is used.
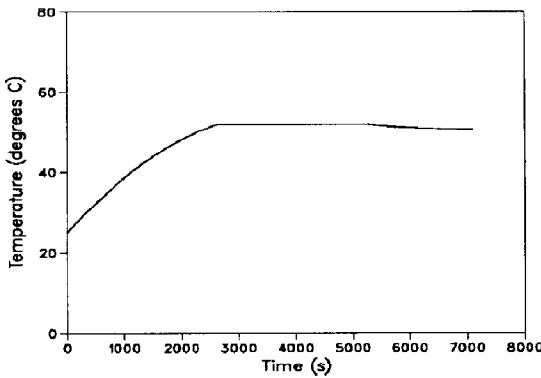
Figure 3 shows the profile of the objective function with time. The final time is determined at the point when there is no further decrease in the objective function. Table 3 shows the various switching times as well as the final product concentration. Figure

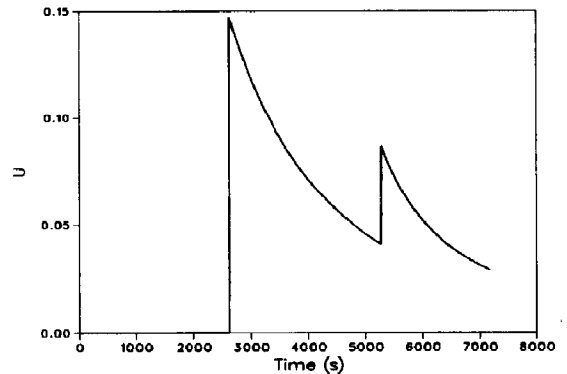Table 2. Initial conditions

C_{A0}	1.0 kg m^{-3}
C_{B0}	0.0 kg m^{-3}
$T(0)$	25°C

Fig. 2. Optimal cooling rate profile (example 1).

Fig. 1. Optimal temperature profile (example 1).

Table 1. Model parameters

k_{10}	1.0 m^3 kg^{-1} s^{-1}
k_{20}	100.0 s^{-1}
E_1	2×10^4 J mol^{-1} K^{-1}
E_2	4×10^4 J mol^{-1} K^{-1}
$-\Delta H$	5×10^4 J mol^{-1} K^{-1}
ρC_p	1000.0 J m^{-3} K^{-1}
ε	1.5×10^{-5} kg s m^{-3}
T_c	15°C
T_{max}	52°C

4 shows the time profile of the first-order condition $\lambda^T g(x)$ and it is observed that in the singular region $\lambda^T g(x) = 0$. It was verified (simulation not shown) that indeed $\left(\frac{\partial \phi}{\partial t} + H\right) = 0$ at the final time.

The constrained optimization problem was compared with the case where there is no state constraint present. Table 3 shows the results. As expected, the objective function takes a longer time to reach its optimum value when the state constraint is present. The robustness of the control law to errors in the kinetic parameters was tested through numerical simulations. In the control law, the values of the parameters k_{10} and k_{20} used were 10% lower than
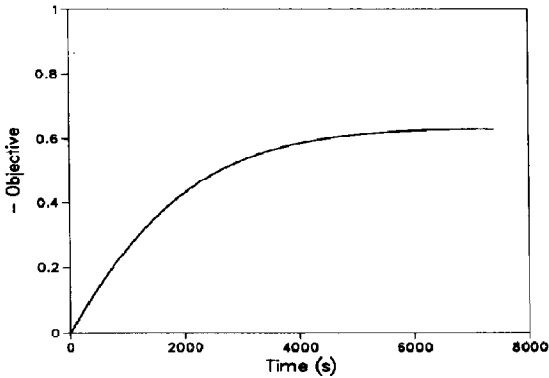
Fig. 3. Profile of objective function (example 1).

Table 3. Constrained vs unconstrained optimization

(Constrained optimization)
Switching time to constrained arc, 2630 s
Switching time to singular arc, 5280 s
Final time, 7170 s
Objective function at final time, −0.629 kg m⁻³

(Unconstrained optimization)
Switching time to singular arc, 4630 s
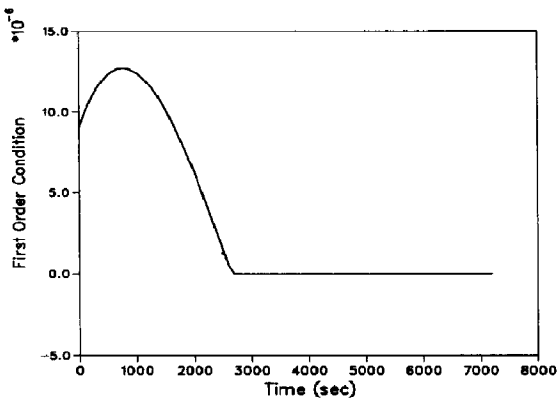Final time, 6750 s
Objective function at final time, −0.629 kg m⁻³

Fig. 4. First-order condition (example 1).

those of the system parameters shown in Table 1. The results are summarized in Table 4. It is observed that the performance index is very close to that obtained in the nominal case, where the true values of the parameters were used in the control law. Similar simulations can be performed by perturbing other parameter values to define a region in the parameter space where the feedback implementation is successful with the *a priori* determined switching times.

Example 2: We consider a yield optimization problem in a semi-batch chemical reactor where the following reactions are occurring:

$$A \rightarrow B$$
$$B \rightarrow C$$
$$A \rightarrow D.$$

The reaction from A to B follows the following kinetics:

$$-r = \frac{k_1 C_A C_B}{k_2 + k_3 C_A + k_4 C_A^2}. \tag{47}$$

All other reactions are first-order reactions. The unsteady state mass balance equations are given by

$$\frac{d(C_A V)}{dt} = -\frac{k_1 C_A C_B V}{k_2 + k_3 C_A + k_4 C_A^2} - k_D C_A V + C_{AF} u$$

$$\frac{d(C_B V)}{dt} = \frac{k_1 C_A C_B V}{k_2 + k_3 C_A + k_4 C_A^2} - k_C C_B V \tag{48}$$

$$\frac{d(C_D V)}{dt} = k_D C_A V$$

$$\frac{dV}{dt} = u.$$

Furthermore, there is a scalar inequality constraint

$$V - V_{max} \leq 0. \tag{49}$$

We will consider two different objective functions.

Case I: (Objective function independent of the final time) The objective function to be minimized at a free final time is

$$J = -C_B V|_{t=t_f} \tag{50}$$

Case II: (Objective function dependent on the final time) The objective function to be minimized at a free

Table 4. Robustness analysis

Parameters in control law	Parameters in process	Performance index
$k_{10} = 1.0$, $k_{20} = 100.0$ All other parameter values from Table 1	$k_{10} = 1.0$, $k_{20} = 100.0$ All other parameter values from Table 1	−0.6296 kg m⁻³
$k_{10} = 0.9$, $k_{20} = 90.0$ All other parameter values from Table 1	$k_{10} = 1.0$, $k_{20} = 100.0$ All other parameter values from Table 1	−0.6295 kg m⁻³

final time is

$$J = - [C_B V - \varepsilon t_f]. \tag{51}$$

Define

$$x_1 = C_A V$$
$$x_2 = C_B V$$
$$x_3 = C_D V \tag{52}$$
$$x_4 = V.$$

The model can be put in the form

$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} -\dfrac{k_1 x_1 x_2 x_4}{k_2 x_4^2 + k_3 x_1 x_4 + k_4 x_1^2} - k_D x_1 \\ \dfrac{k_1 x_1 x_2 x_4}{k_2 x_4^2 + k_3 x_1 x_4 + k_4 x_1^2} - k_C x_2 \\ k_D x_1 \\ 0 \end{bmatrix}$$

$$+ \begin{bmatrix} C_{AF} \\ 0 \\ 0 \\ 1 \end{bmatrix} u. \tag{53}$$

The system model is of the form

$$\dot{x} = f(x) + g(x)u \tag{54}$$

where

$$x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}$$

$$f(x) = \begin{bmatrix} -\dfrac{k_1 x_1 x_2 x_4}{k_2 x_4^2 + k_3 x_1 x_4 + k_4 x_1^2} - k_D x_1 \\ \dfrac{k_1 x_1 x_2 x_4}{k_2 x_4^2 + k_3 x_1 x_4 + k_4 x_1^2} - k_C x_2 \\ k_D x_1 \\ 0 \end{bmatrix}$$

$$g(x) = \begin{bmatrix} C_{AF} \\ 0 \\ 0 \\ 1 \end{bmatrix}.$$

It can be easily shown that for this system $n = 4$ and $s = 1$.

Solution for case I: It is observed that ϕ, f, g are independent of t. Furthermore, $f(x)$, $g(x)$, $ad_f g(x)$ and $ad_f^2 g(x)$ are linearly independent. Thus, from eq. (27),

the optimal static state feedback is given by

$$u = - \frac{\det [f(x) \;\vdots\; g(x) \;\vdots\; ad_f^1 g(x) \;\vdots\; ad_f^2 g(x)]}{\det [f(x) \;\vdots\; g(x) \;\vdots\; ad_f^1 g(x) \;\vdots\; [g; ad_f^1 g](x)]}. \tag{55}$$

Since the reactor starts with a high concentration of A and the reaction rate is decreasing function of A we expect that there will be an initial nonsingular phase which involves feeding of species A. An initial estimate of the switching time was found by performing a one dimensional numerical search as described by Lim *et al.* (1986). This estimate was further refined till the first-order condition $\lambda^T g(x) = 0$ was satisfied on the singular region. When the volume constraint is hit, $u = 0$. The final time, t_f, is determined when the objective function, ϕ reaches its optimum value.

Figures 5 and 6 show the optimal input profile and the profile of the objective function for the system parameters in Table 5 and the initial conditions in Table 6. The various switching times and the objective function at the final time are shown in Table 7. Figures 7 and 8 depict the corresponding time profiles of the switching function ($\lambda^T g(x)$) and the second-order
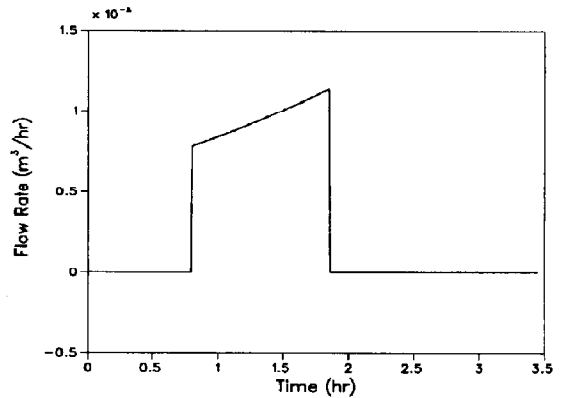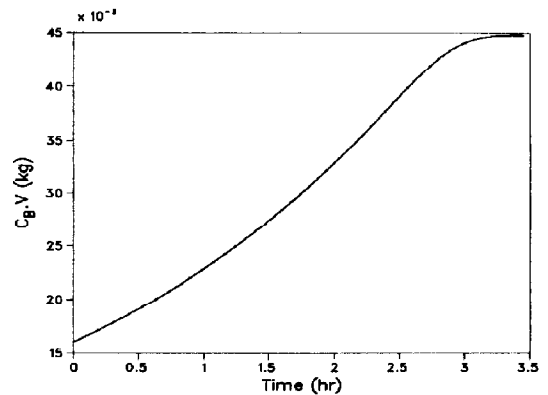

Fig. 5. Optimal input profile (example 2, case I).

Fig. 6. Profile of objective function (example 2, case I).

Table 5. Model parameters

k_1	0.530 m³ kmol⁻¹ h⁻¹
k_2	1.00
k_3	1.00 m³ kmol⁻¹
k_4	1/22 m³ kmol⁻²
k_C	0.01 h⁻¹
k_D	0.01 h⁻¹
ε	2.0

Table 6. Initial conditions

$C_A(0)$	7.5 kg m⁻³
$C_B(0)$	8.0 kg m⁻³
$C_D(0)$	0.0 kg m⁻³
$V(0)$	2.0×10^{-3} m³

Table 7. Constrained optimization (example 2, case I)

Switching time to singular arc, 0.793 h
Switching time to constrained arc, 1.86 h
Final time, 3.39 h
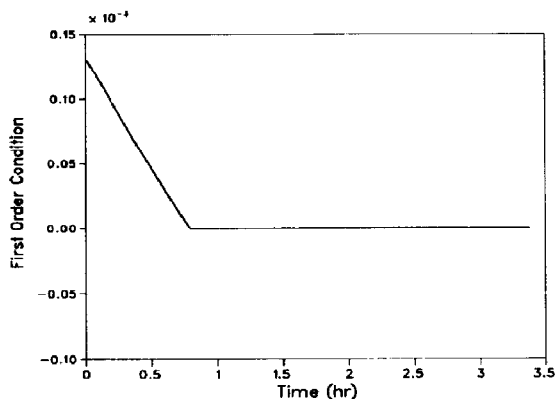Objective function at final time; -44.810×10^{-3} kg
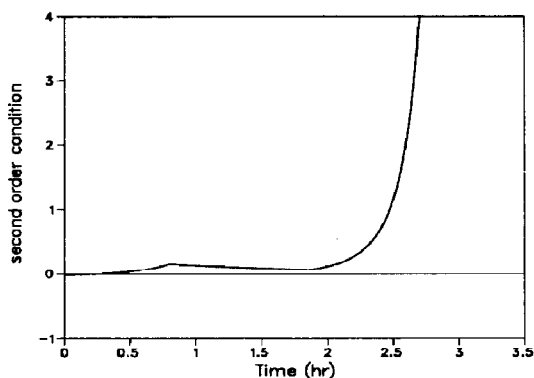

Fig. 7. First-order condition (example 2, case I).

Fig. 8. Second-order condition (example 2, case I).

condition $(-\lambda^T[g, ad_f^1 g](x))$. The switching function vanishes on the singular time interval and is positive everywhere else. The positivity of the switching function is consistent with $u(t)$ taking its minimum value $(u = 0)$ in the nonsingular interval. Furthermore, the second-order condition $-\lambda^T[g, ad_f^2 g](x, t) \geq 0$ is satisfied in the singular region and so the singular extremal is indeed optimal. The final time, t_f, is determined when the objective function ϕ reaches its optimum value. It was verified (simulation not shown) that indeed $H = 0$ everywhere.

The robustness of the state feedback law with respect to errors in the system parameter k_1 was tested through numerical simulations. With the switching time from the nominal case, the static feedback law was implemented using a 13.4% higher k_1 than its true value. The results are summarized in Table 8. It is observed that the performance index is very close to that obtained in the nominal case. Similar simulations can be performed, by perturbing other parameter values, to obtain a region in parameter space where the feedback implementation is successful with the a priori determined switching times.

The sensitivity of the performance index to errors in the switching time to the singular region was checked. Assuming various values of the switching time to the singular region, the feeding profile was calculated using the static state feedback law in the singular region. When the volume constraint was hit, u was set to zero. The final time t_f was determined when the objective function ϕ reached its optimum value. The results are shown in Table 9. It is observed that the final performance index is quite robust to errors in the assumed switching time. From this study we conclude that the performance index is not very sensitive to errors in the switching time and so an a priori estimate of the switching time can be used in closed-loop implementation.

Solution for case II: It can be easily verified that the vector fields $g(x)$, $ad_f^1 g(x)$, $ad_f^2 g(x)$, $ad_f^3 g(x)$ are linearly independent. Thus the optimal state feedback in the singular region will be dynamic. Substituting $n = 4$ and $s = 1$ in eq. (28) we obtain a dynamic feedback law by setting the determinant of

$$
\begin{aligned}
&g(x) \\
&ad_f^1 g(x) \\
&ad_f^2 g(x) + [g, ad_f^1 g](x)u \\
&ad_f^3 g(x) + ([g, ad_f^2 g](x) + [f, [g, ad_f^1 g]])(x) \\
&\quad + [g, [g, ad_f^1 g](x)u]u + [g, ad_f^1 g](x)\frac{du}{dt}
\end{aligned}
\tag{56}
$$

equal to zero.

Figures 9 and 10 show the optimal input profile and the profile of the objective function for the system parameters in Table 5 and the initial conditions in Table 6. The various switching times and the objective function at the final time are shown in Table 10. Figures 11 and 12 depict the corresponding time pro-

Table 8. Robustness analysis

Parameters in control law	Parameters in process	Performance index	Final time
$k_1 = 0.530$ All other parameter values from Table 5	$k_1 = 0.530$ All other parameter values from Table 5	-44.810×10^{-3} kg	3.39 h^{-1}
$k_1 = 0.600$ All other parameter values from Table 5	$k_1 = 0.530$ All other parameter values from Table 5	-44.718×10^{-3} kg	3.39 h^{-1}

Table 9. Sensitivity of error in switching time on performance index

Assumed switching time (h)	Performance index (kg)	Final time (h)
0.75	-44.676×10^{-3}	3.31
0.791	-44.810×10^{-3}	3.39
0.85	-44.760×10^{-3}	3.39
0.90	-44.720×10^{-3}	3.39

Fig. 9. Optical input profile (example 2, case II).

Fig. 10. Profile of objective function (example 2, case II).

Table 10. Constrained optimization (example 2, case II)

Switching time to singular arc, 0.793 h
Switching time to constrained arc, 1.86 h
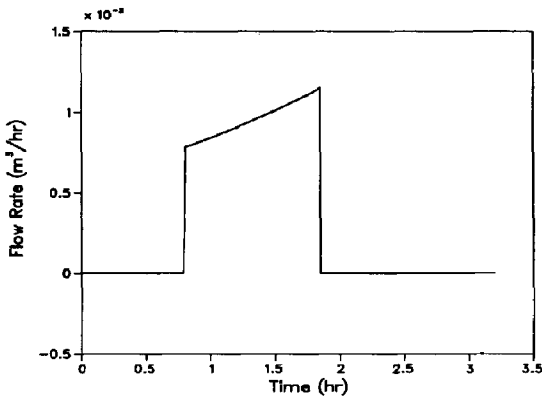Final time, 3.19 h
Objective function at final time, -38.3×10^{-3} kg
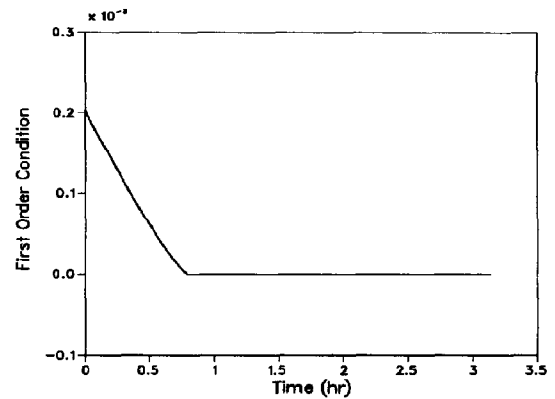
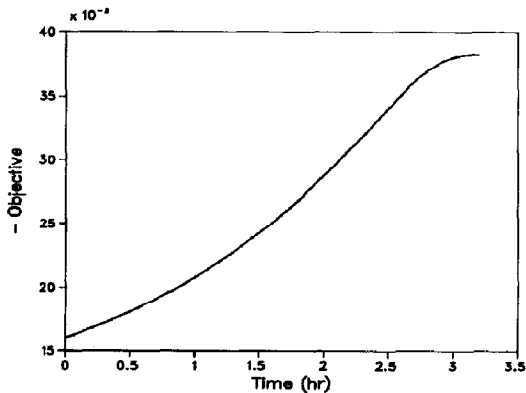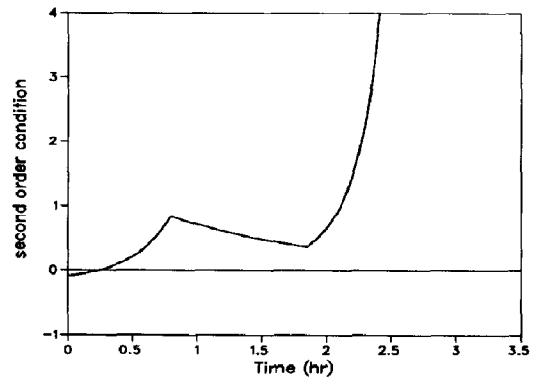Fig. 11. First-order condition (example 2, case II).

Fig. 12. Second-order condition (example 2, case II).

Table 11. Sensitivity of error in initial condition of $u(t)$ on performance index

Assumed initial condition of $u(t)$	Performance index (kg)
0.60	-38.3×10^{-3}
0.75	-38.3×10^{-3}
0.90	-38.3×10^{-3}

Table 12. Robustness analysis

Parameters in control law	Parameters in process	Performance index
$k_1 = 0.530$ All other parameter values from Table 5	$k_1 = 0.530$ All other parameter values from Table 5	-38.3×10^{-3} kg
$k_1 = 0.56$ All other parameter values from Table 5	$k_1 = 0.530$ All other parameter values from Table 5	-38.3×10^{-3} kg
$k_1 = 0.59$ All other parameter values from Table 5	$k_1 = 0.530$ All other parameter values from Table 5	-38.3×10^{-3} kg

files of the switching function $(\lambda^T g(x))$ and the second-order condition $(-\lambda^T[g, ad_f^j g](x))$. The switching function vanishes on the singular time interval and is positive everywhere else. The positivity of the switching function is consistent with $u(t)$ taking its minimum value $(u = 0)$ in the nonsingular interval. Furthermore, the second-order condition $-\lambda^T[g, ad_f^j g](x, t) \geqslant 0$ is satisfied in the singular region and so the singular extremal is indeed optimal. The final time t_f is determined when the objective function ϕ reaches its optimum value. It was verified (simulation not shown) that indeed $\left(\dfrac{\partial \phi}{\partial t} + H\right) = 0$ at the final time.

Since the optimal state feedback is dynamic, we need the initial condition of u to implement the state feedback law. The effect of error in the initial condition of u on the final performance index was studied. The results are shown in Table 11. It is observed that the final performance index is very robust to errors in the assumed initial condition for $u(t)$.

From this study we conclude that the performance index is not sensitive at all to errors in the initial condition for $u(t)$ in the range of initial conditions considered and so an a priori estimate of the initial condition for $u(t)$ can be used in closed-loop implementation.

The robustness of the dynamic state feedback law with respect to errors in the system parameter k_1 was tested. The results are summarized in Table 12. It is observed that the performance index is very close to that obtained in the nominal case. Similar simulations can be performed by perturbing other parameter values to determine the region in parameter space where the feedback implementation is successful.

NOTATION

C_A	concentration of species A, kg m^{-3}
C_{AF}	concentration of species A in feed, kg m^{-3}
C_B	concentration of species B, kg m^{-3}
C_C	concentration of species C, kg m^{-3}
C_D	concentration of species D, kg m^{-3}
C_p	specific heat, J kg^{-1} K^{-1}
E_1, E_2	activation energies, J mol^{-1} K^{-1}
H	Hamiltonian
H_u	first derivative of Hamiltonian with respect to u
H_{uu}	second derivative of Hamiltonian with respect to u
I	identity matrix
J	performance index
k_B	kinetic rate constant of reaction A → B, h^{-1}
$L_f^k C(x)$	kth Lie derivative of $f(x)$ and $C(x)$
T	temperature, K
V	volume, m^3
$ad_f^1 g(x)$	Lie bracket $\{[f, g](x)\}$
$ad_f^k g(x)$	Lie bracket of order k $\{[f, ad_f^{k-1} g](x)\}$
det	determinant
f	vector function in dynamic model
g	vector function in dynamic model
k_1	kinetic rate constant
k_2	kinetic rate constant
k_3	kinetic rate constant
k_4	kinetic rate constant
k_C	kinetic rate constant of reaction B → C, h^{-1}
k_D	kinetic rate constant of reaction A → D, h^{-1}
n	number of state equations (dimension of state vector x)
s	degree of singularity
t	time
t_f	final time
u	manipulated input
x	vector of system states
y	output

Greek symbols

β	adjustable parameter
λ	vector of adjoint states
ϕ	scalar function expressing the performance index in terms of the system states
ρ	density, kg m^{-3}

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APPENDIX A: PROOF OF THEOREM 1

The first-order necessary conditions on the singular extremal are as follows:

$$\lambda^T g(x) = 0$$
$$\lambda^T ad_f^1 g(x) = 0$$
$$\lambda^T ad_f^2 g(x) = 0$$
$$\vdots \qquad (57)$$
$$\lambda^T ad_f^{n-2} g(x) = 0$$
$$\lambda^T ad_f^{n-1} g(x) = 0.$$

Eliminating the *n*-vector of adjoint states, we obtain the singular surface (24) on which the state trajectories corresponding to the singular extremal evolve.

APPENDIX B: PROOF OF THEOREM 2

Proof for (i): The first-order necessary conditions are given by

$$\lambda^T f(x) = 0$$
$$\lambda^T g(x) = 0$$
$$\lambda^T ad_f^1 g(x) = 0$$
$$\lambda^T ad_f^2 g(x) = 0 \qquad (58)$$
$$\vdots$$
$$\lambda^T ad_f^{n-2} g(x) = 0.$$

Eliminating the *n* adjoint states from the above *n* independent equations, we obtain the singular surface (25) on which the state tajectories corresponding to the singular extremal evolve.

Proof for (ii): The first-order necessary conditions are given by

$$\lambda^T g(x) = 0$$
$$\lambda^T ad_f^1 g(x) = 0$$
$$\vdots \qquad (59)$$
$$\lambda^T ad_f^{n-2} g(x) = 0$$
$$\lambda^T ad_f^{n-1} g(x) + \lambda^T [g, ad_f^{n-2} g](x) u = 0.$$

Since these are *n* equations in *n* adjoint states, we can eliminate the adjoint states $\lambda^T = [\lambda_1 \, \lambda_2 \ldots \lambda_n]$ to obtain the static feedback represented by eq. (26).

APPENDIX C: PROOF OF THEOREM 3

Proof for (i): The first-order necessary conditions for $s = n - 3$ can be written as

$$\lambda^T f(x) = 0$$
$$\lambda^T g(x) = 0$$
$$\lambda^T ad_f^1 g(x) = 0$$
$$\vdots \qquad (60)$$
$$\lambda^T ad_f^{n-3} g(x) = 0$$
$$\lambda^T ad_f^{n-2} g(x) + \lambda^T [g, ad_f^{n-3} g](x) u = 0.$$

Since these are *n* equations in *n* adjoint states, we can eliminate the adjoint states $\lambda^T = [\lambda_1, \lambda_2 \ldots \lambda_n]$ to obtain the static state feedback represented by eq. (27).

Proof for (ii): From proposition 2, the first-order necessary conditions for singular extremal are

$$\lambda^T g(x) = 0$$
$$\lambda^T ad_f^1 g(x) = 0$$
$$\vdots \qquad (61)$$
$$\lambda^T ad_f^{n-3} g(x) = 0$$
$$\lambda^T ad_f^{n-2} g(x) + \lambda^T [g, ad_f^{n-3} g](x) u(t) = 0.$$

which constitute $n - 1$ equations in *n* adjoint states. Differentiating the last equation once we obtain an additional equation

$$ad_f^{n-1} g(x) + [g, ad_f^{n-2} g](x) u(t)$$
$$+ \left(I \frac{d}{dt} - \frac{\partial f(x)}{\partial x} - \frac{\partial g(x)}{\partial x} u(t) \right) ([g, ad_f^{n-3} g](x) u(t)).$$
$$(62)$$

The above equations constitute a set of *n* equations in *n* adjoint variables which can be eliminated to give the dynamic state feedback law. This is obtained by setting the determinant of the vector fields in eq. (29) equal to zero.

APPENDIX D: PROOF OF THEOREM 4

Proof for (i): The first-order necessary conditions for singular extremal are

$$\lambda^T f(x) = 0$$
$$\lambda^T g(x) = 0$$
$$\lambda^T ad_f^1 g(x) = 0$$
$$\vdots \qquad (63)$$
$$\lambda^T ad_f^{s-1} g(x) = 0$$
$$\lambda^T ad_f^s g(x) + \lambda^T [g, ad_f^{s-1} g](x) u(t) = 0$$

which constitute $s + 2$ equations in *n* adjoint states. Differentiating the last equation $(n - s - 3)$ times we obtain $(n - s - 3)$ more equations:

$$\lambda^T \left(ad_f^{s+1} g(x) + [g, ad_f^s g](x) u(t) \right.$$
$$\left. + \left(I \frac{d}{dt} - \frac{\partial f(x)}{\partial x} - \frac{\partial g(x)}{\partial x} u(t) \right) ([g, ad_f^{s-1} g](x) u(t)) \right) = 0$$
$$\lambda^T \left(ad_f^{s+2} (g(x)) + [g, ad_f^{s+1} g](x) u(t) \right.$$
$$\left. + \left(I \frac{d}{dt} - \frac{\partial f(x)}{\partial x} - \frac{\partial g(x)}{\partial x} u(t) \right) ([g, ad_f^s g](x) u(t)) \right.$$

$$+ \lambda^T \left(I \frac{d}{dt} - \frac{\partial f(x)}{\partial x} - \frac{\partial g(x)}{\partial x} u(t) \right)^2 ([g, ad_f^{s-1} g](x) u(t)) = 0$$

$$\vdots$$

$$\lambda^T \left(ad_f^{n-2} g(x) + \sum_{k=0}^{n-s-3} \left(I \frac{d}{dt} - \frac{\partial f(x)}{\partial x} - \frac{\partial g(x)}{\partial x} u(t) \right)^k \right.$$

$$\left. \times ([g, ad_f^{n-k-3} g](x) u(t)) \right) = 0. \tag{64}$$

The above equations constitute a set of n equations in n adjoint variables which can be eliminated to give the dynamic state feedback law. This is obtained by setting the determinant of the vector fields in eq. (30) equal to zero.

Proof for (ii): The first order necessary conditions for singular extremal are

$$\lambda^T g(x) = 0$$
$$\lambda^T ad_f^1 g(x) = 0$$
$$\vdots \tag{65}$$
$$\lambda^T ad_f^s g(x) = 0$$
$$\lambda^T ad_f^{s+1} g(x) + \lambda^T [g, ad_f^s g](x) u(t) = 0.$$

which constitute $s + 2$ equations in n adjoint states. Differentiating the last equation $(n - s - 2)$ times we obtain

$(n - s - 2)$ more equations:

$$\lambda^T \left(ad_f^{s+2} g(x) + [g, ad_f^{s+1} g](x) u(t) \right.$$

$$\left. + \left(I \frac{d}{dt} - \frac{\partial f(x)}{\partial x} - \frac{\partial g(x)}{\partial x} u(t) \right) ([g, ad_f^s g](x) u(t)) \right) = 0$$

$$\lambda^T \left(ad_f^{s+3}(g(x)) + [g, ad_f^{s+2} g](x) u(t) \right.$$

$$\left. + \left(I \frac{d}{dt} - \frac{\partial f(x)}{\partial x} - \frac{\partial g(x)}{\partial x} u(t) \right) ([g, ad_f^{s+1} g](x) u(t)) \right)$$

$$\tag{66}$$

$$+ \lambda^T \left(I \frac{d}{dt} - \frac{\partial f(x)}{\partial x} - \frac{\partial g(x)}{\partial x} u(t) \right)^2 ([g, ad_f^s g](x) u(t)) = 0$$

$$\vdots$$

$$\lambda^T \left(ad_f^{n-1} g(x) + \sum_{k=0}^{n-s-2} \left(I \frac{d}{dt} - \frac{\partial f(x)}{\partial x} - \frac{\partial g(x)}{\partial x} u(t) \right)^k \right.$$

$$\left. \times ([g, ad_f^{n-k-2} g](x) u(t)) \right) = 0.$$

The above equations constitute a set of n equations in n adjoint variables which can be eliminated to give the dynamic state feedback law. This is obtained by setting the determinant of the vector fields in eq. (31) equal to zero.