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OPTIMAL CONTROL OF
STATE CONSTRAINED SYSTEMS

by

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A thesis submitted in conformity with the requirements
for the Degree of Master of Applied Science
Department of Chemical Engineering and Applied Chemistry,
in the University of Toronto

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ABSTRACT

In solving optimal control problems with state constraints, penalty function technique is used to transform the problems so that the optimal solution can be sought by using iterative dynamic programming. In this thesis, two types of state constraints, which are frequently encountered in chemical engineering processes, namely final state constraints and inequality state constraints are considered.

For the problems with final state equality constraints, to overcome the difficulty of finding appropriate set of penalty function factors, we propose a systematic scheme for adjusting the penalty function factors, so that all the constraints are satisfied within a specified tolerance, and that the performance index is minimized. Four typical engineering problems, which are used to test the procedure, show that the proposed method of adjusting the penalty function factors can be used for reasonably complex systems to yield reliable results.

To handle inequality state constraints, we propose a method of introducing an auxiliary state variables for each constraint. The derivatives of these state constraint variables are made positive if the constraint is violated, and zero if there is no constraint violation. By incorporating these state variables then as penalty functions in an augmented performance index, we can ensure that the inequality state constraints are satisfied everywhere inside the given time interval. The procedure, as illustrated and tested with three nonlinear optimal control problems, is found to work well even in the presence of a large number of state constraints.
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1. INTRODUCTION

Nonlinear optimal control problems, in which there are some constraints on the state variables to be satisfied and that a given performance index is either minimized or maximized are frequently encountered in process design and operation. The constraints on the state variables may present in the form of final state constraints, where a particular desired state must be reached within some specified tolerance at the final time, or inequality state constraints, where some state variables must be kept within specified bounds throughout the given time interval. Problems involving final state constraints may arise when there are changes in product specification, or in start-up or shut-down process of a chemical plant when some desired state must be reached at the final time. On the other hand, inequality state constraints are found in widely different types of problems. The constraints are usually resulted from the specification of product quality, or some physical limitation of equipment such as valves, reactor volume, etc.

Optimal control problems involving the constraints on state variables are very challenging. There are a number of methods available in literature for solving such state constrained optimal control problems. However choices become somewhat limited when it comes to deal with nonlinear or highly nonlinear systems. Luus et al. (1992) has shown that even in the absence of state constraints, for some nonlinear systems, the global optimum may be difficult to obtain. Goh and Teo (1988) and Teo et al. (1991) used control parameterization technique and could solve nonlinear optimal control problems with several classes of constraints. Logsdon and Biegler (1989) showed that by first converting differential equations into a set of algebraic equations using collocation technique, constrained nonlinear programming could be applied to solve a
number of chemical engineering examples. However using this method, the satisfaction of the state constraints is not guaranteed beyond the collocation points.

An attractive alternative to the use of Pontryagin’s maximum principle and the avoidance of the two-point boundary value problem appears to be dynamic programming. Bellman and Dreyfus (1962), Aris (1961) and Lapidus and Luus (1967) showed that the method can be used successfully to solve several simple staged problems. However there are a number of difficulties associated with the use of dynamic programming in its original form. The most challenging problem is the problem of setting up the grid values for the state and the control without encountering the *curse of dimensionality*. To have meaningful results, the state grid must be sufficiently fine. For optimization then, at each time step, for each grid point in the state, the state equations must be integrated for each allowable value for control. Therefore, a large number of integrations must be performed at each time step. Of further concern is the interpolation problem when the state trajectory does not reach a grid point at the next stage. Interpolation as shown by Lapidus and Luus (1967) could be used for simple problems, but it is time-consuming and the resulting approximation is unreliable. Edgar and Himmelblau (1987) further reaffirmed the problems with dynamic programming and stated that, even with our present-day computers, systems with more then three of four state variables cannot be optimized with dynamic programming even when a scalar control is involved.

To overcome the state dimensionality problem, Luus (1989) introduced the iterative dynamic programming method using region contraction. In this method, a relatively small number of grid points for the state vector were generated by assigning different values for control, and at each grid point, candidates for the control variables were chosen from a uniform distribution
inside an allowable region. In addition, to overcome the interpolation problem, it was recommended to simply use the best control policy available at the grid point closest to the point as was done by de Tremblay and Luus (1989). After each iteration, the region was contracted so that a refined answer could be obtained after a small number of iterations. Recently Bojkov and Luus (1992) showed that by choosing the candidates for control over a random distribution rather than a uniform distribution, high dimensional linear and nonlinear systems could be solved quite readily. In fact, by using the suggested procedure with a piecewise linear continuous control policy and a multipass method, Luus (1993a) could solve a 130 dimensional linear system having 130 control variables successfully. In this thesis, we shall extend the use of IDP to solve problems with final state and inequality state constraints.

To handle state constraints in an optimal control problem when solved with IDP, a convenient and effective way is by constructing an augmented performance index where the state constraints are included in a penalty function, and then minimizing the augmented performance index. If the penalty function is properly chosen, then minimization of the augmented performance index yields the minimum of the originally chosen performance index and also forces the constraints to be satisfied. Luus (1991) and Rosen and Luus (1991) used penalty function technique with IDP and could solve some optimal control problems with state constraints quite readily. Recently, Dadebo and McAuley (1995a) showed that absolute deviation from the desired state is a better choice than the square of the deviation in the penalty function, and suggested that each penalty function factor be chosen to be approximately the same size as the performance index. However, in one of their examples where six final state constraints were to be satisfied, only four were within acceptable tolerance. The deviations from the desired values for two of the
variables exceeded 0.02 (Dadebo, 1995). It is clear that the problem of choosing appropriate penalty function factors for final state constraints has not yet been solved.

On the other hand, to deal with inequality state constraints, Luus (1991) and Dadebo and McAuley (1995a) also used penalty function technique and obtained better results than previously reported for several inequality state constrained problems. However, by penalizing the violation of the constraints only at the end of each time stage, the satisfaction of the constraints inside the time interval is not guaranteed. In fact, it was pointed out by Keil (1994) that although the constraints were satisfied at the end of each time stage, constraint violation occurred inside a time stage in the example used by Luus (1993b).

In this thesis, we wish to address these problems of using penalty function technique in solving final state constrained, and inequality state constrained optimal control problems. To handle final state constraints, we shall propose a systematic way of choosing penalty function factors so that the optimum value for the performance index can be obtained, and all the state variables are transferred to the desired values within a specified tolerance of the final state constraints. On the other hand, to ensure that the inequality state constraints are satisfied inside each time stage, we present the method of introducing additional state variables which are used as penalty functions in an augmented performance index. We shall use the proposed schemes with iterative dynamic programming, and to test its viability, we consider four engineering examples with final state constraints, and three optimal control problems involving inequality state constraints.
2. PROBLEMS INVOLVING FINAL STATE CONSTRAINTS

Optimal control problems involving final state constraints are generally difficult to solve. The difficulty is increased as the number of such constraints is increased. To handle final state constraints using penalty function technique, in this chapter, we shall present the systematic scheme for adjusting penalty function factors so that all of the final state constraints are satisfied within some tolerance, and that the given performance index is minimized. The proposed scheme will be used with IDP in a multipass manner, and the viability of the procedure will be tested with four engineering optimal control problems.

2.1. Problem Statement

Let us consider the system described by the differential equation

\[ \frac{dx}{dt} = f(x,u) \]  \hspace{1cm} (2.1.1)

where the initial state \( x(0) \) is given. The state vector \( x \) is an \( (n \times 1) \) vector and \( u \) is an \( (m \times 1) \) control vector bounded by

\[ \alpha_j \leq u_j \leq \beta_j \hspace{0.5cm} j = 1, 2, \ldots, m \]  \hspace{1cm} (2.1.2)

At the final time \( t_f \), each state variable is to be within a tolerance \( \varepsilon_i \) of the desired final state \( x_i^d \); i.e.,

\[ \left| x_i(t_f) - x_i^d \right| \leq \varepsilon_i \hspace{0.5cm} i = 1, 2, \ldots, s \]  \hspace{1cm} (2.1.3)
where the variables are arranged so that the constraints are placed on the first \( s \) variables. The optimal control problem is to find the control policy \( u(t) \) in the time interval \( 0 \leq t \leq t_f \) that minimizes the final value performance index

\[
I = \Phi(x(t_f))
\]  

(2.1.4)

2.2. Construction of Augmented Performance Index

To ensure that the constraints specified by eq (2.1.3) are satisfied, we construct the augmented performance index

\[
J = I + \sum_{i=1}^{s} \theta_i \left| x_i(t_f) - x_i^f \right|
\]  

(2.2.1)

where \( \theta_i > 0 \) are penalty function factors that should be determined so that the final state constraints are satisfied and so that the performance index \( I \) is minimized when \( J \) is minimized. In this thesis we propose a systematic way of changing the penalty function factors during the course of optimization.

For optimization we choose iterative dynamic programming (IDP) as developed by Luus (1989). This method was found to be well suited for constrained optimal control problems by Luus and Rosen (1991) and by Dadebo and McAuley (1995a). We divide the time interval into \( P \) stages of equal length and use IDP in a multipass fashion, as was used by Luus (1996) for high dimensional systems, to find piecewise constant control over the \( P \) time stages so that the augmented performance index in eq (2.2.1) is minimized.
Intuitively it is felt that greater penalty factors should be placed on those variables that do not meet the constraint criterion to drive them closer to the constraint. Therefore, we propose the scheme of adjusting the penalty function factors after every pass of IDP according to

\[
\theta_i^{(q+1)} = (1 + \delta)\theta_i^{(q)} \quad \text{if} \quad |x_i(t_f) - x_i^d| > \varepsilon_i \quad (2.2.2)
\]

and

\[
\theta_i^{(q+1)} = (1 - \delta)\theta_i^{(q)} \quad \text{if} \quad |x_i(t_f) - x_i^d| \leq \varepsilon_i \quad (2.2.3)
\]

where \(\delta\) is a small positive factor and \(q\) is the pass number. This means that the value of each penalty factor is either increased in value if the tolerance is not met or decreased in value if the tolerance is met. Furthermore, we propose to decrease \(\delta\) after every pass to reduce the fluctuations in the control policy. It is expected that as passes continue, the adjustment in the penalty factors will eventually yield a set of appropriate values for which all the final states are in the vicinity of the desired values within the specified tolerance \(\varepsilon_r\).

2.3. Algorithm

The basic iterative dynamic programming algorithm using systematic region contraction and randomly chosen test values for the admissible control as described by Bojkov and Luus (1992) and modified to incorporate the multipass procedure by Luus (1996) is modified further to incorporate the proposed scheme for adjusting the penalty function factors. The algorithm involves 11 steps:

1. Divide the time interval [0, \(t_f\)] into \(P\) time stages, each of equal length \(L\).

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2. Choose the number of grid points at each time stage $N$ and the number of random test values for $u$ denoted by $R$. Choose the initial region size $r^{(0)}$ and an initial control policy $u^{(0)}$ for each time stage. Also choose the region contraction factor $\gamma$ used after every iteration, the region restoration factor $\eta$ used after every pass, the number of iterations to be used in every pass and the number of passes.

3. Choose the initial values for penalty function factors $\theta^{(0)}$, the initial value for $\delta$, and the reduction factor for $\delta$.

4. Set the pass number index $q = 1$ and the iteration number index $j = 1$.

5. By choosing $N$ values of control evenly distributed inside the allowable region $r$, integrate eq (2.1.1) from $t = 0$ to $t = t_f$ with the given initial condition, to generate the x-grid for each time stage. Thus we have $N$ grid points at each time stage, except the first one. For the first time stage we have a single grid point consisting of the given initial condition.

6. Starting at the beginning of the last time stage $P$, corresponding to time $t_f - L$, for each x-grid point integrate eq (2.1.1) from $t_f - L$ to $t_f$ once with each of the $R$ allowable values of control chosen at random inside the allowable region $r$. Choose the control that gives the minimum value of the augmented performance index and store the corresponding value of control for use in step 7.

7. Proceed to stage $P - 1$, corresponding to time $t_f - 2L$. For each x-grid point integrate eq (2.1.1) once with each of the $R$ allowable values of control from $t_f - 2L$ to $t_f - L$. To continue integration from $t_f - L$ to $t_f$ choose the control from step 6 that corresponds to the grid point that is closest to the resulting $x$ at $t_f - L$. Compare the $R$ values of the augmented performance index and store the value of control that gives the minimum value.
8. Repeat the procedure for stages $P - 2$, $P - 3$, etc., until stage 1, corresponding to the initial time $t = 0$, is reached. Store the control policy that gives the minimum value for the augmented performance index.

9. Reduce the region $r$ by a factor $\gamma$; i.e.,

$$r^{(j+1)} = \gamma r^{(j)}$$

10. Increment the iteration index $j$ by 1 and go to step 5. Continue the procedure for the number of iterations specified in step 2 to finish a pass.

11. Increment the pass number index $q$ by 1, adjust the penalty function factors to be used for the next pass according to eq (2.2.2) or (2.2.3) and reduce the value of $\delta$ by the factor specified in step 3. Restore the region sizes to $\eta \times 100\%$ of the values at the beginning of the pass. Then go to step 5, continue the procedure for the number of passes specified in step 2 and interpret the results.

2.4. Numerical Examples

The computations in Chapter 2 were performed in double precision on Pentium/120 personal computer using WATCOM FORTRAN compiler version 9.5. For integration the standard fourth order Runge Kutta method was used. The built-in compiler random number generator was used for the generation of random numbers.
2.4.1. Nonlinear CSTR Problem

Let us consider the continuous stirred tank reactor (CSTR) first modelled by Aris and Amundson (1958) and used as a typical nonlinear chemical engineering system by Lapidus and Luus (1967) for optimal control studies. This system was also used by Luus and Cormack (1972) and by Luus and Galli (1991) to illustrate multiplicity of solutions in optimal control, and by Luus and Rosen (1991) to examine the handling of final state constraints by IDP. The equations describing the CSTR are

\[
\frac{dx_1}{dt} = g(x) - (2 + u)(x_1 + 0.25) \quad (2.4.1.1)
\]

\[
\frac{dx_2}{dt} = 0.5 - x_2 - g(x) \quad (2.4.1.2)
\]

\[
\frac{dx_3}{dt} = x_1^2 + x_2^2 + 0.1 \, u^2 \quad (2.4.1.3)
\]

where the reaction term is given by

\[
g(x) = (x_2 + 0.5) \exp \left(\frac{25x_1}{x_1 + 2}\right) \quad (2.4.1.4)
\]

The initial state \(x(0) = [0.09 \quad 0.09 \quad 0.0]^T\) is given. The state variables \(x_1\) and \(x_2\) are deviations from the dimensionless steady-state temperature and concentration respectively, and \(x_3\) is the additional variable introduced to give the performance index at the specified final time \(t_f = 0.78\). Therefore, the performance index to be minimized is

\[
I = x_3(t_f) \quad (2.4.1.5)
\]
The desired final state is the origin given by $x_1(0.78) = 0$ and $x_2(0.78) = 0$.

By using a quadratic penalty function, Luus and Rosen (1991) obtained at the final time the performance index $I = 0.14490$ and the state variables $x_1 = -0.00371$ and $x_2 = -0.00368$.

To use the proposed procedure, we introduce the augmented performance index

$$J = I + \theta_1|x_1(t_f)| + \theta_2|x_2(t_f)|$$

(2.4.1.6)

where the two positive penalty function factors $\theta_1$ and $\theta_2$ are to be determined.

We took 20 time stages ($P = 20$), each of length 0.039, and used an integration step length of 0.00975. In using IDP, we chose a single grid point and 20 randomly chosen candidates for control ($N = 1, R = 20$). For all the runs we used a region contraction factor $\gamma = 0.80$ and a region restoration factor $\eta = 0.98$; i.e., after each iteration the control region was reduced by 0.80 and after every pass, the region was restored to 0.98 of its value used at the beginning of the previous pass. We chose 200 passes, each consisting of 30 iterations. The initial value for $\delta$ was chosen as 0.10 and at the end of each pass we reduced $\delta$ by a factor 0.95 (i.e., 5% reduction). To avoid the local optimum we chose as the initial control policy $u^{(0)} = 3$, and the initial region size $\lambda^{(0)} = 1$.

By choosing the tolerances $\epsilon_1 = \epsilon_2 = 0.001$, $\theta_1^{(0)} = \theta_2^{(0)} = 1.0$, after 200 passes requiring 1134 s of CPU time, we obtained the performance index $I = 0.14369$ with the final values for the states $x_1 = -0.001002$ and $x_2 = -0.001000$. The final values for the penalty function factors were $\theta_1 = 0.33348$ and $\theta_2 = 0.40802$. It is noted that the performance index 0.14369 is slightly better than the 0.14490 reported by Luus and Rosen (1991) and the final states are closer to the origin.
By using a different starting condition for the penalty function factors, namely $\theta_{1}^{(0)} = \theta_{2}^{(0)} = 0.2$, we obtained identical results as before, except that the final value for $x_1$ was -0.001001.

We now reduced the tolerances to $\varepsilon_1 = \varepsilon_2 = 0.0001$, and repeated the above runs. In each case we obtained $I = 0.14438$. With the first starting point we obtained the final values for the states $x_1 = -0.000100$ and $x_2 = -0.000100$, and the penalty function factors $\theta_1 = 0.35374$ and $\theta_2 = 0.42868$; with the second starting condition we obtained the same value for the performance index with the final values $x_1 = -0.000102$ and $x_2 = -0.000100$, and the penalty function factors $\theta_1 = 0.35372$ and $\theta_2 = 0.42866$. It is interesting to note that the resulting penalty function factors are very slightly larger than in the previous case.

Next we took $\varepsilon_1 = \varepsilon_2 = 0.00001$ with initial choices for the penalty function factors as found in the run with $\varepsilon_1 = \varepsilon_2 = 0.0001$, namely $\theta_{1}^{(0)} = 0.35372$ and $\theta_{2}^{(0)} = 0.42866$. It was expected that, since these values are close to the ones that should result at the optimum, convergence should be obtained more rapidly. Surprisingly, after 200 passes, a performance index $I = 0.146044$ was obtained, the constraint tolerance was violated, and it was clear that convergence was not obtained. The run was repeated with initial values for the penalty function factors chosen to be $\theta_{1}^{(0)} = \theta_{2}^{(0)} = 0.3$. Although these values are not as good as the ones used before, convergence was systematic and the tolerance was almost satisfied within 200 passes. We obtained the performance index $I = 0.14445$ with $x_1 = -0.000010$ and $x_2 = -0.000012$, and the penalty function factors $\theta_1 = 0.35575$ and $\theta_2 = 0.43073$. The previous case that did not converge was rerun with the use of 50 iterations per pass, rather than 30. Leaving all the other conditions the same, convergence to $I = 0.14445$ was obtained with no difficulty, yielding the same values.
for the penalty function factors. In fact, after 80 passes a value of the performance index $I = 0.14446$ was reached with $x_1 = -0.000000$ and $x_2 = -0.000004$, and after 103 passes the performance index was reduced to $0.14445$ with $x_1 = 0.000000$ and $x_2 = -0.000008$. It is interesting to note that this value of the performance index is still slightly better than the one obtained with the use of a quadratic penalty function by Luus and Rosen (1991). The resulting control policy is given in Figure 2.4.1.1, and the trajectories for the first two state variables are shown in Figure 2.4.1.2.
Figure 2.4.1.1: Optimal control policy for the CSTR problem.
Figure 2.4.1.2: Trajectories of the first 2 state variables for the CSTR problem; —— \( x_1 \), ——\( x_2 \).
2.4.2. Nonlinear Two-Stage CSTR Problem (1)

Let us consider the two-stage CSTR considered by Oh and Luus (1975) for time-suboptimal control studies. The system is described by

\[
\frac{dx_1}{dt} = 0.5 - x_1 - R_1 
\]

(2.4.2.1)

\[
\frac{dx_2}{dt} = -2(x_2 + 0.25) - u_1 (x_2 + 0.25) + R_1 
\]

(2.4.2.2)

\[
\frac{dx_3}{dt} = x_1 - x_3 - R_2 + 0.25 
\]

(2.4.2.3)

\[
\frac{dx_4}{dt} = x_2 - 2x_4 - u_2 (x_4 + 0.25) + R_2 - 0.25 
\]

(2.4.2.4)

\[
\frac{dx_5}{dt} = x_1^2 + x_2^2 + x_3^2 + x_4^2 + 0.1(u_1^2 + u_2^2) 
\]

(2.4.2.5)

where the reaction rate term in the first tank is given by

\[
R_1 = (x_1 + 0.5) \exp \left( \frac{25x_2}{x_2 + 2} \right) 
\]

(2.4.2.6)

and in the second tank

\[
R_2 = (x_3 + 0.25) \exp \left( \frac{25x_4}{x_4 + 2} \right) 
\]

(2.4.2.7)

The normalized controls are bounded by

\[-1 \leq u_1 \leq 1 \]

(2.4.2.8)

\[-1 \leq u_2 \leq 1 \]

(2.4.2.9)
and the initial condition is given by

\[ x(0) = [-0.15 \ 0.05 \ -0.10 \ 0.02]^T \]  \hfill (2.4.2.10)

The state variables \( x_1 \) and \( x_3 \) are normalized concentration variables in tanks 1 and 2 respectively, \( x_2 \) and \( x_4 \) are normalized temperature variables in tanks 1 and 2 respectively. We have introduced the additional variable \( x_5 \) to represent the performance index at the specified final time \( t_f = 1 \). Therefore, the performance index to be minimized is

\[ I = x_5(t_f) \] \hfill (2.4.2.11)

Incorporating the constraints into the performance index yields the augmented performance index:

\[ J = I + \sum_{i=1}^{4} \theta_i |x_i(t_f)| \] \hfill (2.4.2.12)

Therefore, in this case, there are four penalty function factors in the augmented performance index to be determined.

For all runs, we choose \( P = 20, N = 1, R = 20, \gamma = 0.70, \eta = 0.95, r_1^{(0)} = r_2^{(0)} = 2 \) and use 30 iterations per pass. As initial control policy, we chose \( u_1^{(0)} = u_2^{(0)} = 0 \). Initially, \( \delta \) was set to 0.5 and it was reduced in value by a factor of 0.98 after every pass.

First, we take the tolerance \( \varepsilon = 0.001 \) and \( \theta^{(0)} = [1.0 \ 1.0 \ 1.0 \ 1.0]^T \). After 197 passes, requiring the CPU time of 3281 s, we obtained the performance index \( I = 0.05783 \) with the state variables at the final time brought to within the tolerance of the desired final state with \( x(1) = [0.000681 \ -0.000842 \ -0.000994 \ -0.000991]^T \). The final values for the penalty function factors
were $\theta = [0.14011 \ 0.03657 \ 1.82944 \ 1.26306]^T$. We reran the above case using $\varepsilon = 0.0001$. Without any difficulty, after 155 passes, we obtained $I = 0.06109$ with $x(1) = [0.000087 \ 0.000000 \ -0.000063 \ -0.000067]^T$.

Next, to bring the final state variables closer to the origin, we attempted to use $\varepsilon = 0.00001$. After 156 passes, requiring 2470 s of CPU time, we obtained $I = 0.06192$ with $x(1) = [0.000003 \ 0.000000 \ -0.000004 \ 0.000000]^T$. The final values for the penalty function factors were $\theta = [0.21066 \ 0.03961 \ 2.03842 \ 1.29848]^T$. The resulting control policy after 157 passes is shown in Figure 2.4.2.1 and the corresponding trajectories for the first four state variables are shown in Figure 2.4.2.2.
Figure 2.4.2.1: Optimal control policy for the two-stage CSTR problem (1); \( u_1 \), \( u_2 \).
Figure 2.4.2.2: Trajectories of the first 4 state variables for the two-stage CSTR problem (1);

- \( x_1 \), \( x_2 \), \( x_3 \), \( x_4 \).
2.4.3. Nonlinear Two-stage CSTR Problem (2)

Let us now consider the two-stage CSTR system used for optimal control studies by Edgar and Lapidus (1972), Luus (1974a, b), Nishida et al. (1976), Rosen and Luus (1991), Bojkov and Luus (1994) and Dadebo and McAuley (1995b). The system is described by

\[
\frac{dx_1}{dt} = -3x_1 + g_1(x) \tag{2.4.3.1}
\]

\[
\frac{dx_2}{dt} = -11.1558x_2 + g_1(x) - 8.1558(x_2 + 0.1592)u_1 \tag{2.4.3.2}
\]

\[
\frac{dx_3}{dt} = 1.5(0.5x_1 - x_3) + g_2(x) \tag{2.4.3.3}
\]

\[
\frac{dx_4}{dt} = 0.75x_2 - 4.9385x_4 + g_2(x) - 3.4385(x_4 + 0.122)u_2 \tag{2.4.3.4}
\]

\[
\frac{dx_5}{dt} = x_1^2 + x_2^2 + x_3^2 + x_4^2 + 0.1(u_1^2 + u_2^2) \tag{2.4.3.5}
\]

where the reaction rate term in the first tank is given by

\[
g_1(x) = 1.5 \times 10^7 (0.5251 - x_1) \exp \left( \frac{-10}{x_2 + 0.6932} \right) - 1.5 \times 10^{10} (0.4748 + x_1) \exp \left( \frac{-15}{x_2 + 0.6932} \right) - 1.4280 \tag{2.4.3.6}
\]

and in the second tank

\[
g_2(x) = 1.5 \times 10^7 (0.4236 - x_2) \exp \left( \frac{-10}{x_4 + 0.6560} \right) - 1.5 \times 10^{10} (0.5764 + x_3) \exp \left( \frac{-15}{x_4 + 0.6560} \right) - 0.5086 \tag{2.4.3.7}
\]
The normalized controls are bounded by

\[ -1 \leq u_1 \leq 1 \quad (2.4.3.8) \]

\[ -1 \leq u_2 \leq 1 \quad (2.4.3.9) \]

and the initial condition is given by

\[ x(0) = [0.1962 \quad -0.0372 \quad 0.0946 \quad 0.0 \quad 0.0]^T \quad (2.4.3.10) \]

The state variables \( x_1 \) and \( x_3 \) are normalized concentration variables in tanks 1 and 2 respectively, and \( x_2 \) and \( x_4 \) are normalized temperature variables in tanks 1 and 2 respectively. We have introduced the additional variable \( x_5 \) to represent the performance index at the final time \( t_f \). Therefore, the performance index to be minimized is

\[ I = x_5(t_f) \quad (2.4.3.11) \]

At the final time \( t_f \), we want the concentration variables and the temperature variables to be zero.

Incorporating the constraints into the performance index yields the augmented performance index:

\[ J = I + \sum_{i=1}^{4} \theta_i |x_i(t_f)| \quad (2.4.3.12) \]

Therefore, in this case, there are four penalty function factors in the augmented performance index to be determined.

This problem has been widely used for time optimal control studies. Edgar and Lapidus (1972) obtained a minimum time \( t_f = 0.342 \) and brought all the variables to within 0.0017 of the origin. Luus (1974a) reported a better minimum time \( t_f = 0.325 \) for the \( 10^{-3} \) tolerance. Recently, Bojkov and Luus (1994) took a tighter tolerance of \( 10^{-4} \), and obtained a minimum time \( t_f = \)

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0.32715 by using IDP with 10 stages of flexible stage length. Here we choose the final time \( t_f = 0.325 \) and attempt to bring the state variables as close to the origin as possible at the final time.

To see whether we could reach the origin to more than six figures, we set the tolerances \( \varepsilon_i = 10^{-7} \) for \( i = 1, 2, \ldots, 4 \) and took \( P = 20, N = 1, R = 20, \gamma = 0.70, \eta = 0.95, r_1^{(0)} = r_2^{(0)} = 2 \). The initial values for the controls and the penalty function factors were chosen to be \( u_1^{(0)} = u_2^{(0)} = 0.0 \) and \( \Theta^{(0)} = [1.0 \ 1.0 \ 1.0 \ 1.0]^T \) respectively. Initially, \( \delta \) was set to 0.2 and it was reduced in value by a factor of 0.98 after every pass. The step size of 0.00325 was used for integration. By using 250 passes, each consisting of 30 iterations, we obtained the performance index \( I = 0.046892 \) with all of the state variables within \( 10^{-7} \) of the desired final state with \( x(0.325) = \begin{bmatrix} -0.741 \times 10^{-7} \\ 0.249 \times 10^{-12} \\ 0.888 \times 10^{-7} \\ 0.252 \times 10^{-12} \\ 0.046892 \end{bmatrix} \) and the penalty function factors \( \Theta = [11.64047 \\ 0.25091 \\ 8.38370 \\ 3.45059]^T \). The resulting optimal control policy is shown in Figure 2.4.3.1. It compares favorably to the policy reported by Luus (1974a), but the control \( u_1 \) increases more gradually than the policies reported by Rosen and Luus (1991) and Bojkov and Luus (1994). However the optimal control policy is substantially different from the control policies obtained by Edgar and Lapidus (1972), Luus (1974b) and Nishida et al. (1976). The trajectories of the first four state variables are given in Figure 2.4.3.2. In Figure 2.4.3.3, the Euclidean norm of the first four state variables at the final time is plotted against the pass number to show the convergence properties of the proposed method. Although the norm of the final states is oscillatory in nature, the reduction is quite systematic. The CPU time required for 250 passes was 6093 s.
Figure 2.4.3.1: Optimal control policy for the 2-stage CSTR problem (2); $u_1$, $u_2$. 
Figure 2.4.3.2: Trajectories of the first 4 state variables for the 2-stage CSTR problem (2);

- $x_1$, $x_2$, $x_3$, $x_4$. 

- $X_2$, $X_3$, $X_4$. 

$2.432$
Figure 2.4.3.3: Convergence profile of final state variables to the desired final state for the 2-stage CSTR problem (2).
2.4.4. Container Crane Problem

We next consider a more difficult optimal control problem where it is required to determine the optimal operation of a container crane system in which there are two inequality constraints on the state variables and six final state equality constraints. The problem was first presented by Sakawa and Shindo (1982) and was considered by Goh and Teo (1988), Teo et al. (1991), Luus (1991) and most recently by Dadebo and McAuley (1995a). A hoist and a trolley motor are used in the container crane to transfer a container from a ship to a truck. The movement of the crane by these two control variables is described by the dynamic equations:

\[
\frac{dx_1}{dt} = 9x_4
\]  
(2.4.4.1)

\[
\frac{dx_2}{dt} = 9x_5
\]  
(2.4.4.2)

\[
\frac{dx_3}{dt} = 9x_6
\]  
(2.4.4.3)

\[
\frac{dx_4}{dt} = 9(u_1 + 17.2656x_3)
\]  
(2.4.4.4)

\[
\frac{dx_5}{dt} = 9u_2
\]  
(2.4.4.5)

\[
\frac{dx_6}{dt} = -\frac{9(u_1 + 27.0756x_3 + 2x_5x_6)}{x_2}
\]  
(2.4.4.6)

\[
\frac{dx_7}{dt} = 4.5(x_3^2 + x_6^2)
\]  
(2.4.4.7)

where \(x_1\) and \(x_2\) are the horizontal and vertical distances respectively that the container moves and \(x_3\) is the swing angle of the container, \(x_4\) and \(x_5\) are the horizontal and vertical velocities.
respectively of the container, and \( x_6 \) is the angular velocity of the container. The last variable \( x_7 \) is introduced here as an additional variable representing the behavior of the container during the transfer, where the integral of \( x_7 \) is to be minimized.

The initial state of the container is given as

\[
x(0) = [0 \ 22 \ 0 \ 0 \ -1 \ 0 \ 0]^T \tag{2.4.8}
\]

The controls consisting of the torque of the hoist and trolley motors are bounded by

\[
-2.834 \leq u_1 \leq 2.834 \tag{2.4.9}
\]
\[
-0.809 \leq u_2 \leq 0.713 \tag{2.4.10}
\]

At the final time \( t_f = 1 \), the state variables must be brought to the desired final state:

\[
x^d(1) = [10 \ 14 \ 0 \ 2.5 \ 0 \ 0 \ \text{free}]^T \tag{2.4.11}
\]

In addition, there are inequality constraints on \( x_4 \) and \( x_5 \):

\[
-2.5 \leq x_4 \leq 2.5 \tag{2.4.12}
\]
\[
-1.0 \leq x_5 \leq 1.0 \tag{2.4.13}
\]

For safety reason, we want the container to oscillate as little as possible during the transfer, so that the performance index to be minimized is

\[
l = x_7(t_f) \tag{2.4.14}
\]
Here we choose the augmented performance index to be

\[ J = x_7(t_f) + \sum_{i=1}^{6} \theta_i |x_i(t_f) - x_i^d| + p_1 \sum_{k=1}^{p} p_{4k} + p_2 \sum_{k=1}^{p} p_{5k} \]  \tag{2.4.15}

where

\[ p_{4k} = \begin{cases} 
2.5 - x_4(t_k) & \text{if } x_4(t_k) < -2.5 \\
0 & \text{if } -2.5 \leq x_4(t_k) \leq 2.5 \\
x_4(t_k) - 2.5 & \text{if } x_4(t_k) > 2.5 
\end{cases} \]  \tag{2.4.16}

and

\[ p_{5k} = \begin{cases} 
1.0 - x_5(t_k) & \text{if } x_5(t_k) < -1.0 \\
0 & \text{if } -1.0 \leq x_5(t_k) \leq 1.0 \\
x_5(t_k) - 1.0 & \text{if } x_5(t_k) > 1.0 
\end{cases} \]  \tag{2.4.17}

In the augmented performance index, there are eight penalty function factors. Normally, \( p_i \) and \( p_j \) are relatively easy to choose since inequality constraints are not as restrictive as equality constraints, and a wide range for \( p_i \) and \( p_j \) is possible. Here we simply choose \( p_i = p_j = 1 \), which is large enough to ensure that the inequality constraints are satisfied. Thus the problem now is to determine the six values for \( \theta_i \).

A few preliminary runs showed that a reasonable choice for the starting values for penalty factors is \( \theta^{(0)} = [5 \times 10^{-4} \ 5 \times 10^{-4} \ 5 \times 10^{-2} \ 5 \times 10^{-3} \ 1 \times 10^{-3} \ 6 \times 10^{-2}]^T \). Now let us take \( P = 10 \) stages, the tolerances \( \epsilon_i = 10^{-3} \) for \( i = 1, 2, \ldots, 6 \), the integration step length of 0.01, and take \( r_1^{(0)} \) and \( r_2^{(0)} \) to be 20 percent of the allowed range for each control, \( N = 3, \ R = 20, \ \gamma = 0.7, \ \eta = 0.95, \ u_1^{(0)} = 0.5, \ u_2^{(0)} = 0 \) and use 20 iterations per pass. The adjustment for penalty factors was made after every pass. Initially, \( \delta \) was taken to be 0.05 and it was reduced in value by the factor 0.95 after every 5 passes. After 150 passes, the minimum value for the performance index was \( J = 0.005376 \)
where $x(1) = [10.000968, 14.000000, -0.000974, 2.499055, -0.000785, -0.000994, 0.005376]^T$. All the final state constraints are satisfied within the specified tolerances and there is no violation of the inequality constraints on $x_4$ and $x_5$. The computation time required for 150 passes was 948 sec. At pass 150, the penalty function factors were $\theta = [5.774 \times 10^{-4}, 4.888 \times 10^{-3}, 6.366 \times 10^{-2}, 6.668 \times 10^{-3}, 2.478 \times 10^{-4}, 7.424 \times 10^{-5}]^T$. It is noted that the magnitudes of the penalty function factors are widely different. This shows that the strategy of simply choosing the same penalty function factor for every constraint as used by Dadebo and McAuley (1995a) is not the best choice for this problem. Figure 2.4.4.1 shows the resulting optimal control policy. The corresponding trajectories for the state variables $x_1$, $x_2$, $x_4$ and $x_5$ are shown in Figure 2.4.4.2 and the trajectories for the state variables $x_3$ and $x_6$ are shown in Figure 2.4.4.3.

Next we tightened up the final state constraints by setting $\varepsilon_i = 10^{-6}$ for $i = 1, 2, \ldots, 6$. In this case, a slightly higher value of performance index $I = 0.005523$ resulted with $x(1) = [10.000000, 14.000000, 2.500000, 0.000000, 0.000000, 0.005523]^T$. The optimal control policy for this case, as shown in Figure 2.4.4.4, is very similar to the optimal control policy in the previous case. By dividing the time interval into 20 stages of equal length and using $\varepsilon_i = 10^{-4}$ for $i = 1, 2, \ldots, 6$, a lower value of the performance index $I = 0.005264$ could be obtained with $x(1) = [10.000000, 14.000000, 2.500000, 0.000000, 0.000000, 0.005264]^T$ and again there was no violation of the inequality constraints on $x_4$ and $x_5$. The values for the penalty function factors were $\theta = [5.459 \times 10^{-4}, 4.887 \times 10^{-3}, 5.388 \times 10^{-2}, 6.360 \times 10^{-3}, 2.579 \times 10^{-4}, 8.089 \times 10^{-5}]^T$. The penalty function factors obtained in this case are quite close to those obtained with 10 stages. The performance index obtained here is slightly better than the value reported by Goh and Teo (1988) of $I = 0.00540$ and by Teo et al. (1991) of $I = 0.005361$. Although Dadebo and McAuley (1995a)
reported a lower value for the performance index of $I = 0.004234$, the states $x_3(1) = -0.038490$ and $x_6(1) = -0.020262$ (Dadebo, 1995) are quite far from the desired state. The optimal control policy is shown in Figure 2.4.4.5. It is noted that the control profiles are somewhat different from the control policies obtained by Luus (1991) and by Dadebo and McAuley (1995a). The difficulty in solving this problem arises not only because of the large number of state constraints, but also from the low sensitivity of the performance index to the change in the control policy.

To see whether we can obtain a lower performance index with approximately the same level of constraint violation on $x_3$ and $x_6$ as reported by Dadebo and McAuley (1995a), we relax the tolerances for $x_3$ and $x_6$ by choosing $\varepsilon = [10^{-6} \ 10^{-6} \ 0.03 \ 10^{-6} \ 10^{-6} \ 0.02]^T$ and choose as the initial value $\theta^{(0)} = [0.005 \ 0.005 \ 0.005 \ 0.005 \ 0.005 \ 0.005]^T$. The initial value for $\delta$ was taken to be 0.2 and it was reduced by the factor 0.98 after every pass. After 55 passes, we obtained the final state $x(1) = [10.000000 \ 14.000000 \ -0.026689 \ 2.500000 \ 0.000000 \ -0.019664 \ 0.003459]^T$ with $\theta = [2.066\times10^{-4} \ 6.520\times10^{-5} \ 2.148\times10^{-4} \ 2.307\times10^{-3} \ 1.187\times10^{-4} \ 2.784\times10^{-2}]^T$. The performance index $I = 0.003459$ is 22% lower than the value reported by Dadebo and McAuley (1995a) and the state is somewhat closer to the desired final state. The corresponding control policy, as shown in Figure 2.4.4.6, is significantly different from the policy given by Dadebo and McAuley (1995a). The control policy for $u_1$ here also differs considerably from the optimal control policy for the case of using $10^{-6}$ tolerances for all the constraints, by starting off at a higher value, and the dip in value of $u_1$ at stage 19 is not as steep. Therefore, by being able to specify the tolerance for each individual constraint separately, we are able to take advantage of this flexibility to reduce the value of the performance index.
Figure 2.4.4.1: Optimal control policy for the container crane problem when using 10 stages and the deviation of each state variable from the desired final state is less than $10^3$; $l = 0.005376$; —— $u_1$, —— $u_2$. 
Figure 2.4.4.2: Trajectories of the state variables $x_1$, $x_2$, $x_4$ and $x_5$ for the container crane problem; $x_1$, $x_2$, $x_4$, $x_5$. 
Figure 2.4.4.3: Trajectories of the state variables $x_3$ and $x_6$ for the container crane problem:

--- $x_3$, ----------- $x_6$. 
Figure 2.4.4.4: Optimal control policy for the container crane problem when using 10 stages and the deviation of each state variable from the desired final state is less than $10^{-6}$; $I = 0.005523$; $u_1$, $u_2$. 
Figure 2.4.4.5: Optimal control policy for the container crane problem when using 20 stages and the deviation of each state variable from the desired final state is less than $10^{-6}$; $\epsilon = 0.005264$; $u_1$, $u_2$. 
Figure 2.4.4.6: Optimal control policy for the container crane problem when setting the initial tolerance vector as $\mathbf{v} = [10^{-6} \ 10^{-6} \ 0.03 \ 10^{-6} \ 10^{-6} \ 0.02]^T$; $u_1$, $u_2$. 

$\mathbf{v} = [10^{-6} \ 10^{-6} \ 0.03 \ 10^{-6} \ 10^{-6} \ 0.02]^T$
3. PROBLEMS WITH INEQUALITY STATE CONSTRAINTS

Inequality state constraints are frequently encountered in solving optimal control problems. In many cases, the strict satisfaction of such constraints is crucial since the violation may result in the failure of equipment or degradation of a product. To handle the inequality state constraints, we shall present the method of introducing additional state variables to express the constraint violation. By incorporating these variables as penalty functions in an augmented performance index, we can ensure that the inequality state constraints are satisfied everywhere inside the given time interval. The procedure will be illustrated and tested with three nonlinear optimal control problems.

3.1. Problem Statement

Let us consider the system described by the differential equation

\[
\frac{dx}{dt} = f(x, u)
\]  

(3.1.1)

where the initial state \( x(0) \) is given. The state vector \( x \) is an \( (n \times 1) \) vector and \( u \) is an \( (m \times 1) \) control vector bounded by

\[
\alpha_j \leq u_j \leq \beta_j \quad j = 1, 2, \ldots, m
\]  

(3.1.2)

In addition, there are \( s \) inequality constraints on the state variables

\[
\psi_i(x) \leq 0 \quad i = 1, 2, \ldots, s
\]  

(3.1.3)
The performance index associated with this system is a scalar function of the state at final time $t_f$ given by

$$I = \Phi(x(t_f))$$  \hspace{1cm} (3.1.4)$$

The optimal control problem is to find the control policy $u(t)$ in the time interval $0 \leq t \leq t_f$ that minimizes (or maximizes) the performance index in eq (3.1.4).

3.2. Construction of Augmented Performance Index

To deal with inequality constraints in eq (3.1.3), we shall use the penalty function approach. Since there are $s$ inequality constraints, we introduce $s$ additional variables $x_{n+1}, x_{n+2}, \ldots, x_{n+s}$, which we call state constraint variables, through the relationship

$$\frac{dx_{n+i}}{dt} = \begin{cases} \psi_i(x) & \text{if } \psi_i(x) > 0 \\ 0 & \text{if } \psi_i(x) \leq 0 \end{cases} \quad i = 1, 2, \ldots, s$$  \hspace{1cm} (3.2.1)$$

with the initial condition

$$x_{n+i}(0) = 0 \quad i = 1, 2, \ldots, s$$  \hspace{1cm} (3.2.2)$$

The final value $x_{n+s}(t_f)$ therefore gives the total violation of the $i^{th}$ inequality state constraint integrated over time. For minimization of the performance index in eq (3.1.4), we choose the augmented performance index

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\[ J = I + \sum_{i=1}^{t} \rho_i x_{n+1}(t_f) \]  \hspace{1cm} (3.2.3)

where \( \rho_i > 0 \) are penalty function factors for inequality state constraints.

For optimization we choose iterative dynamic programming (IDP) as developed by Luus (1989), and has been found to be well suited for constrained optimal control problems by Luus (1991) and by Dadebo and McAuley (1995a). In the last two examples, we shall use IDP in a multipass fashion as used by Luus (1996) for high dimensional systems. We divide the time interval \( 0 \leq t \leq t_f \) into \( P \) stages of equal length and seek piecewise constant control over the \( P \) time stages so that the augmented performance index in eq (3.2.3) is minimized. If \( J \) is equal to \( I \), then it is clear that all of the inequality constraints are satisfied everywhere. Maximization of the performance index in eq (3.1.4) creates no difficulty, because then we simply minimize the augmented performance index

\[ J = -I + \sum_{i=1}^{t} \rho_i x_{n+1}(t_f) \]  \hspace{1cm} (3.2.4)

where the penalty function is chosen as before.

Of interest is whether the use of the penalty function in the performance index yields the optimum value of the performance index, and the range of penalty function factors for which convergence will result. To investigate the viability of the approach and to illustrate the procedure, we therefore choose three nonlinear optimal control problems that have been examined by other methods.

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3.3. Algorithm

The iterative dynamic programming algorithm used in this chapter is the same as the one used in chapter 2 except that in this chapter, $\Theta$ is replaced by $\rho$, and the value of $\rho$ is not adjusted after every pass according to eq (2.2.2) or (2.2.3) as in the previous chapter.

3.4. Numerical Examples

The computations in Chapter 3 were performed in double precision on Pentium/120 personal computer using WATCOM FORTRAN compiler version 9.5. The FORTRAN subroutine DVERK of Hull et al. (1976) was used for the integration of the differential equations. The built-in compiler random number generator URAND was used for the generation of random numbers.

3.4.1. Plug-Flow Tubular Reactor Problem

Let us first consider the plug-flow tubular reactor problem as studied by Ko and Stevens (1971), Reddy and Husain (1981), Modak et al. (1989) and by Luus (1991). The system is described by the two differential equations:

\[
\frac{dx_1}{dt} = (1 - x_1)k_1 - x_1k_2
\]

\[
\frac{dx_2}{dt} = 300[(1 - x_1)k_1 - x_1k_2] - u(x_2 - 290)
\]

where

\[
k_1 = 1.7536 \times 10^5 \exp \left( \frac{-1.1374 \times 10^4}{1.9872 x_2} \right)
\]
and
\[ k_2 = 2.4885 \times 10^{10} \exp\left( \frac{-2.2748 \times 10^4}{1.9872 x_2} \right) \]  \hspace{1cm} (3.4.1.4)

with the initial condition
\[ x(0) = [0 \hspace{0.2cm} 380]^T \]  \hspace{1cm} (3.4.1.5)

The control \( u \) is bounded by
\[ 0 \leq u \leq 0.5 \]  \hspace{1cm} (3.4.1.6)

In addition, there is the state constraint on the temperature
\[ x_2(t) \leq 460 \]  \hspace{1cm} (3.4.1.7)

The performance index to be maximized is the yield given by
\[ I = x_1(t_f) \]  \hspace{1cm} (3.4.1.8)

where the final time \( t_f = 5 \) min.

In order to deal with the inequality state constraint in eq (3.4.1.7), we introduce a state constraint variable \( x_3 \) by
\[
\frac{dx_3}{dr} = \begin{cases} 
  x_2 - 460 & \text{if } x_2 - 460 > 0 \\
  0 & \text{if } x_2 - 460 \leq 0 
\end{cases}
\]  \hspace{1cm} (3.4.1.9)

with the initial condition \( x_3(0) = 0 \). Therefore, whenever the state constraint is violated, \( x_3 \) is increased in value.

Since the performance index in eq (3.4.1.8) is to be maximized we choose the augmented performance index to be minimized as
\[ J = -I + \rho x_3(t_f) \]  \hspace{1cm} (3.4.1.10)
where \( p \) is chosen to be positive.

Let us divide the given time interval into 25 time stages \( (P = 25) \) each of length 0.2 min, and take \( N = 3, R = 20, \gamma = 0.9 \). The local error tolerance of \( 10^{-8} \) was used for integration in subroutine DVERK. By choosing \( u^{(0)} = 0.25, r^{(0)} = 0.5 \) as the initial control policy and the initial control region respectively, and using \( \rho = 10 \), after 34 iterations requiring 96 s of computation time, we obtained the performance index \( I = 0.67684 \) with no violation on the inequality constraint at all (i.e. \( x_3(t_f) = 0 \)). By using a lower value for the penalty function factor \( \rho = 0.1 \), we obtained almost the same performance index \( I = 0.67685 \) also with \( x_3(t_f) = 0 \). Therefore, the choice of the penalty function factor is not very important for this problem. Although, Luus (1991) reported a slightly higher performance index \( I = 0.6770 \), this better value is attributed to a slight violation of the inequality state constraint within the time stages 12 and 13, i.e., at the time \( 2.2 < t < 2.4 \) and \( 2.4 < t < 2.6 \). The optimal control policy obtained here is given in Table 3.4.1.1, and the corresponding state trajectory of \( x_2 \) is shown in Figure 3.4.1.1. The state trajectory was generated by using the optimal control policy to integrate the system equations with the time interval divided into 500 time steps in order to obtain an accurate profile. As can be seen, the peak of the trajectory just touches the 460 boundary but does not go over.
**Table 3.4.1.1**: Optimal control policy for the plug-flow tubular problem.

<table>
<thead>
<tr>
<th>Stage Number</th>
<th>Time $t_k$</th>
<th>Control $u(t_k,i)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.2</td>
<td>0.0000</td>
</tr>
<tr>
<td>2</td>
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<td>0.0000</td>
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<tr>
<td>9</td>
<td>1.8</td>
<td>0.0000</td>
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<td>0.2714</td>
</tr>
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<td>2.2</td>
<td>0.5000</td>
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<tr>
<td>12</td>
<td>2.4</td>
<td>0.5000</td>
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<td>13</td>
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<tr>
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<td>0.3214</td>
</tr>
<tr>
<td>17</td>
<td>3.4</td>
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<tr>
<td>22</td>
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</tr>
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<td>23</td>
<td>4.6</td>
<td>0.1957</td>
</tr>
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<td>24</td>
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<td>0.1522</td>
</tr>
<tr>
<td>25</td>
<td>5.0</td>
<td>0.1643</td>
</tr>
</tbody>
</table>
Figure 3.4.1.1: Temperature profile for the plug-flow tubular problem.
3.4.2. Mathematical System with Nonlinear Inequality Constraint

This system involving a nonlinear inequality constraint was studied by Mehra and Davis (1972), Goh and Teo (1988), Vlassenbroeck (1988), Teo et al. (1991) and Elnagar et al. (1995).

The differential equations describing the system are

\[ \frac{dx_1}{dt} = x_2 \]  \hspace{1cm} (3.4.2.1)

\[ \frac{dx_2}{dt} = -x_2 + u \]  \hspace{1cm} (3.4.2.2)

\[ \frac{dx_3}{dt} = x_1^2 + x_2^2 + 0.005 \, u^2 \]  \hspace{1cm} (3.4.2.3)

with the initial condition

\[ x(0) = [0 \ -1 \ 0]^T \]  \hspace{1cm} (3.4.2.4)

The nonlinear inequality constraint to be satisfied is

\[ h(x) = x_2 + 0.5 - 8(t - 0.5)^2 \leq 0 \]  \hspace{1cm} (3.4.2.5)

The control is bounded by

\[ -20 \leq u \leq 20 \]  \hspace{1cm} (3.4.2.6)

The performance index to be minimized is

\[ I = x_3(t_f) \]  \hspace{1cm} (3.4.2.7)

where \( t_f = 1 \).
To deal with the inequality state constraint in eq (3.4.2.5), we introduce a state constraint variable $x_4$ by

$$\frac{dx_4}{dt} = \begin{cases} h(x) & \text{if } h(x) > 0 \\ 0 & \text{if } h(x) \leq 0 \end{cases}$$

(3.4.2.8)

with the initial condition $x_4(0) = 0$.

Since the performance index in eq (3.4.2.7) is to be minimized, we choose the augmented performance index to be minimized as

$$J = I + \rho \, x_4(t_f)$$

(3.4.2.9)

Now let us take $P = 20$, $R = 20$, $\gamma = 0.7$, $\eta = 0.5$, the penalty function factor $\rho = 10$ and $N = 21$ since the optimum was not obtained when using fewer than 21 grid points. We chose $u(0) = 0$, $v(0) = 40$ as the initial control policy and initial control region respectively. The tolerance $10^{-8}$ was used in subroutine DVERK for integration. By allowing 4 passes, consisting of 50 iterations per pass, we obtained the performance index $I = 0.17241$ with $x_4(1) = 6.31\times10^{-10}$. Already, after 16 iterations of pass 4, the final value for the state constraint variable $x_4(1) = 0$ was obtained with the same value of the performance index. This performance index is 5.3 % lower than the value reported by Goh and Teo (1988) of $I = 0.1816$ and marginally lower than the performance index $I = 0.1730$ obtained by Teo et al. (1991) with a mild violation in the inequality state constraint. The optimal control policy is given in Table 3.4.2.1. The computation time required for 4 passes was 1922 s. The trajectory of the function of state $h(x)$ is shown in Figure 3.4.2.1. As can be seen, the constraint is satisfied throughout the time interval.
To refine the results, we divided the time interval into 40 stages. By starting from the control policy obtained from the previous run, we obtained the performance index $I = 0.17085$, and again there was no violation in the inequality state constraint throughout the entire period of time. This value of the performance index is very slightly lower than the performance index $I = 0.17185$ reported by Elnagar et al. (1995) for a smooth control profile when using nonlinear programming along with the collocation technique.
Table 3.4.2.1: Optimal control policy for the mathematical system with nonlinear inequality constraint.

<table>
<thead>
<tr>
<th>Stage Number</th>
<th>Time $t_k$</th>
<th>Control $u(t_{k+1})$</th>
</tr>
</thead>
<tbody>
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</tr>
<tr>
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<td>3</td>
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<td>0.5580</td>
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<td>-2.8815</td>
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<td>7</td>
<td>0.35</td>
<td>-3.0754</td>
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<tr>
<td>8</td>
<td>0.40</td>
<td>-2.3706</td>
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<td>9</td>
<td>0.45</td>
<td>-1.6628</td>
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<td>10</td>
<td>0.50</td>
<td>-0.8970</td>
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<tr>
<td>11</td>
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<td>15</td>
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<td>2.2640</td>
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<td>16</td>
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<td>17</td>
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<td>0.3972</td>
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<td>18</td>
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<tr>
<td>20</td>
<td>1.00</td>
<td>-0.0260</td>
</tr>
</tbody>
</table>
Figure 3.4.2.1: Trajectory of the function $h(x)$ for the mathematical system with nonlinear inequality constraint.
3.4.3 Fed-Batch Fermentor Problem

Let us consider next the problem of determining the feed rate to a fed-batch fermentor in which the maximum production of penicillin is desired. The presence of six state inequality constraints makes this a challenging optimal control problem. This problem was studied by Lim et al. (1986), Cuthrell and Biegler (1989), Luus (1993b), Dadebo and McAuley (1995a) and most recently by Gupta (1995). The system is described by the four differential equations:

\[
\frac{dx_1}{dt} = h_1 x_1 - \left( \frac{x_1}{500x_4} \right) u 
\]

\[
\frac{dx_2}{dt} = h_2 x_1 - 0.01x_2 - \left( \frac{x_2}{500x_4} \right) u 
\]

\[
\frac{dx_3}{dt} = \frac{h_1 x_1}{0.47} - \frac{h_2 x_1}{1.2} - \frac{0.029x_3 x_1}{0.0001 + x_3} + \left( 1 - \frac{x_3}{500} \right) \frac{u}{x_4} 
\]

\[
\frac{dx_4}{dt} = \frac{u}{500} 
\]

where

\[
h_1 = \frac{0.11x_3}{0.006x_1 + x_3} 
\]

\[
h_2 = \frac{0.0055x_3}{0.0001 + x_3(1+10x_3)} 
\]

with the initial state

\[
x(0) = [1.5 \ 0 \ 0 \ 7]^T 
\]

The constraints on the feed rate are
and the constraints on the state variables are

\[ 0 \leq x_1 \leq 40 \]  \hspace{1cm} (3.4.3.9)

\[ 0 \leq x_3 \leq 25 \]  \hspace{1cm} (3.4.3.10)

\[ 0 \leq x_4 \leq 10 \]  \hspace{1cm} (3.4.3.11)

The performance index to be maximized is the total amount of penicillin produced at the final time \( t_f \) given by

\[ l = x_2(t_f) x_4(t_f) \]  \hspace{1cm} (3.4.3.12)

Since there are two inequality constraints imposed on each of the variables \( x_1, x_3 \) and \( x_4 \), we must deal with six inequality constraints. However, for simplicity, instead of introducing six auxiliary variables, we introduce only three state constraint variables, \( x_5, x_6 \) and \( x_7 \), through the differential equations

\[
\frac{dx_5}{dt} = \begin{cases} 
    x_1 - 40 & \text{if} \quad x_1 > 40 \\
    0 & \text{if} \quad 0 \leq x_1 \leq 40 \\
    -x_1 & \text{if} \quad x_1 < 0
\end{cases} \hspace{1cm} (3.4.3.13)
\]

\[
\frac{dx_6}{dt} = \begin{cases} 
    x_3 - 25 & \text{if} \quad x_3 > 25 \\
    0 & \text{if} \quad 0 \leq x_3 \leq 25 \\
    -x_3 & \text{if} \quad x_3 < 0
\end{cases} \hspace{1cm} (3.4.3.14)
\]

\[
\frac{dx_7}{dt} = \begin{cases} 
    x_4 - 10 & \text{if} \quad x_4 > 10 \\
    0 & \text{if} \quad 0 \leq x_4 \leq 10 \\
    -x_4 & \text{if} \quad x_4 < 0
\end{cases} \hspace{1cm} (3.4.3.15)
\]

with the initial conditions \( x_5(0) = 0, x_6(0) = 0, x_7(0) = 0 \).
Since the performance index in eq (3.4.3.12) is to be maximized, the augmented performance index to be minimized is chosen as

\[ J = -l + \rho_1 x_5(t_f) + \rho_2 x_6(t_f) + \rho_3 x_7(t_f) \]  

(3.4.3.16)

First let us choose \( t_f = 126 \) h and divide the time interval into 10 stages, i.e., \( P = 10 \), and take \( R = 5, \gamma = 0.8, \eta = 0.8, r^{(0)} = 2.5, 20 \) iterations per pass and \( N = 9 \) since the optimum was not obtained when using less then 9 grid points. The control policy given by Luus (1993b) was used as the initial control profile, and the error tolerance of \( 10^{-6} \) was used for integration. A few preliminary runs showed that, in order to ensure that all state constraints would be satisfied, the penalty function factors must be of the order of \( 10^5 \). However, to avoid convergence difficulties resulting when the penalty terms are much larger than the magnitude of the performance index, and also to obtain the state trajectories that satisfy all of the state constraints, we first set each \( \rho_i \) to be at about the same magnitude as the performance index and then systematically increased \( \rho_i \) after every pass. We simply chose for the first pass \( \rho_1 = \rho_2 = \rho_3 = 10 \), and increased these values by a factor of 2 after every pass. After 14 passes requiring the computation time of 18144 s, we obtained the performance index \( I = 87.78851 \) with \( x_3(126) = x_6(126) = x_7(126) = 0 \). This performance index is slightly better than the performance index \( I = 87.76 \) reported by Luus (1993b) and by Dadebo and McAuley (1995a). Although the control policy reported by Luus (1993b) does not cause any constraint violation at the end of each time stage, it yields the state constraint variable \( x_6(126) = 2.92 \) which shows some violation of the constraint on \( x_3 \). This state violation inside the time stages in this example was first pointed out by Keil (1994). The optimal
control policy obtained here is given in Table 3.4.3.1 and the resulting trajectories of the state variables $x_1, x_3$ and $x_4$ are shown in Figure 3.4.3.1.

Let us now take $T = 132$ h and divide this time interval into 20 stages. For this case, Luus (1993b) reported the performance index $I = 87.948$, and Gupta (1995) obtained $I = 88.00$. Their control policies were checked by integrating the system equations (eqs (3.4.3.1) - (3.4.3.4)) and the state constraint differential equations (eqs (3.4.3.13) - (3.4.3.15)). The control policy given by Luus (1993b) yielded $x_6(132) = 3.28$ showing that the constraint on $x_3$ is violated inside a time stage, while the policy reported by Gupta (1995) gave $x_7(132) = 0.127 \times 10^3$, showing a very slight violation of the upper bound on $x_4$. In fact, $x_5(132) = 10.002208$. By starting with the control policy given by Gupta (1995), we obtained convergence to the performance index $I = 87.955$, with no violation of the constraints throughout the time interval ($x_3(132) = x_6(132) = x_7(132) = 0$). The optimal control policy is given in Table 3.4.3.2.

Although, IDP was used for the three examples for optimization, the proposed method of introducing the state constraint variables to handle state constraints is not restricted to any particular optimization procedure.
Table 3.4.3.1: Optimal control policy for the fed-batch fermentor problem using 10 stages.

<table>
<thead>
<tr>
<th>Stage Number</th>
<th>Time $t_k$</th>
<th>Control $u(t_k)$</th>
</tr>
</thead>
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</table>

Table 3.4.3.2: Optimal control policy for the fed-batch fermentor problem using 20 stages.

<table>
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<th>Stage Number</th>
<th>Time $t_k$</th>
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</tr>
</thead>
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</tr>
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<tr>
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<td>9.4516</td>
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Figure 3.4.3.1: Trajectories of state variables; — $x_1$, $x_3$, and $x_4$ for the fed-batch fermentor problem.
4. CONCLUSIONS

Penalty function technique when used with iterative dynamic programming provides a good means for solving state constrained optimal control problems.

To handle final state constraints, the proposed method of determining the penalty function factors appears to be an effective procedure. By using different values for the tolerance, different levels of constraint satisfaction is possible. The systematic way of determining the penalty function factors is also useful in situations where the requirements for the accuracy of the final states is not the same for each state variable.

In solving optimal control problems with inequality state constraints, we introduce state constraint variables which are used as penalty functions in an augmented performance index. The proposed procedure works well, and no computational difficulties were encountered with the test problems. In each case the state constraint variables were zero at the final time, showing that the state constraints were satisfied everywhere inside the given time period.

The proposed two procedures with iterative dynamic programming are easy to use and optimal control of several meaningful engineering problems can be carried out on a personal computer in reasonable computational time. In many cases, the methods yield better results than previously reported in literature.
5. NOMENCLATURE

\( I \) = performance index

\( J \) = augmented performance index

\( k \) = index used for stage number

\( m \) = number of control variables

\( n \) = number of state variables

\( N \) = number of grid point used in IDP

\( p \) = penalty function

\( P \) = number of time stages

\( r \) = region over which allowable values for the control are taken

\( r \) = region vector, \( m \times 1 \)

\( R \) = number of sets of random allowable values for the control

\( s \) = number of state constraints

\( t \) = time

\( t_f \) = final time

\( u \) = scalar control variable

\( u \) = control vector, \( m \times 1 \)

\( x \) = state variable

\( x \) = state vector, \( n \times 1 \)

\textit{Greek Letters}

\( \alpha_j \) = lower bound on control \( u_j \)
$\beta_j$ = upper bound on control $u_j$

$\gamma$ = reduction factor for the control region after every iteration

$\delta$ = adjustment parameter used in eqs (2.2.2) and (2.2.3)

$\epsilon$ = tolerance for final state constraint violation

$\eta$ = restoration factor used after every pass

$\Theta$ = penalty function for final state constraints

$\theta$ = penalty function vector for final state constraints, $s \times 1$

$\rho$ = penalty function for state inequality state constraints

$\Phi$ = performance index

$\psi$ = inequality constraint function

Subscripts

$f$ = final

$i$ = general index, state variable number

$j$ = general index, control variable number

$k$ = index used for stage number

Superscripts

$d$ = desired value

$(j)$ = iteration number

$(q)$ = pass number
6. REFERENCES


