The Suboptimal Control of Nonlinear Systems Using Liapunov-Like Functions

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A technique which calculates approximate solutions to optimal control problems is developed in this work. The technique, which uses an empirically found weighted quadratic Liapunov function to transform the original *n*-dimensional optimization problem into a scalar optimization problem, is applied to a number of optimal control problems typical of those encountered in chemical engineering practice. The problems considered include both linear and nonlinear, lumped and distributed systems with minimum time, and quadratic and final value type performance indices. The solutions of these control problems show that the Liapunov-like suboptimal method, in general, requires less computer time and storage than that required by iterative and noniterative optimal methods currently used to solve optimal control problems. The reduction in computer storage and time enables the Liapunov-like technique to handle large dimensional control problems with relatively little effort.

Recently considerable interest has been shown in the suboptimal control of dynamic systems. Even though efficient algorithms have been developed to calculate the optimal control policies for dynamic systems, many classes of linear and nonlinear problems, especially those with state or control constraints, still require excessive computer time and/or storage when these algorithms are applied. Suboptimal control is an attempt to approximate the solution to these problems with a reduced amount of computer storage and computer time. The use of suboptimal control is justified in many cases, because system equations may not be very accurate, or because state measurements may not be precise. If the suboptimal control can be chosen so that a closed-loop policy results, the difficulties that arise in the application of open-loop control laws, when preciseness or accuracy is poor, can be circumvented. In addition, the use of suboptimal control may be justified for those problems where the performance index being optimized is insensitive to small perturbations in the control policy (*19*).

This paper illustrates a procedure which utilizes Liapunov-like or quadratic state functions to produce suboptimal solutions to control problems that closely approximate the optimal solutions. The suboptimal method has been developed so that state and control constraints are easily handled, and so that the suboptimal control policy is closed loop. No attempt, however, has been made to develop a suboptimal method which converges to the true optimum after many iterations.

Bass (*1*) was the first to point out the possibility of dynamic system optimization using Liapunov functions. He suggested that a stable control policy could be generated by minimizing the derivative of a positive definite Liapunov function for the system under investigation, with respect to the control. Koepcke and Lapidus (*9*) extended this approach for control of a variable coefficient extraction train, and Stevens and Wanninger (*18*) applied the method to a stirred-tank reactor. Paradis and Perlmutter (*14*) also used Liapunov functions for control of a stirred-tank reactor, but they further extended the method to the control of a lumped approximation to a tubular reactor. None of these works related the Liapunov function chosen to an optimal performance index. Denn (*3*), however, has recently related this type of Liapunov function-generated control policy to a truly optimal performance index for continuous, control constrained systems.

Attempts have been made to make the Liapunov function optimization method proposed by Bass more responsive to the type of performance desired. Nahi (*13*) showed that if the system under investigation meets certain requirements, minimization of a quadratic Liapunov function will produce the true time optimal response of that system. Unfortunately the requirements are so specific as to limit direct application to a very small number of specially structured problems. The generation of suboptimal minimum time control policies with Liapunov functions has been further investigated by Chant and Luus (*2*). They investigated several ways of choosing the weighting function to be used in a quadratic discrete time Liapunov function. They found that a numerical hill climbing method was necessary to find a weighting function that would give a suitable suboptimal minimum time response. Durbeck (*5*) also used a numerical gradient technique to find the best weighting to use for a general class of optimization problems, but a different polynomial had to be chosen for each problem.

In brief, the use of Liapunov functions, as proposed by Bass, has been used with considerable success to generate suitable suboptimal control policies. Little however has been done to generalize these interesting results, so that an a priori selection of the appropriate Liapunov function can be made. This paper attempts to show how an a priori selection of the Liapunov function can be made, and then to show how the resulting theory extends the Liapunov-like suboptimal control method to other optimization problems, where the performance index to be extremized is chosen in advance. Both lumped and distributed systems are considered with numerical results presented to show the application of this approach.

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THEORETICAL DEVELOPMENT

In a concurrent fashion we can develop the equations to be used for either a continuous or discrete approach. Thus we consider the system model as

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

$$\mathbf{x}(k+1) = \mathbf{h}[\mathbf{x}(k), \mathbf{u}(k)] \tag{1a}$$

The initial state $\mathbf{x}(0)$ is the boundary condition. We seek to select $\mathbf{u}(t)$ or $\mathbf{u}(k)$ such that a scalar performance index

$$I = \int_0^{t_f} g(\mathbf{x}, \mathbf{u})\, dt \tag{2}$$

$$I = \sum_{k=0}^{N} S[\mathbf{x}(k), \mathbf{u}(k)] \tag{2a}$$

is minimized subject to the constraints of (1) or (1*a*). Control and/or state constraints may also be added.

The Liapunov suboptimal method replaces the original state vector $\mathbf{x}$ with a scalar quadratic function:

$$V(\mathbf{x}) = \langle \mathbf{x}, \mathbf{Q}\mathbf{x} \rangle \tag{3}$$

$$V(k) = \langle \mathbf{x}(k), \mathbf{Q}\mathbf{x}(k) \rangle \tag{3a}$$

where $\langle \mathbf{x}, \mathbf{Q}\mathbf{x} \rangle$ represents a scalar product. The dynamic behavior of this new scalar system is described by

$$\dot{V}(\mathbf{x}) = \langle \mathbf{x}, \mathbf{Q}\mathbf{f} \rangle + \langle \mathbf{f}, \mathbf{Q}\mathbf{x} \rangle \tag{4}$$

$$V(k+1) = \langle \mathbf{h}(k), \mathbf{Q}\mathbf{h}(k) \rangle \tag{4a}$$

with the initial condition

$$V\{\mathbf{x}(0)\} = \langle \mathbf{x}(0), \mathbf{Q}\mathbf{x}(0) \rangle \tag{5}$$

Note from Equations (4) and (4*a*) that the Liapunov discrete dynamics will have terms containing the control to the second power whereas the equivalent continuous form multiplies these control terms by only the state vector.

Following a technique similar to that used in the development of the maximum principle (*10*), we combine Equations (2) and (4) to form the Hamiltonian

$$H(t) = z(t)\dot{V}(\mathbf{x}, \mathbf{u}) + g(\mathbf{x}, \mathbf{u}) \tag{6}$$

$$H(k+1) = z(k+1)V(k+1) + S(k) \tag{6a}$$

Note that this is a significant reduction in dimension as compared to the classical maximum principle approach since $z(t)$ is a sealer variable. In order to minimize the performance index, the Hamiltonian is minimized with respect to the control variables, usually by differentiation:

$$\frac{\partial H}{\partial u} = 0 \tag{7}$$

$$\frac{\partial H(k+1)}{\partial \mathbf{u}(k)} = 0 \tag{7a}$$

In some cases, when control or state constraints operate, this minimizing must be done numerically. This will yield an "optimal" control policy

$$\mathbf{u}^0 = \mathbf{u}(\mathbf{x}, z) \tag{8}$$

for the system defined by Equations (2) and (4), the reduced scalar system and the original performance index. In the discrete case, (8) is always a closed-loop policy, since the control term appears to a power other than 1 in (6*a*). Equation (8), however, will not in general be the optimal control for the system defined by Equation (1), because the Liapunov function transformation used in this work cannot account for all the dynamics of the original n-dimensional optimization problem. The classical maximum principle also dictates that the adjoint equation be defined by

$$\dot{z}(t) = -\frac{\partial H}{\partial V} \tag{9}$$

$$z(k) = \frac{\partial H(k+1)}{\partial V(k)} \tag{9a}$$

with the boundary conditions

$$z(t_f) = 0 \tag{10}$$

$$z(N) = 0 \tag{10a}$$

At this point, the continuous Liapunov method can be summarized. The optimal control policy for the transformed scalar system will in general be a function of the state vector and scalar adjoint variable. As is the case with the n-dimensional maximum principle, the state equation and adjoint equation make up a two-point boundary-value problem, with boundary conditions for the state being given at the initial time, and the boundary condition for the adjoint being given at the final time. However, the boundary-value problem which the Liapunov method produces is easy to solve. Since the adjoint variable is a scalar quantity, only one initial boundary condition is missing. Furthermore, results to be presented later in this paper indicate that the adjoint equation is essentially stable over the time intervals considered, when integrated in the forward direction. The solution to the boundary-value problem which the continuous Liapunov method produces is accomplished by assuming initial values for the adjoint variable, integrating the system equation, (1), and the adjoint equation, (9), in the forward direction while in the process generating the optimal control policy via (8). This procedure is repeated with different values of the initial adjoint variable, until the final boundary condition on the adjoint variable, (10), is satisfied.

The procedure is identical in the discrete case with one exception. Because of the resulting form of (9*a*), a series of iterations is required in addition to the overall iterations required to meet the final boundary specification. These new iterations involve assuming a $z(k+1)$ and calculation of the terms in (9*a*), until the value of $z(k)$ specified by calculations in the previous time step is satisfied.

SPECIFIC EXAMPLES

The control policy generated by the transformed system, defined by the scalar Liapunov function and the performance index, may or may not be the optimal policy for the original n-dimensional system. If however, the original system equation is scalar to begin, optimality should result. To illustrate this point a linear problem and a nonlinear problem are presented here.

The quadratic performance index

$$I = (1/2)\int_0^{t_f} (px^2 + ru^2)\, dt \tag{11}$$

is to be minimized subject to the linear equation

$$\dot{x} = ax + bu \tag{12}$$

Picking the Liapunov function as

$$V = qx^2 \tag{13}$$

and substituting (12) into the time derivative expression of (13), we get

$$\dot{V} = 2q(ax^2 + bux)$$

Formation of the Hamiltonian

$$H = 2q(ax^2 + bxu)z + (1/2)px^2 + (1/2)ru^2 \quad (14)$$

and differentiation, with respect to the control, give

$$u^0 = -2qbzx/r \quad (15)$$

Substitution of (15) into the Hamiltonian (14), and differentiation with respect to V, yield

$$\dot{z} = -2az + (2qb^2z^2/r) - (p/2q) \quad (16)$$

Letting $q = 1/2$, (16) can be recognized as the Riccati equation, given in (17), that would result from the application of the continuous maximum principle to the linear quadratic problem defined by (11) and (12) (see reference *10*).

$$\dot{z} + 2az - r^{-1}b^2z^2 + p = 0 \quad (17)$$

Thus the Liapunov procedure yields the true optimal control policy for this scalar linear optimal control problem.

The nonlinear example involves finding the temperature profile for a plug-flow tubular reactor that will maximize the yield of B. The reversible reaction taking place is $A \rightleftarrows B$, and the rate constants are

$$k_i = k(i) \exp[-E_i/RT] \quad i = 1, 2$$

with T being the controllable temperature in the reactor. The system equation is

$$\dot{x} = k_1(1 - x) - k_2x$$

with x the concentration of B. Selection of the Liapunov function to be

$$V = qx^2$$

yields a Hamiltonian of the following form:

$$H = 2qx[k_1(1 - x) - k_2x]z$$

Differentiation with respect to the temperature yields

$$T^0 = (E_1 - E_2)\left[R \ln\left\{(x/1 - x)\frac{k(2)E_2}{k(1)E_1}\right\}\right]$$

This result is the same as that derived by Fan (*6*) for this problem, using the continuous maximum principle. Thus the Liapunov procedure again yields the true optimal control policy.

Further comparisons can also be made with nonscalar problems but we prefer to show these later in the paper.

NUMERICAL SYSTEMS

Here we present the details for a number of different systems which have been used to test the current suboptimal procedure. These are taken from a larger set (*16*) which also contains further specific results.

Lumped-Parameter Systems

Two-Variable Problem. The nonlinear reaction system

$$A \rightarrow 2B \rightarrow C$$

carried out isothermally in a tubular reactor is the first lumped-parameter system considered. The pressure profile that maximizes the yield of B is desired. A material balance on A and B gives (*11*)

$$\dot{x}_1 = -2k_1P\frac{x_1}{B + x_2}$$

$$\dot{x}_2 = 4k_1P\frac{x_1}{B + x_2} - 4k_2P^2\frac{x_2^2}{(B + x_2)^2} \quad (18)$$

where $B = 2x_1(0) + 2x_2(0)$. Numerical values used in all the calculations are $x_1(0) = 0.010$, $x_2(0) = 0.002$, $k_1 = 0.01035$, $k_2 = 0.04530$, and $t_f = 8$ min.

Five-Variable Problem. Sage (*15*) presents a linear five-variable system which results from the lumping of a distributed linear diffusion process described by

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial y^2} + u(y, t)$$

Spatial discretization yields a linear system

$$\dot{\mathbf{x}}(t) = \mathbf{Ax} + \mathbf{Bu} \quad (19)$$

where $\mathbf{x}$ is the vector representing the temperature profile T. $\mathbf{A}$ is a tridiagonal matrix of the form

$$\mathbf{A} = \begin{bmatrix} -1 & 1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 1 & -1 \end{bmatrix}$$

and $\mathbf{B} = \mathbf{I}_5$. The Δy term, which results from discretizing, equals 1.0 for this problem. The performance index to be minimized is

$$I = (1/2)\int_0^1 (\langle\mathbf{x}, \mathbf{Px}\rangle + \langle\mathbf{u}, \mathbf{Ru}\rangle)dt \quad (20)$$

and the initial condition for $\mathbf{x}$ is

$$\mathbf{x}^T(0) = [1\,2\,3\,4\,5]$$

The choices of $\mathbf{P}$ and $\mathbf{R}$ will be presented later.

Six-Variable Problem. A linear model of a six-plate absorber is the next multidimensional system considered. This system has been described in detail by Lapidus and Luus (*10*). The system has the same form as (19); all matrices and initial conditions are as given in reference *10*. Two types of performance indices are investigated: the minimization of a quadratic index

$$I = (1/2)\int_0^{t_f} (\langle\mathbf{x}, \mathbf{Px}\rangle + \langle\mathbf{u}, \mathbf{Ru}\rangle)dt \quad (21)$$

and the minimum time index $I = t_f$. The various choices of $\mathbf{P}$ and $\mathbf{R}$ used in (21) are discussed later.

Distributed Parameter Systems

Linear System. A double-pipe heat exchanger described by two linear hyperbolic equations is the first distributed parameter system investigated. The system is composed of an inner tube with a spatially distributed temperature profile T_1, and an outer tube containing a heating medium which heats the wall to a temperature T_2. Control is achieved by varying the temperature of the outer fluid $u(t)$. After the simplifying assumptions made by Lesser (12) are included, an energy balance yields

$$\frac{\partial T_1}{\partial t} = -\frac{\partial T_1}{\partial y} + C_1[T_2 - T_1]$$

$$\frac{\partial T_2}{\partial t} = C_2[u - T_2] - C_3[T_2 - T_1] \quad (22)$$

where C_1, C_2, and C_3 are heat transfer coefficients and $u(t)$ is the dimensionless temperature of the outer fluid, constrained between $+(2/3)$ and $-(4/3)$. The boundary conditions for this system are

$$T_1(0, y) = T_{1ss}(y)$$
$$T_2(0, y) = T_{2ss}(y)$$
$$u(0) = U_0$$

where U_0 is the steady state control and T_{1ss} and T_{2ss} are related to U_0, C_1, C_2, C_3 *(16)*. Numerical values used in all the calculations are $C_1 = 1.2876642$, $C_2 = 5.5035774$, $C_3 = 2.5207966$, and $U_0 = -0.666667$. The desired final state for both T_1 and T_2 is zero. The optimization problem is concerned with the minimization of the quadratic index

$$I = \int_0^1 T_1^2(\text{exit})\,dt \tag{23}$$

Nonlinear System. The next distributed system investigated is made up of two nonlinear elliptic equations which describe the behavior of a tubular reactor with radial diffusion in which a reversible reaction $A \rightleftarrows B$ is taking place. Denn *(4)* and Seinfeld *(17)* have investigated this same nonlinear distributed system with different optimal techniques. A material balance on B and energy balance applied to this system yields

$$\frac{\partial C}{\partial t} = \frac{a}{Pe}\left[\frac{\partial^2 C}{\partial r^2} + \frac{1}{r}\frac{\partial C}{\partial r}\right] + bR(C, T)$$
$$\frac{\partial T}{\partial t} = \frac{a}{Pe'}\left[\frac{\partial^2 T}{\partial r^2} + \frac{1}{r}\frac{\partial C}{\partial r}\right] + b'R(C, T) \tag{24}$$

where

$$R(C, T) = \exp\,[E_1/RT_0]\{(1 - C)\exp(-E_1/RTT_0) - kC\exp(-E_2/RTT_0)\}$$

Pe, b and Pe', b' are Peclet and Damkohler numbers for mass and heat transfer, respectively. T_0 is a characteristic temperature and a is the length of reactor/radius of the reactor.

The boundary conditions for this system are

$$\begin{array}{ll} C(0, r) = 0 & T(0, r) = 1 \\ \{\partial C(t, 0)/\partial r\} = 0 & \{\partial T(t, 0)/\partial r\} = 0 \\ \{\partial C(t, 1)/\partial r\} = 0 & \{\partial T(t, 1)/\partial r\} = -Q(t) \\ \{\partial C(1, r)/\partial t\} = 0 & \{\partial T(1, r)/\partial t\} = 0 \end{array} \tag{25}$$

The optimal control problem is concerned with selecting the dimensionless wall flux $Q(t)$, constrained between 0 and 1.5, which maximizes the integral average outlet conversion

$$I = 2\int_0^1 rC(1, r)\,dr \tag{26}$$

Numerical values used in all the calculations are $E_1/R = 12{,}000$, $E_2/R = 25{,}000$, $Pe = 110$, $Pe' = 84.5$, $T_0 = 620°\text{K.}$, $b = 0.5$, $b' = 0.25$, $k = 3.85 \times 10^9$, and $a = 50$.

THE SOLUTION OF LINEAR LUMPED CONTROL PROBLEMS

Here we shall illustrate the application of the Liapunov suboptimal method to linear lumped systems. Only discretized problems will be analyzed, although continuous problems can be easily handled *(16)*. The form of the system equations is thus

$$\mathbf{x}(k+1) = \boldsymbol{\varphi}\mathbf{x}(k) + \boldsymbol{\Delta}\mathbf{u}(k) \quad k = 0, 1, \ldots, N-1 \tag{27}$$

where $\boldsymbol{\varphi}$ and $\boldsymbol{\Delta}$ are matrices relating to the system parameters. Alternately these matrices may be related to an original continuous system as detailed in reference *10*.

Choosing the Weighting Matrix

One of the primary questions in the Liapunov suboptimal methods is the selection of the weighting matrix $\mathbf{Q}$. This matrix strongly influences the degree of suboptimality because the original n-dimensional optimization problem is approximated in the scalar domain differently by different weighting matrices. The relation between the weighting matrix and the degree of suboptimality will be illustrated when numerical results are presented. However, only weighting matrices with nonzero diagonal elements and zero off-diagonal elements are considered here. Thus only n nonzero elements in the weighting matrix need be specified.

A method of choosing the weighting matrix that could be generalized to all discrete linear control problems, independent of the number of equations under consideration, was found and consequently used for all the optimization problems in this work. The diagonal weighting matrix found to give suboptimal answers with the lowest degree of suboptimality on a large number of different problems is of the form

$$\mathbf{Q} = [Q_{i,i}]\mathbf{P}$$

where

$$Q_{i,i} = Q_{1,1}^{\;d_i} \qquad (i = 1, 2, \ldots, n) \tag{28}$$
$$d_i = \ln[\textstyle\sum_j \Delta_{1,j}]/\ln[\sum_j \Delta_{i,j}]$$

and, of course, $Q_{i,j} = 0$ for $i \neq j$. This form requires only a one-dimensional gradient search for the $Q_{1,1}$ element which will give the best suboptimal performance index, since the d_i may be calculated from $\boldsymbol{\Delta}$. The details of this search technique will be presented in the next section but it should be pointed out that this contrasts with the work of Chant and Luus *(2)* and with the work of Durbeck *(5)*, both of which required a large dimensional gradient search.

The empirical nature of the procedure used to find the Liapunov function weighting matrix is a disadvantage of the suboptimal method presented in this work. Attempts were made to relate the weighting matrices which gave the best results, to optimal feedback matrices gotten from the maximum principle, but only on linear problems with quadratic performance indices was any relationship found. Thus for a two-variable problem the relationship above can be developed directly. For higher dimensional systems however, this approach could not be carried out. The major justification for using the weighting matrix of (28) was that all the computational results obtained had a very low degree of suboptimality.

Minimum Time Problems

For unconstrained linear minimum time problems, the performance index is time, the linear discrete system is described by (27), and the Hamiltonian becomes

$$H(k+1) = z(k+1)[\mathbf{x}^T(k)\,\boldsymbol{\varphi}^T\mathbf{Q}\boldsymbol{\varphi}\mathbf{x}(k) + 2\mathbf{x}^T(k)\,\boldsymbol{\varphi}^T\mathbf{Q}\boldsymbol{\Delta}\mathbf{u}(k) + \mathbf{u}^T(k)\,\boldsymbol{\Delta}^T\mathbf{Q}\boldsymbol{\Delta}\mathbf{u}(k)] \tag{29}$$

Minimizing (29) with respect to the control yields the optimal policy

$$\mathbf{u}^0(k) = -(\boldsymbol{\Delta}^T\mathbf{Q}\boldsymbol{\Delta})^{-1}\boldsymbol{\Delta}^T\mathbf{Q}\boldsymbol{\varphi}\mathbf{x}(k) \tag{30}$$

This result is closed loop and does not require that the adjoint equation be solved at all. This special type of control policy will occur for all control problems where the performance index lacks terms containing the control vector.

The explicit solution of all unconstrained discrete linear control problems with a control policy similar to (30) may be obtained by a single iteration procedure. This is due to

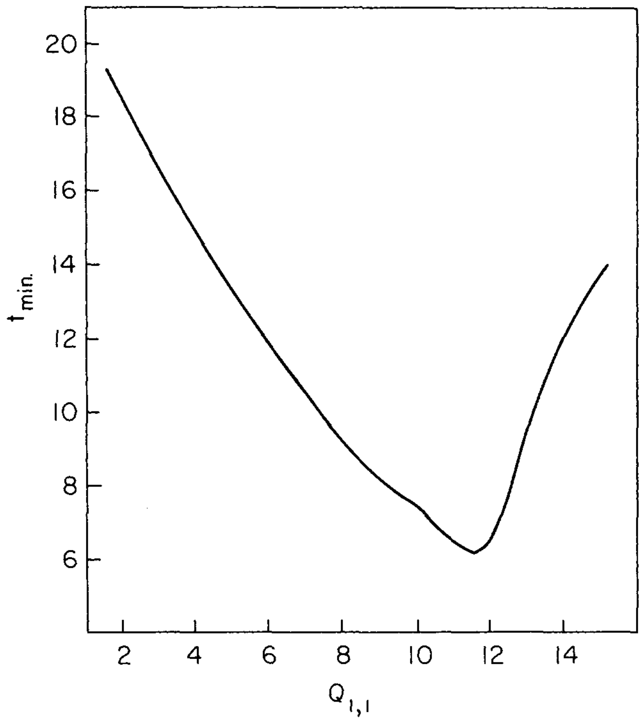

Fig. 1. $Q_{1,1}$ versus suboptimal minimum time for the six-variable minimum time problem.

the fact that the adjoint variable is not needed. To begin the iteration a value for $Q_{1,1}$ is assumed, and the appropriate **Q** matrix is calculated. With (30) specifying the control policy, the system equation is integrated starting at $\mathbf{x}(0)$. Terms in the performance index are calculated along the path of the trajectory, if such a quantity is required by the optimization problem. For minimum time problems, the time required to reach a previously chosen stopping condition is stored in the computer memory, along with the $Q_{1,1}$ element which produced that suboptimal minimum time. If another type of performance index is being optimized, the value of $Q_{1,1}$ and the corresponding value of the performance index at the final time specified by the statement of the problem are stored. Different values of $Q_{1,1}$ are now chosen, and the whole problem is solved again for each of these different $Q_{1,1}$ elements, until the value of $Q_{1,1}$ which gives the lowest minimum time, or the best performance index, is found. The search for the best $Q_{1,1}$ is facilitated by using a one-dimensional gradient technique constructed to provide a direction for the iteration sequence.

The six-plate absorber system was used to illustrate the Liapunov approach to discrete minimum time problems. A sampling time interval T of 0.25 min. was used in discretizing this system. A suboptimal minimum time of 6.25 min. was the best result found by the Liapunov method using a $Q_{1,1}$ element of 11.50 and a stopping condition of $\max_i[|x_i|] < 0.001$. This compares favorably with the true minimum time of 5 min. calculated by Lesser (*12*) for this problem with the same sampled time interval of 0.25. Figure 1 shows the effect of $Q_{1,1}$ on the suboptimal minimum time.

Quadratic Performance Index Control Problems

Application of the Liapunov method to an unconstrained linear discrete system with the specific discrete quadratic performance index

$$I = \sum_{k=0}^{N} \{<\mathbf{x}(k), \mathbf{P}\mathbf{x}(k)> + <\mathbf{u}(k), \mathbf{R}\mathbf{u}(k)>\}$$

yields a Hamiltonian described by

$$H(k+1) = z(k+1)[\mathbf{x}^T(k)\boldsymbol{\varphi}^T\mathbf{Q}\boldsymbol{\varphi}\mathbf{x}(k) + 2\mathbf{x}^T(k)\boldsymbol{\varphi}^T\mathbf{Q}\boldsymbol{\Delta}\mathbf{u}(k) + \mathbf{u}^T(k)\boldsymbol{\Delta}^T\mathbf{Q}\boldsymbol{\Delta}\mathbf{u}(k)] + \mathbf{x}^T(k)\mathbf{P}\mathbf{x}(k) + \mathbf{u}^T(k)\mathbf{R}\mathbf{u}(k) \quad (31)$$

Minimization of this expression with respect to the control yields the optimal policy

$$\mathbf{u}^0(k) = -z(k+1)[(z(k+1)\boldsymbol{\Delta}^T\mathbf{Q}\boldsymbol{\Delta} + \mathbf{R}]^{-1}\boldsymbol{\Delta}^T\mathbf{Q}\boldsymbol{\varphi}\mathbf{x}(k) \quad (32)$$

This equation prescribes a nonstationary control law, since $z(k+1)$, the scalar adjoint variable, is a function of the time step. If no cost is attached to the amount of control used, the optimal control policy becomes

$$\mathbf{u}^0(k) = -(\boldsymbol{\Delta}^T\mathbf{Q}\boldsymbol{\Delta})^{-1}\boldsymbol{\Delta}^T\mathbf{Q}\boldsymbol{\varphi}\mathbf{x}(k) \quad (33)$$

since $\mathbf{R} = \mathbf{0}$. This result is identical to the expression obtained for the minimum time problem. The adjoint equation is

$$z(k) = \frac{\partial[z(k+1)V(k+1) + \mathbf{x}^T(k)\mathbf{P}\mathbf{x}(k) + \mathbf{u}^T(k)\mathbf{R}\mathbf{u}(k)]}{\partial V(k)} \quad (34)$$

The five-variable system described by (19) and (20) was used to illustrate the Liapunov approach to unconstrained linear problems with quadratic performance indices. **P** and **R** were chosen as diagonal matrices with diagonal elements [0.5, 1, 1, 1, 0.5]. A sampling time interval of 0.05 was used. The solution of the adjoint equation can be

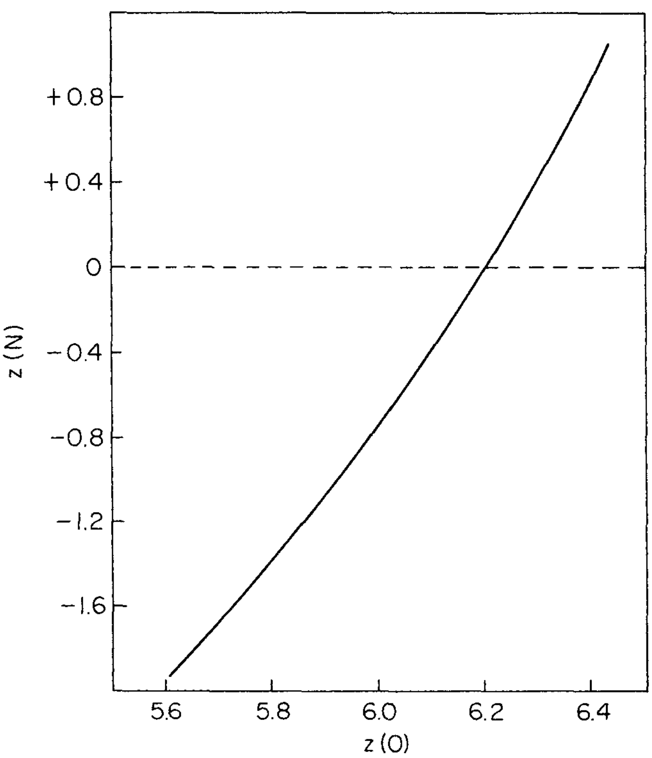

Fig. 2. $z(N)$ versus $z(0)$ for the five-variable quadratic performance index problem. $Q_{1,1} = 1.00$.

TABLE 1. THE SUBOPTIMAL CONTROL AND ADJOINT VARIABLE FOR THE FIVE-VARIABLE PROBLEM
(Sampled Period = 0.05 min. and $Q_{1,1}$ = 1.00)

t	z	u_1	u_2	u_3	u_4	u_5
0.00	6.2000	−0.6725	−1.1969	−1.8034	−2.3694	−3.0205
0.05	6.0790	−0.6646	−1.1411	−1.7163	−2.2534	−2.8476
0.10	5.9420	−0.6533	−1.0861	−1.6293	−2.1367	−2.6788
0.15	5.7870	−0.6388	−1.0315	−1.5422	−2.0194	−2.5134
0.20	5.6120	−0.6212	−0.9768	−1.4549	−1.9014	−2.3510
0.25	5.4160	−0.6006	−0.9219	−1.3671	−1.7826	−2.1909
0.30	5.1960	−0.5769	−0.8662	−1.2786	−1.6630	−2.0326
0.35	4.9520	−0.5503	−0.8097	−1.1891	−1.5424	−1.8756
0.40	4.6820	−0.5208	−0.7520	−1.0986	−1.4207	−1.7197
0.45	4.3840	−0.4883	−0.6930	−1.0068	−1.2980	−1.5644
0.50	4.0590	−0.4528	−0.6325	−0.9136	−1.1740	−1.4994
0.55	3.7060	−0.4145	−0.5704	−0.8190	−1.0490	−1.2547
0.60	3.3260	−0.3732	−0.5065	−0.7230	−0.9228	−1.1000
0.65	2.9190	−0.3291	−0.4409	−0.6255	−0.7955	−0.9454
0.70	2.4890	−0.2822	−0.3735	−0.5266	−0.6674	−0.7909
0.75	2.0360	−0.2327	−0.3043	−0.4265	−0.5386	−0.6365
0.80	1.5660	−0.1805	−0.2336	−0.3254	−0.4094	−0.4826
0.85	1.0810	−0.1260	−0.1613	−0.2234	−0.2800	−0.3293
0.90	0.5860	−0.0692	−0.0878	−0.1208	−0.1508	−0.1770
0.95	0.0863	−0.0103	−0.0130	−0.0178	−0.0221	−0.0259

handled numerically by assuming that

$$V(k+1) \approx a(k)V(k)$$

and that

$$[\mathbf{x}^T(k)\mathbf{P}\mathbf{x}(k) + \mathbf{u}^T(k)\mathbf{R}\mathbf{u}(k)] \approx b(k)V(k)$$

Equation (34) then becomes

$$z(k) = z(k+1)a(k) + b(k) \quad (35)$$

where

$$a(k) = V(k+1)/V(k)$$

$$b(k) + [\mathbf{x}^T(k)\mathbf{P}\mathbf{x}(k) + \mathbf{u}(k)^T\mathbf{R}\mathbf{u}(k)]/V(k)$$

To solve this type of discrete adjoint equation, an iteration procedure is involved. Briefly, each time step involves an iteration in order to find the $z(k+1)$ which meets the specifications of (35), and the entire problem is iterated until the final boundary condition $z(N) = 0$ is satisfied. A plot of $z(N)$ versus $z(0)$ is shown in Figure 2. The procedure used to find the best nonstationary suboptimal control policy for the system under discussion involves picking values for $Q_{1,1}$ and solving the corresponding adjoint equations until the value of $Q_{1,1}$ which gives the best suboptimal response is found. The best suboptimal control policy for the five-variable problem that was generated by this approach is given in Table 1, along with the value of the corresponding adjoint variable. This control policy yielded a performance index of $I = 6.5190$. This compares well with the true optimal index of $I^0 = 6.5115$, and comparison of these two indices gives a % degree of suboptimality of 0.11%. The % degree of suboptimality as used here and in the remainder of the work is defined as

$$\begin{matrix}\%\text{ Degree of} \\ \text{suboptimality}\end{matrix} = \left[\frac{I - I^0}{I^0}\right] 100 \quad (36)$$

Lapidus and Luus (*10*) show, for a stable linear control problem with a quadratic performance index and a large final time, that a stationary feedback control matrix will result from the application of the maximum principle and the Riccati transformation. This stationary control law results when the Riccati equation, being integrated in the reverse time direction, reaches a steady state. In the course of this investigation, it became evident that the Liapunov approach would behave in an analogous way. A method for implementing this behavior was developed, with the result that for those problems where a stationary feedback matrix can be assumed, the necessity of solving the scalar adjoint equation is removed. Briefly, it is assumed that if the scalar adjoint equation, (34), were solved in the backward direction, a steady state value for the adjoint variable $z(ss)$ would eventually be reached. Instead of doing this, however, the steady state adjoint variable $z(ss)$ is assumed to be an unknown parameter in the feedback control expression which has to be chosen optimally. The stationary optimal control law then becomes

$$\mathbf{u}^0(k) = -z(\text{ss})[z(ss)\boldsymbol{\Delta}^T\mathbf{Q}\boldsymbol{\Delta} + \mathbf{R}]^{-1}\boldsymbol{\Delta}^T\mathbf{Q}\boldsymbol{\varphi}\mathbf{x}(k) \quad (37)$$

In effect, linear problems with quadratic indices where an adjoint variable is required, but a stationary control law is assumed, have two parameters, $Q_{1,1}$ and $z(ss)$, which have to be found by a gradient technique if a performance index with a low degree of suboptimality is to result.

A further consequence of this stationary feedback law assumption is the ability to relate the resulting suboptimal control policy to a truly optimal performance index. The discrete recurrence equations that result when the Riccati transformation matrix $\mathbf{J}(t)$ reaches a steady state $\mathbf{J}(\text{ss})$ are (*10*)

$$\mathbf{u}^0(k) = -\mathbf{K}(\text{ss})\mathbf{x}(k) \quad (38)$$

$$\mathbf{K}(\text{ss}) = [\boldsymbol{\Delta}^T(\mathbf{J}(\text{ss}) + \mathbf{P})\boldsymbol{\Delta} + \mathbf{R}]^{-1}\boldsymbol{\Delta}^T(\mathbf{J}(\text{ss}) + \mathbf{P})\boldsymbol{\varphi} \quad (39)$$

$$\mathbf{J}(\text{ss}) = \boldsymbol{\varphi}^T(\mathbf{J}(\text{ss}) + \mathbf{P})[\boldsymbol{\varphi} - \boldsymbol{\Delta}\mathbf{K}(\text{ss})] \quad (40)$$

Comparison of (38) and (39) with (37) indicates that if $\mathbf{J}(\text{ss})$ is set equal to $\{z(\text{ss})\mathbf{Q} - \mathbf{P}\}$ the optimal control laws given by these equations are identical. This result leads to the conclusion that the control law which the Liapunov method generates, (37), specifies the exact optimal control policy for a discrete linear system

$$\mathbf{x}(k+1) = \boldsymbol{\varphi}\mathbf{x}(k) + \boldsymbol{\Delta}\mathbf{u}(k)$$

with a performance index to be minimized of

$$I = \sum_{k=0}^{N} \{\langle \mathbf{x}, \mathbf{P}(\text{true})\mathbf{x}\rangle + \langle \mathbf{u}, \mathbf{R}\mathbf{u}\rangle\}$$

where

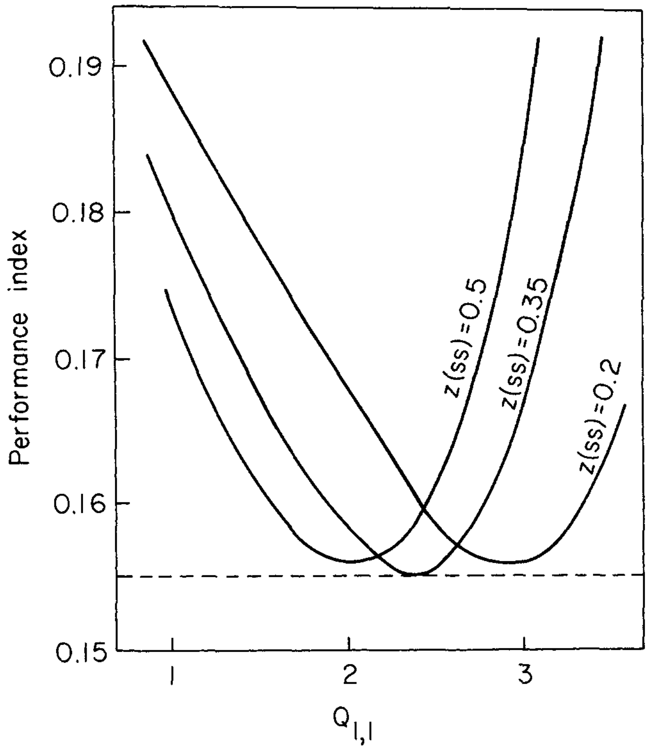

Fig. 3. $Q_{1,1}$ **versus performance index with** z**(ss) as a parameter for the six-variable quadratic index problem.** $\mathbf{P} = \mathbf{I}$ **and** $\mathbf{R} = \mathbf{I}$**.**

$$\mathbf{P}(\text{true}) = z(\text{ss})\{\mathbf{Q} - \boldsymbol{\varphi}^T\mathbf{Q}\boldsymbol{\varphi} + \boldsymbol{\varphi}^T\mathbf{Q}\boldsymbol{\Delta} [z(\text{ss})\boldsymbol{\Delta}^T\mathbf{Q}\boldsymbol{\Delta} + \mathbf{R}]^{-1}\boldsymbol{\Delta}^T\mathbf{Q}\boldsymbol{\varphi}z(\text{ss})\} \quad (41)$$

This last equation defining $\mathbf{P}$(true) results from substituting the relationship

$$\mathbf{J}(\text{ss}) = z(\text{ss})\mathbf{Q} - \mathbf{P}$$

into Equations (39) and (40), and then solving for the $\mathbf{P}$ matrix.

The six-variable adsorber system with $T = 1.0$ min. was used to illustrate the generation of stationary feedback control laws by the Liapunov suboptimal approach. The procedure for finding the best $Q_{1,1}$ elements described previously for the minimum time problem was used to find the best suboptimal control policies for those problems with performance indices having no control weighting, $\mathbf{R} = \mathbf{0}$, because no z(ss) term was required. For problems with indices containing the weighted control term $\mathbf{R} \neq 0$, the best suboptimal control policy was calculated by first using a gradient search technique to find the best z(ss) to use for each $Q_{1,1}$, and then by performing another one-dimensional search for the best $Q_{1,1}$. The values of these parameters that yielded the lowest performance index were considered to be the best values. A plot of $Q_{1,1}$ versus index with z(ss) as a parameter and with $\mathbf{P} = \mathbf{I}$ and $\mathbf{R} = \mathbf{I}$ is shown in Figure 3. Table 2 shows the results obtained for the different performance indices considered. The same notation used in Lapidus and Luus (*10*) is used to describe the weighting matrix. $\mathbf{R} = [-2, 1]$ means a diagonal matrix with elements 10^{-2} and 10^1. One interesting result shown in Table 2 is that the suboptimal method yields larger errors for those indices where $\mathbf{R} \neq \mathbf{0}$. Some effect for the $\mathbf{R}$ matrix should probably be included in the choice of the $\mathbf{Q}$ matrix, but this was not investigated during the course of the present work. The low degree of suboptimality obtained for these problems indicates that the Liapunov approach and the method used to pick the $\mathbf{Q}$ weighting matrix, taken together, provide a suitable way to approximate the optimal solution to linear-quadratic control problems.

For this linear six-variable system, the Liapunov method requires more computer time to generate good suboptimal control policies for problems with quadratic indices than the Riccati tranformation true optimal method, because several iterations are required to find the best $Q_{1,1}$ and $z(ss)$ elements. The nature of the several iteration paths which have been presented indicate that these iterations can be quickly implemented, and can be started almost anywhere, because the curves of $Q_{1,1}$ versus the performance index are smooth and have only one minimum. For problems with a large n, say 20 or 30, the Liapunov suboptimal method will require less computer time than the Riccati transformation technique, because the Riccati technique requires many more matrix manipulations than that required by the Liapunov method. As was the case with the minimum time problem, the suboptimal method does, however, require considerably less computer storage than the Riccati transformation approach. In general, the Riccati approach requires three times the storage required by the suboptimal method to generate a control policy. The implementation of the nonstationary suboptimal policy, as illustrated by the five-variable problem, is easier than the implementation of the nonstationary Riccati-generated policy. The suboptimal policy requires the "playing back" of only an n-dimensional matrix and a time varying multiplicative scalar at each time step, while the Riccati generated policy requires the storage and "playing back" of a series of time varying n-dimensional matrices, one for each time step. Kleinman and Athans (*7*, *8*) have developed a suboptimal technique which produces "piecewise constant" feedback matrices, and as a consequence a reduction in the number of matrices that have to be stored when implementing the suboptimal control policy. Instead of having a matrix which changes at each time step, their technique finds the best constant feedback matrix to use over a certain preselected time period which is longer than the time step under consideration. With this method however, a different matrix is still required for each time period. The number of matrices required is less than that required by the Riccati approach, so the storage problems associated with nonstationary feedback control laws are

TABLE 2. SUMMARY OF THE SUBOPTIMAL RESULTS FOR THE SIX-VARIABLE LINEAR ABSORBER
(Sampled Period = 1.00 min.)

P	R	$Q_{1,1}$	z(ss)	Degree of suboptimality, %
I	0	1.91	——	0.02
I	I	2.35	0.352	0.04
5I	I	3.00	0.550	0.09
I	[−2, 1]	3.25	0.700	0.15
5I	[−2, 1]	3.00	0.700	0.70
[−7, −1, −1, −1, −1, −7]	0	1.90	——	0.04

alleviated somewhat. The Liapunov approach, however, practically eliminates the storage problems.

THE SOLUTION OF NONLINEAR LUMPED-CONTROL PROBLEMS

Final Value Index Control Problem

Problems with a final value index can be handled in two ways by the continuous Liapunov suboptimal method. The first way uses an approach similar to that presented earlier for unconstrained problems. A Hamiltonian is formed by combining the derivative of the Liapunov function and the final value performance index

$$H(t) = z(t)\dot{V}(\mathbf{x}, \mathbf{u}) \tag{42}$$

The final value index prescribes a boundary condition on the adjoint variable, $z(t_f)$. Extremizing this Hamiltonian yields, for the nonlinear systems considered in this work, a suboptimal control policy which is not a function of the adjoint variable

$$\mathbf{u}^0 = \mathbf{u}(\mathbf{x}) \tag{43}$$

It must be emphasized that this result is encountered only when differentiation of the nonlinear system euqations with respect to the control vector yields a system of equations which still contains the control vector as a parameter. The procedure used to find the best suboptimal performance index is to iterate on the problem with different **Q** matrix weightings until the best value for the final valued index is found. An alternate approach to final value index control problems proceeds by defining an integral performance index which is equivalent to the final value index and then using the integral index in the optimization procedure presented previously. For example, if the final value of x_2 was to be maximized, the integral index

$$I = \int_0^t \dot{x}_2 dt \tag{44}$$

could be maximized to yield the desired result. The final value index and the integral index are shown to be equivalent, by integrating (44) to yield

$$\max_u \left\{ \int_0^{t_f} \dot{x}_2 dt \right\} = \max_u \left\{ x_2\Big|_{t_f} - x_2\Big|_0 \right\}$$

Applying the Liapunov method to an optimization problem with an integral index similar to (44) will, in most cases, yield a control policy that is dependent on the scalar adjoint variable, thus requiring that the adjoint equation be solved in the process of finding the control policy.

The nonlinear system used to illustrate both of the above approaches to final value index problems was the reaction system described by (18). The pressure profile which maximized x_2 at the end of the reactor was desired. Since this problem was not linearized in any manner, the effect of the control could not be isolated or assigned to any one term, as is possible with linear systems when the effect of the control is isolated in the $\mathbf{\Delta}$ matrix. Because no control term could be isolated, a constant diagonal **Q** weighting matrix was used, and since only two diagonal elements were required by this problem $Q_{1,1}$ was set to 1.0, and $Q_{2,2}$ was the free element to be found via a gradient search in a manner similar to the problems previously presented. With the use of the first Liapunov approach for final valued index problems, the continuous Liapunov method yields a Hamiltonian of the form

$$H = -2k_1x_1^2 P\, Q_{1,1}/[x_2 + B] + 4Q_{2,2}$$
$$[k_1x_1x_2P - k_2x_2^3P^2/(x_2 + B)]/(x_2 + B) \tag{45}$$

Maximizing this expression yields the optimal control policy

$$P = \frac{x_1k_1[2x_2Q_{2,2} - x_1Q_{1,1}](x_2 + B)}{4x_2^3k_2Q_{2,2}} \tag{46}$$

With this equation specifying the control policy, the whole problem is iterated by assuming values for $Q_{2,2}$ and integrating the state equations in a forward direction until the value of $Q_{2,2}$ which gives the highest value of the final value performance index is found. A fourth-order Runge-Kutta method was used to integrate the state equations. The best suboptimal policy, presented in Table 3 along with the corresponding trajectory, was generated using a $Q_{2,2}$ of 2.50 and gave a yield of 0.010718. Comparison of this with the optimal yield, 0.01132, gives a degree of suboptimality of 5.3%.

The second Liapunov approach to final value index problems yields a Hamiltonian similar to (45), except with the integral index of (44) adjoint to it. Minimization yields an optimal pressure policy of

$$P = \frac{x_1k_1[2x_2Q_{2,2}z - x_1Q_{1,1}z - 2](x_2 + B)}{4x_2^2k_2[Q_{2,2}x_2z - 1]} \tag{47}$$

This expression requires that the adjoint equation be solved, so following the procedure used before, the adjoint equation becomes

$$\dot{z}(t) = \frac{-[(\partial H/\partial x_1)\dot{x}_1 + (\partial H/\partial x_2)\dot{x}_2]}{[(\partial V/\partial x_1)\dot{x}_1 + (\partial V/\partial x_2)\dot{x}_2]} \tag{48}$$

Both this equation and the system equations were integrated in the forward direction with a fourth-order Runge-Kutta method. A value for the initial adjoint boundary condition was assumed to start these integrations for each value of $Q_{2,2}$ chosen, and the whole problem was iterated with different initial conditions until the final adjoint boundary condition of zero was satisfied. These iterations were carried out for each different value of $Q_{2,2}$ until the $Q_{2,2}$ which gave the highest value for the performance index was found. The best suboptimal policy calculated using a $Q_{2,2}$ of 0.0225 gave a yield of 0.0113154, which resulted in a degree of suboptimality of 0.04%. Figure 4 presents the optimal pressure profile along with the best suboptimal policy. This suboptimal pressure profile not only produces

TABLE 3. THE SUBOPTIMAL PRESSURE PROFILE AND CORRESPONDING TRAJECTORIES FOR THE NONLINEAR REACTION SYSTEM $A \rightarrow 2B \rightarrow C$

($Q_{2,2} = 2.510$)

t	P, atm.	x_1	x_2
0.00	0.02730	0.01000	0.00200
0.50	0.54807	0.00755	0.00565
1.00	0.35542	0.00644	0.00700
1.50	0.27557	0.00575	0.00778
2.00	0.23009	0.00527	0.00833
2.50	0.19992	0.00489	0.00874
3.00	0.17809	0.00459	0.00907
3.50	0.16139	0.00434	0.00935
4.00	0.14810	0.00412	0.00958
4.50	0.13722	0.00393	0.00978
5.00	0.12810	0.00377	0.00996
5.50	0.12033	0.00362	0.01012
6.00	0.11360	0.00348	0.01026
6.50	0.10772	0.00336	0.01039
7.00	0.10251	0.00325	0.01051
7.50	0.09786	0.00315	0.01062
8.00	0.09368	0.00305	0.01072

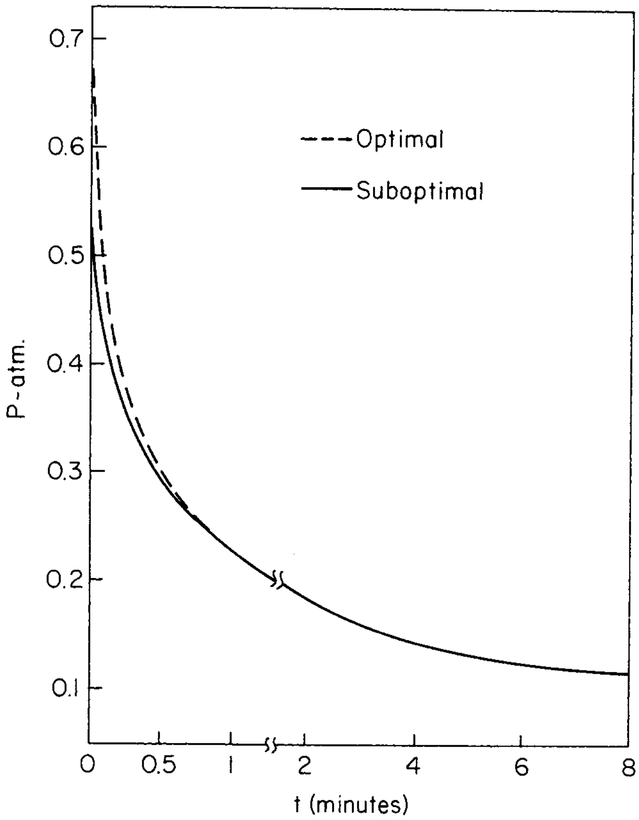

Fig. 4. Comparison of the suboptimal and optimal pressure profiles for the nonlinear reaction system: $A \rightarrow 2B \rightarrow C$. $Q_{2,2} = 0.0225$, $z(0) = -185.854$, and $z(8) = 0.013$.

a final value performance index with a low degree of suboptimality, 0.040%, but it also closely approximates the optimal pressure profile.

The amount of computer time required by the suboptimal method to generate the results presented above is less than that required by optimal methods that have been applied to this nonlinear problem. The procedure Fan (*6*) used to solve the above problem required iteration on two parameters, the initial conditions for the adjoint variables resulting from the maximum principle formulation. The second Liapunov method presented for final value index problems also requires iteration on two quantities, the initial condition for the scalar adjoint variable and the $Q_{2,2}$ element, but these two parameters do not interact like the two adjoint variables in Fan's formulation. More specifically, the iterations required by the Liapunov technique take place on two distinct parameters, for each value of $Q_{2,2}$, $z(0)$ is iterated until $z(t_f)$ is zero. Picking different $Q_{2,2}$ elements defines another iteration sequence, independent of the iteration on $z(0)$, so one-dimensional gradient searches can be used on these parameters separately. Fan's procedure iterates on two interdependent quantities, the maximum principle specified adjoint variables, and thus the iteration of these two quantities must be carried out simultaneously. In this situation a two-dimensional gradient search must be used. The path of iterations which result from the Liapunov technique will be monotonic for each of the parameters, $Q_{2,2}$ and $z(0)$, and as a result, the convergence to the best suboptimal answer is faster than the convergence of Fan's method by a factor of approximately 2. As the number of variables increases, the Liapunov method becomes more advantageous, since at most only two parameters, $Q_{1,1}$ and $z(0)$, have to be iterated.

Lee (*11*) solved the nonlinear problem presented in this section using quasilinearization. The number of iterations required to yield an optimal answer is approximately equal to that required by the suboptimal method, but the convergence of the Liapunov method to the best suboptimal answer is not dependent on the initial values chosen for $Q_{2,2}$ or $z(0)$. This contrasts with Lee's results, since he found that the assumed initial control policy strongly influences convergence.

THE SOLUTION OF DISTRIBUTED-PARAMETER CONTROL PROBLEMS

Although a comprehensive theory can be developed for the Liapunov suboptimal control of distributed-parameter systems (see *16*), some type of discretizing of the equations is ultimately necessary before a digital solution can take place. In view of this, all the distributed systems were replaced by a corresponding set of ordinary differential equations. These ordinary differential equations resulted when the spatial partial derivatives in the distributed systems were approximated by finite differences. The method of generating the suboptimal control and the form of the **Q** weighting matrices that were used in the application of the discrete Liapunov method to these problems were the same as those presented in earlier sections for linear control problems.

Linear Hyperbolic System

The linear hyperbolic system defined by (22) and (23) was used to illustrate the Liapunov method on a control constrained quadratic performance index problem. This distributed system was reduced to 62 ordinary differential equations, with 31 representing the temperature in the outer pipe and 31 representing the temperature of the inner pipe wall of the double-pipe heat exchanger.

A sampling time interval of 0.05 min. was used. The application of the Liapunov technique to the discretized system equation

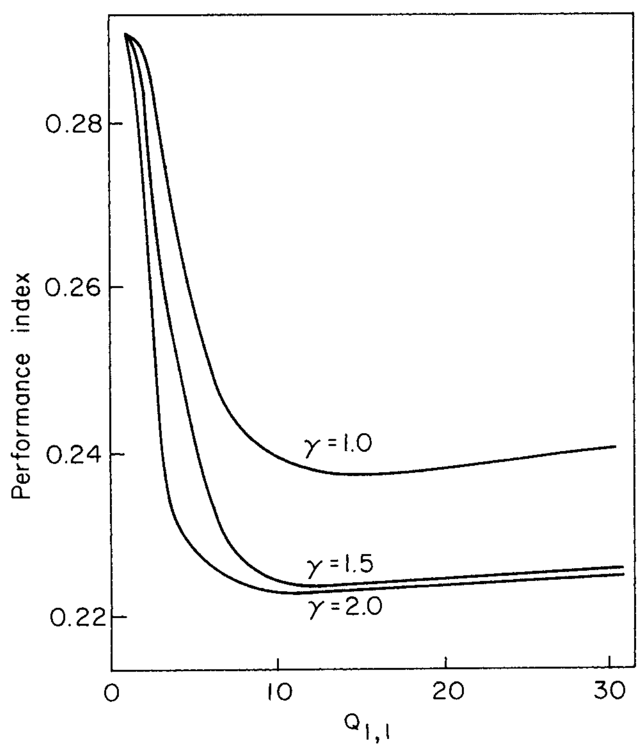

Fig. 5. Performance index versus $Q_{1,1}$, with γ as a parameter for the double-pipe heat exchanger quadratic performance index problem.

$$\mathbf{x}(k+1) = \boldsymbol{\varphi}\mathbf{x}(k) + \boldsymbol{\Delta}\mathbf{u}(k)$$

and the performance index

$$I = \sum_{0}^{N} [x(62, k)]^2 \tag{49}$$

yielded an optimal control policy of

$$\mathbf{u}^0(k) = -(\boldsymbol{\Delta}^T\mathbf{Q}\boldsymbol{\Delta})^{-1}\boldsymbol{\Delta}^T\mathbf{Q}\boldsymbol{\varphi}\mathbf{x}(k) \tag{50}$$

For ease in calculation the weighting matrix $\mathbf{Q}$ in the Liapunov function was chosen with the constant diagonal elements $Q_{1,1}$ with the lower corner element raised to a power γ. The best suboptimal minimum performance index was found by iterating on $Q_{1,1}$ and γ, while solving this control constrained problem in the manner described earlier for control constrained systems until the lowest value for the performance index was found. A plot of $Q_{1,1}$ versus the index with γ as a parameter is shown in Figure 5. The best suboptimal control policy, generated by a $Q_{1,1}$ of 10.0 and a γ of 2.0, is shown in Figure 6 along with the best optimal policy generated by Seinfeld (*17*). The suboptimal policy yielded a performance index of 0.022330, while Seinfeld's control policy yielded an index of 0.0022464. It should be noted that the performance index generated by the Liapunov technique is actually lower than Seinfeld's result. The reason for this will be presented shortly.

At this point a discussion of the results obtained for the distributed linear parabolic system is appropriate. The Liapunov suboptimal solution of the control problems which involved this type of distributed system points up two advantages of the Liapunov method. First, the Liapunov suboptimal solution of the control problems is capable of handling large dimensioned dynamic systems. Most proposed noniterative or iterative optimal methods are basically incapable of handling optimization problems with 60 variables, using existing computer facilities, because large amounts of information have to be stored during the solution of the optimization problem. The Liapunov method requires the storage of only scalar quantities, such as the performance index, the scalar adjoint variable, and the $Q_{1,1}$ element, so these large dimensioned problems can be handled by the existing computer facilities. Second, in addition to the capability of the Liapunov method to handle large dimensional optimization problems, the generalized procedure used to find the best $\mathbf{Q}$ weighting matrix for these problems gave answers with a low degree of suboptimality.

The reduced amount of computer time necessary to generate the suboptimal results obtained for the problems just presented can be appreciated when comparison is made with Seinfeld's (*17*) solutions to distributed parameter control problems. His direct search method involved the same type of repetitive system integrations required in the Liapunov technique, so a comparison of the iterations required for solution is appropriate. Taking the solution of the double-pipe heat exchanger quadratic index problem as typical, Seinfeld required around 400 iterations to generate his best optimal solution with the direct search technique. The Liapunov method required only 30 iterations to generate the best suboptimal solution (a relative computing time decrease of about 13 to 1), which, as mentioned before, yielded a performance index that was actually lower than the index resulting from Seinfeld's solution. The explanation for this occurrence is that the direct search technique requires that the control variable be limited to a finite number of discrete values. The analytical control law given in Equation (50), which results from the Liapunov approach, can specify any control value within the constraints placed on the problem. This "infinitely fine grid" capability of the Liapunov approach allowed a lower performance index.

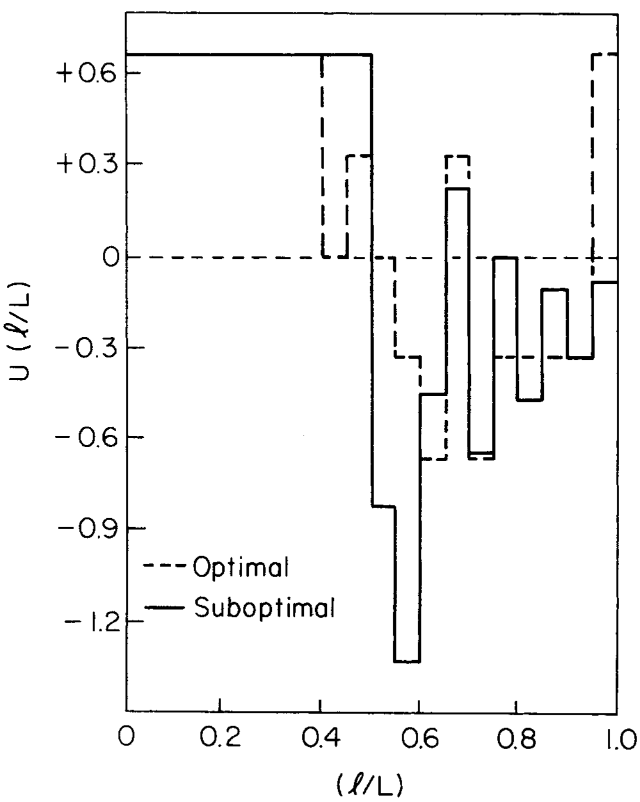

Fig. 6. The best suboptimal and Seinfeld's optimal control policies for the double-pipe heat exchanger. $Q_{1,1} = 10.0$, $\gamma = 2.0$.

Nonlinear Parabolic System

The nonlinear tubular reactor with radial diffusion, presented in (24) to (26), was used to illustrate the solution of a final value index control problem by the Liapunov suboptimal technique. This distributed system was reduced to a nonlinear system of 22 ordinary differential equations which can be written in matrix form as

$$\dot{\mathbf{x}}(t) = \mathbf{A}(\mathbf{x})\mathbf{x} + \mathbf{B}\mathbf{u} + \mathbf{F}(\mathbf{x}) \tag{51}$$

Equation (51) was integrated and discretized, using a sampling time interval of 0.05 min., to yield

$$\mathbf{x}(k+1) = \boldsymbol{\varphi}[\mathbf{x}(k)]\mathbf{x}(k) + \boldsymbol{\Delta}[\mathbf{x}(k)]\mathbf{u}(k) + \boldsymbol{\lambda}[\mathbf{x}(k)] \tag{52}$$

where $\boldsymbol{\varphi}[\mathbf{x}(k)]$, $\boldsymbol{\Delta}[\mathbf{x}(k)]$, and $\boldsymbol{\lambda}[\mathbf{x}(k)]$ were recalculated at each time step. The application of the first Liapunov method described for final valued index problems yields a Hamiltonian of

$$H(k+1) = z(k+1)[\mathbf{x}(k+1)\mathbf{Q}\mathbf{x}(k+1)] \tag{53}$$

Since this problem is control constrained, the Hamiltonian was maximized numerically by finding the value of the discretized control variable that yields the largest value for $H(k+1)$ at each time step. The best suboptimal performance index was found by varying the $Q_{1,1}$ element, which yields the $\mathbf{Q}$ matrix, and integrating the problem until the highest value for the final valued performance was found. The best suboptimal performance index, generated by a $Q_{1,1}$ element of 1.545×10^{-6}, gave a final valued performance index of 0.44682. This is better than Seinfeld's index of 0.44583 for the same reason presented

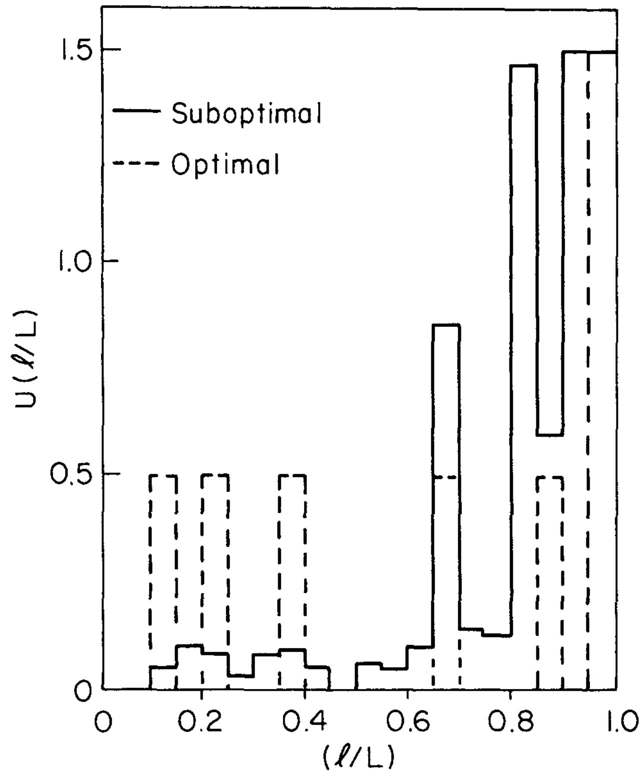

Fig. 7. The best suboptimal and Seinfeld's optimal control policies for the tubular reactor with radial diffusion. $Q_{1,1} = 1.454 \times 10^{-6}$.

for the heat exchanger problem. While the numerical maximization of the Hamiltonian used in the Liapunov method applied to this problem used a discretized control value, the discretization interval of 0.01 used in this approach was smaller than the 0.5 interval used by Seinfeld. Hence, the finer grid used in the Liapunov approach gave a better performance index. Figure 7 presents the best suboptimal and Seinfeld's optimal control policy. The Liapunov method required approximately 20 iterations of the problem to find the best suboptimal result, while the direct search method used by Seinfeld required about 280 iterations of the problem. This corresponded to a relative computation time decrease of about 14 to 1.

SUMMARY AND CONCLUSIONS

A technique which calculates approximate solutions to optimal control problems has been developed in this work. The technique, which uses an empirically found weighted quadratic Liapunov function to transform the original n-dimensional optimization problem into a scalar optimization problem, was successfully applied to a large number of optimal control problems typical of those encountered in chemical engineering practice. The problems considered included both linear and nonlinear, lumped and distributed systems with minimum time, quadratic and final value type performance indices. In addition, the investigation of constrained, singular, and recycle control problems has been reported by Schlossmacher (*16*). The solutions of these optimal control problems show that the Liapunov suboptimal technique has the following advantages:

1. The solution to the discrete minimum time problem is closed loop, as opposed to the classical solution, which is open loop. Dependence on the exact system equations is therefore reduced.
2. Control and state constraints are easily handled because of the forward nature of the integrations required by the method.
3. The reduction of computer storage necessary for solution, over that required by other optimization methods presented in the literature, permits the handling of large dimensional problems.
4. Distributed system control problems which have been lumped into a set of ordinary differential equations are easily handled by the method. The number of ordinary differential equations of the lumped system may be very large (for example, 40 or 60), since the method will at most require only one scalar adjoint equation be solved. The difficulties associated with the boundary-value problem of size $2n$ which results from the maximum principle are avoided in the Liapunov procedure even for large values of n.
5. Nonlinear systems may be handled without linearization.

The application of the Liapunov suboptimal method to two particular systems, a problem that would ordinarily encounter regions of singularity, and a recycle problem, shows two additional advantages:

6. The regions of singular control that would ordinarily be encountered by the original unreduced system are avoided, because the suboptimal control law obtained for this type of system is not a function of the adjoint variable, and thus no singularities are encountered in the generation of the suboptimal control policy.
7. Recycle problems require fewer iterations when handled by the method than that required by other proposed iterative techniques.

Above all, the Liapunov suboptimal technique as presented in this work is capable of approximating with a low degree of suboptimality the solutions of optimal control problems, generally with a smaller amount of computer storage and time than that required by the optimal techniques currently being used to solve such problems.

NOTATION

$\mathbf{F}(\mathbf{x})$ = arbitrary vector function of $\mathbf{x}$
$\mathbf{f}(\mathbf{x}, \mathbf{u})$ = arbitrary vector function of $\mathbf{x}$ and $\mathbf{u}$
$g(\mathbf{x}, \mathbf{u})$ = arbitrary scalar function of $\mathbf{x}$ and $\mathbf{u}$
$\mathbf{h}\{\mathbf{x}(k), \mathbf{u}(k)\}$ = arbitrary discretized vector function of $\mathbf{x}(k)$ and $\mathbf{u}(k)$
H = Hamiltonian function
I = performance index
$\mathbf{J}$ = Riccati transformation matrix of dimension $n \times n$
$\mathbf{K}$ = feedback matrix of dimension $n \times n$
k = time step or stage number
N = total number of time steps
n = dimension of state vector
o = optimal value of some quantity
$\mathbf{P}$ = weighting matrix of dimension $n \times n$ used in quadratic performance index
$\mathbf{Q}$ = quadratic Liapunov function weighting matrix of dimension $n \times n$
$\mathbf{R}$ = weighting matrix of dimension $r \times r$ used in quadratic performance index
r = dimension of control vector
ss = steady state of some quantity
$S\{\mathbf{x}(k), \mathbf{u}(k)\}$ = arbitrary discretized scalar function of $\mathbf{x}(k)$ and $\mathbf{u}(k)$
T = transposition of a matrix (superscript)
t = time
$\mathbf{u}$ = control vector of dimension r
V = scalar Liapunov function
$\mathbf{x}$ = state vector of dimension n
$\mathbf{x}(0)$ = initial value of the state vector
$\dot{\mathbf{x}}(t)$ = time derivative of the state vector
$z(t)$ = scalar adjoint variable

Greek Letters

φ = transition matrix of dimension $n \times n$

Δ = forcing function weighting matrix of dimension $n \times r$

λ = discretized vector function

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A Corresponding States Correlation of Saturated Liquid Volumes

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A corresponding states correlation is presented for the prediction of saturated liquid volumes. Parameters required are the critical temperature, the acentric factor, and a scaling volume. The correlation is valid over the entire useful range of reduced temperatures from 0.2 to 1.0. The full temperature range has not been covered by previous corresponding states correlations. Average absolute deviations in predicted liquid volumes is one-quarter of 1% for 26 compounds. The correlation is also useful for calculating critical temperatures, pressures, and volumes when experimental critical data are lacking. The proposed method also provides a convenient means for calculating rapidly and accurately the statistical mechanical parameters used in the cell model correlation developed by Renon, Eckert, and Prausnitz.

Liquid densities or liquid molar volumes are often needed for a wide variety of engineering calculations, such as the design of storage facilities, flow metering, high pressure vapor-liquid equilibrium studies, and fluid flow analyses. Not infrequently densities and other properties are required at temperatures for which no experimental data exist. In such cases the three-parameter corresponding states formulation of Pitzer et al. (*4, 15*) is widely used for predicting the thermodynamic properties of dense gases and liquids. However, Pitzer's correlation for saturated liquid compressibility factors, and similar correlations by Lyckman, Eckert, and Prausnitz (*12*) and by Halm and Stiel (*6*), are valid only over a range of reduced temperatures of 0.56 to 1.00.

THE CORRELATION

A new correlation is presented here which is valid over essentially the entire useful range of 0.20 to 1.00 in the reduced temperature. This correlation has the following form linear in the acentric factor

$$V/V_{SC} = V_R^{(0)}(1.0 - \omega\ \delta) \qquad (1)$$

The generalized functions $V_R^{(0)}$ and δ, which are dependent only upon the reduced temperature, are tabulated in Table 1. These values were calculated from density data for the following 10 substances: argon, methane, nitrogen, propane, *n*-pentane, *n*-heptane, *n*-octane, benzene, ethyl ether and ethylbenzene.

To establish the correlation at the lowest temperatures, the functions $V_R^{(0)}$ and δ are extrapolated from a T_R of 0.225 to a T_R of 0.20. Density data for slightly subcooled propane liquid determine $V_R^{(0)}$ at a reduced temperature of 0.225, and the product $\delta\ V_R^{(0)}$ is virtually constant below a reduced temperature of 0.5.

The scaling volume V_{SC} is used in Equation (1) rather than the critical volume. It is widely recognized that the experimental determination of critical volumes is very difficult and subject to rather large errors. For this reason

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