y_n = extract concentration leaving n^{th} stage
ρ = density

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The Control of Nonlinear Systems.

Part II: Convergence by Combined First and Second Variations

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It is shown that the first variation method can be used to provide an excellent starting condition for the second variation control of nonlinear systems. Numerical examples illustrate the basic features of the methods.

In Part I (*10*) we presented a simple and straightforward algorithm for determining the optimal control trajectory of nonlinear systems subject to control and state constraints. The basic concept involved a direct search on the control function. In the present paper we outline a more rational method for choosing the variations in the control function. The performance index is expanded to first- or second-order terms in the control vector; the direction in which the control vector is driven and its magnitude are then chosen so as to extremize the change in performance index at each step.

A method suitable for determining the optimal control trajectory which currently is in much favor is the *gradient* or *first variation* procedure (*9*). The logic in this method is easy to follow and programming on a digital computer is straightforward. A certain step is always taken in the *direction* of the most rapid change of the function to be extremized, and if the optimum region is overstepped, the step size is halved and the procedure is continued until some criterion is satisfied. However, the simplicity of the formulation is offset by two serious disadvantages. First, it is found in practice that a very large number of such steps or iterations must be taken before convergence occurs. Second, and more important, the trajectory *approaches* the optimum, but *does not actually reach it.* In some cases, after as many as 50 to 150 iterations, the trajectory is still far from the optimum and the rate of convergence becomes too slow to warrant further iterations.

To overcome these drawbacks of the first variation method Bryson et al. (*4, 12*), Kelley et al. (*7*), Merriam (*13, 14*) Kopp and McGill (*8*), and Jaswinski (*6*) have developed an iteration scheme which incorporates into the formulation not only the gradient of the function, but also the *curvature* or magnitude of the function. This formulation is called the *second variation method,* since second-order terms are used in the development. Convergence to the optimal trajectory now occurs in a quadratic fashion.

There are certain disadvantages of the second variation method which remove some of the theoretical attractiveness it may have. First, and most important, the initially assumed trajectory must be sufficiently close to the optimal trajectory for convergence to be obtained. Second, the number of equations to be integrated is considerably greater than required for the first variation method. Third, the equations themselves are more complicated. Hence, the programming of the iteration scheme with the required equations can be quite complicated. Finally, instability can arise from bad starting values, that is, from an insufficiently good guess for the initial trajectory.

In this paper we wish to show how the uncertainty of the choice of the initial trajectory can be removed by using the first variation method for the first few iterations and then changing over to the second variation method. This combination provides rapid convergence to the optimum from almost any realistic starting trajectory.

To illustrate the advantages of using the combined first and second variation methods, the control of a continuous stirred-tank reactor (CSTR) will be analyzed. In particular, we shall consider the control of the CSTR at a naturally unstable steady state. This choice will make the selection of the initial control policy very crucial if the second variation method is used alone. With the combined method, however, the choice of the initial control policy can be relaxed considerably.

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We should briefly mention that in the present method the inclusion of the control or state constraints is most difficult. Usually this is accomplished by means of penalty functions but we do not desire to amplify this point here.

PROBLEM DEFINITION

We shall consider the control of the CSTR as originally formulated by Aris and Amundson (*1*). A first-order, irreversible exothermic reaction is carried out in the reactor and the control is to be achieved by the manipulation of the flow of cooling fluid through a cooling coil inserted in the reactor.

The state equations for the CSTR are given by

$$\dot{T} = -(T + 0.25) + (C + 0.5) \exp\left(\frac{25T}{T+2}\right) - u_1(T + 0.25) \quad (1)$$

$$\dot{C} = 0.5 - C - (C + 0.5) \exp\left(\frac{25T}{T+2}\right) \quad (2)$$

where u_1, the control action (based on the temperature deviation), has a minimum value of 0 when the coolant valve is completely closed. Although Aris and Amundson have specified that u_1 has a maximum value of 2.0 when the valve is completely open, here we shall assume that u_1 is not bounded from above; as will be seen, a suitable weighting of the performance index will accomplish the same purpose.

The performance index of interest in the present problem is taken as

$$I[\mathbf{x}(0), t_f] = \int_o^{0.78} \{(T^2 + C^2) + r(u_1 - 1)^2\}\, dt \quad (3)$$

where the vector $\mathbf{x}(t)' = [T(t)\ C(t)]$ has been introduced. r is a weighting parameter on the control term in the performance index and the final time of control t_f is chosen as $t_f = 0.78$. For initial conditions on the control trajectory we choose

$$\mathbf{x}(0)' = [0.05 \quad 0] \quad (4)$$

and note that

$$\mathbf{x}(t)' = [0 \quad 0],\ u_1 = 1.0 \quad (5)$$

defines an unstable steady state at which we wish to keep the system. If we now define a normalized control action

$$u = u_1 - 1 \quad (6)$$

we may write Equations (1) and (2) in the general form

$$\dot{\mathbf{x}}(t) = \mathbf{f}[\mathbf{x}(t),\ \mathbf{u}(t)] \quad (7)$$

and the integrand of the performance index as

$$J[\mathbf{x}(t),\ \mathbf{u}(t)] = T^2 + C^2 + ru^2 \quad (8)$$

THE SECOND VARIATION METHOD

The derivation of the second variation algorithm may be specified in a number of different ways. We shall here follow the work of Merriam (*13, 14*) since we have found this specific version to be relatively easy to use on a digital computer. Only the main equations will be detailed since the explicit and lengthy derivations can be found in reference 9.

From a conceptual point of view, however, we shall discuss a generalized variational approach to the second variation equations. Thus one starts with the normal nonlinear problem with no constraints and expands the performance index to second-order terms (see below); if the canonical equations of the maximum principle are then envoked the result is the minimum accessory optimal control problem (*2, 3, 5, 9, 11, 15*). This new accessory problem consists of a linearized system equation and a quadratic performance index, the solution to which is well known in the literature. Thus the original nonlinear problem is converted over to a problem whose characteristics are well known. The material below is actually a specific version of this generalized approach.

The performance index which we wish to minimize is of the form

$$I[\mathbf{x}(0), t_f] = \int_o^{t_f} J[\mathbf{x}(t),\ \mathbf{u}(t)]\, dt \quad (9)$$

where, for the CSTR, we have chosen t_f to be 0.78 and have defined J by Equation (8). The minimization is to be carried out subject to the system constraints as expressed by the state Equation (7) or explicitly as Equations (1) and (2).

We can incorporate these constraints directly in the performance index by considering the augmented performance index

$$I^* = \int_o^{t_f} \{J(\mathbf{x}, \mathbf{u}) + \mathbf{z}'(\mathbf{f} - \dot{\mathbf{x}})\}\, dt \quad (10)$$

where we are penalizing ourselves if Equation (7) does not hold. Here $\mathbf{z}$ is a vector of n Lagrange multipliers or adjoint variables.

If we add a superscript $(j + 1)$ to all items in Equation (10) the problem is to construct an iteration algorithm such that

$$I^{*(0)} > I^{*(1)} > \ldots . I^{*(j)} > I^{*(j+1)} > \ldots . \quad (11)$$

where the superscript refers to the stage of iteration.

We start by expressing the values of functions at stage $(j + 1)$ in terms of the j^{th} iteration by Taylor's series expansions through second-order terms. To simplify the notation we use J_x† $= (\partial J/\partial \mathbf{x})$, $J_{xx} = (\partial^2 J/\partial \mathbf{x}^2)$, etc., and use a linear operator δ on the iteration numbers, that is, $\delta J = J^{(j+1)} - J^{(j)}$, $\delta \mathbf{x} = \mathbf{x}^{(j+1)} - \mathbf{x}^{(j)}$, etc. Thus, it follows directly that

$$\delta J = J_x'\ \delta \mathbf{x} + J_u'\ \delta \mathbf{u} + \frac{1}{2}\delta \mathbf{x}'\ J_{xx}\ \delta \mathbf{x} + \delta \mathbf{u}'\ J_{ux}\ \delta \mathbf{x} + \frac{1}{2}\delta \mathbf{u}'\ J_{uu}\ \delta \mathbf{u} \quad (12)$$

where all items on the right hand are evaluated at j^{th} iteration and the prime indicates the transpose of the vector or matrix. In the same manner, if we define

$$\overline{H} = \mathbf{z}'\mathbf{f} \quad (13)$$

and note that $\overline{H} = \overline{H}(\mathbf{z}, \mathbf{x}, \mathbf{u})$ then

$$\delta \overline{H} = \overline{H}_x'\ \delta \mathbf{x} + \overline{H}_u'\ \delta \mathbf{u} + \overline{H}_z'\ \delta \mathbf{z} + \frac{1}{2}\delta \mathbf{x}'\ \overline{H}_{xx}\ \delta \mathbf{x} + \delta \mathbf{u}'\ \overline{H}_{ux}\ \delta \mathbf{x} + \frac{1}{2}\delta \mathbf{u}'\ \overline{H}_{uu}\ \delta \mathbf{u} + \delta \mathbf{u}'\ \overline{H}_{uz}\ \delta \mathbf{z} + \delta \mathbf{x}'\ \overline{H}_{xz}\ \delta \mathbf{z} \quad (14)$$

The system Equation (7) may be linearized by expansions to terms of first order to yield

$$\delta \dot{\mathbf{x}} = \mathbf{f}_x\ \delta \mathbf{x} + \mathbf{f}_u\ \delta \mathbf{u} \quad (15)$$

with $\delta \mathbf{x}(0) = \mathbf{0}$, since our initial conditions are constant. Finally, we envoke the relationship

$$\delta \mathbf{z} = \mathbf{P}\ \delta \mathbf{x} \quad (16)$$

† Note: The italic subscripts x and u have the same definitions (see Notation) as their bold face counterparts.

where $\mathbf{P} = \mathbf{z}_x =$ a symmetric matrix. At this point $\mathbf{P}$ is unknown but Equation (16) allows us to remove δz in all our equations in terms of δx.

With these expansions, Equations (12) and (16) are substituted into Equation (10) with the $(j + 1)$ superscript. The result is

$$\delta I^* = \int_o^{t_f} \left\{ H_x' \ \delta x + H_u' \ \delta u + \frac{1}{2} \delta x' \ H_{xx} \ \delta x + \delta u' \ H_{ux} \ \delta x + \frac{1}{2} \delta u' \ H_{uu} \ \delta u + \delta u' \ f_u' \ P \ \delta x + \delta x' \ f_x' \ P \ \delta x - z' \ \delta \dot{x} - \delta x' \ P' \ \delta \dot{x} \right\} dt \quad (17)$$

where H is the normal Hamiltonian for this problem, namely

$$H = J + z'f \quad (18)$$

So far we have not used the canonical equations which are necessary for an optimal trajectory. To bring these to bear we prefer to go through the Hamilton-Jacobi formulation. Thus, if we define

$$I^o = \min_{\mathbf{u}} I$$

$$H^o = \min_{\mathbf{u}} H$$

the Hamilton-Jacobi partial differential equation has the form

$$I_t^o + H^o = 0 \quad (19)$$

It is fairly easy to show that under mild conditions the characteristic equations of Equation (19) are the canonical equations of the maximum principle; this is simply illustrated by the equivalence

$$z = I_x^o$$

But if we now envoke $H_u = 0$ then it follows that

$$J_u + f_u' \ z = 0 \quad (20)$$

Further the total time derivative of z is given by

$$\dot{z} = z_t + z_x \ \dot{x} \quad (21)$$

Differentiating Equation (19) with respect to x and using (20) and (21), we obtain

$$\dot{z} = -J_x - f_x' \ z \quad (22)$$

If we follow the same steps for P, noting that $P = z_x$, there also results

$$\dot{P} = -H_{xx} - \{P \ f_x + f_x' \ P\} + K \ R \quad (23)$$

where

$$K = R' \ H_{uu}^{-1} \quad (24)$$

$$R = H_{ux} + f_u' \ P \quad (25)$$

Equation (23) is the well-known Riccati equation.

When all of these new items are substituted into Equation (17) we obtain

$$\delta I^* = \int_o^{t_f} \left\{ \frac{1}{2} \delta u' \ T \ \delta u + \frac{1}{2} \delta x' \ K \ R \ \delta x + \delta u' \ R \ \delta x + s' \ \delta u \right\} dt \quad (26)$$

where

$$T = H_{uu} \quad (27)$$

$$s = H_u \quad (28)$$

Thus at this point we have converted the nonlinear system equation to the linear form, Equation (15), and converted the performance index to the modified quadratic form of Equation (26). This new problem must now be solved to solve the originally stated problem. Obviously, the right-hand side of Equation (26) needs to be negative in order for the iterations to converge, that is

$$\delta I^* = I^{*(j+1)} - I^{*(j)} < 0$$

In addition, we would like the convergence to be as fast as possible, so we consider the minimization of the integral of Equation (26) in the form

$$V(\delta x, t) = \int_t^{t_f} \{ \qquad \} d\lambda \quad (29)$$

through the proper choice of δu. We denote this minimum as $V^o(\delta x, t)$. Since $V(\delta x, t)$ as given in Equation (29) is quadratic in δx, we may write the minimum of $V(\delta x, t)$ as a quadratic expression:

$$V^o(\delta x, t) = q(t) + q'(t) \ \delta x + \delta x' Q(t) \ \delta x \quad (30)$$

where

$q(t)$ = scalar ; $q(t_f) = 0$
$\mathbf{q}(t)$ = vector ; $\mathbf{q}(t_f) = 0$
$\mathbf{Q}(t)$ = symmetric matrix ; $\mathbf{Q}(t_f) = 0$

From Equation (30)

$$V_t^o = \dot{q}(t) + \dot{q}(t)' \ \delta x + \delta x' \ \dot{Q}(t) \ \delta x \quad (31)$$

$$V_{\delta x}^o = q(t) + 2 \ Q(t) \ \delta x \quad (32)$$

Now minimization of $V(\delta x, t)$ as given by Equation (29) yields

$$\frac{1}{2} \delta u^{o\prime} T \delta u^o + \frac{1}{2} \delta x' K R \delta x + \delta u^{o\prime} R \delta x + s' \delta u^o + (q'(t) + 2\delta x' Q(t)) \delta \dot{x} + \dot{q}(t) + \dot{q}(t)' \delta x + \delta x' \dot{Q}(t) \delta x = 0 \quad (33)$$

where

$$\delta u^o = -T^{-1} [s + R\delta x + f_u'(q(t) + 2Q(t)\delta x)] \quad (34)$$

and

$$\delta \dot{x} = f_x \ \delta x + f_u \ \delta u \quad (35)$$

When the optimal control as given by Equation (34) is substituted into Equation (33) and the coefficients of δx and $\delta x' \delta x$ along with terms not containing δx are set to zero (to satisfy the identity for any δx), there results

$$\dot{q} = \frac{1}{2} \{s'T^{-1}s + s'T^{-1}f_u'q + q'f_u'T^{-1}s + q'f_uT^{-1}f_u'q\} \quad (36)$$

$$\dot{q} = R'T^{-1}s + R'T^{-1}f_uq - f_xq + 2Q[f_uT^{-1}s + f_uT^{-1}f_u'q] \quad (37)$$

$$\dot{Q} = 2\{Qf_uT^{-1}R + Qf_uT^{-1}f_u'Q - Qf_x\} \quad (38)$$

At this point it is noted that the matrix Q contributes only insignificantly to the control and appears as a second-order term. Therefore, to facilitate programming on the digital computer we shall discard these $\frac{n(n+1)}{2}$ equations and put Q to zero. Thus Equation (37) takes the form

$$\dot{q} = R'T^{-1}s + R'T^{-1}f_uq - f_xq \quad (39)$$

and Equation (34) becomes

$$\delta u^o = -T^{-1} (s + R \ \delta x + f_u' \ q) \quad (40)$$

Only one final change need be made to finish this development. To prevent overstepping of the control and to maintain the system linearization we introduce a constant ϵ where $0 < \epsilon < 1$ such that

$$\delta u^0 = -\epsilon\ \mathbf{T}^{-1}(\mathbf{s} + \mathbf{f}_u'\mathbf{q}) - \mathbf{T}^{-1}\mathbf{R}\ \delta\mathbf{x} \qquad (41)$$

Now we may summarize the details of the second variation algorithm. It may take the following steps:

1. An initial guess is made for $\mathbf{u}(t)$.
2. Equations (7) and (9) are integrated forward from $t = 0$ to $t = t_f$ using the initial $\mathbf{u}(t)$. This involves the integration of $(n + 1)$ equations, namely

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

$$\dot{I} = J(\mathbf{x}, \mathbf{u})$$

3. While these integrations are carried out, the values of $\mathbf{x}(t)$ are retained in computer memory.
4. The adjoint Equation (22) plus the additional equations (23) and (39) are integrated backward, that is, $2n + \dfrac{n(n+1)}{2}$ equations are integrated backward in time from $t = t_f$ to $t = 0$.
5. During the backward integration the values of **T**, **s**, **q**, and **R** are stored in the computer memory.
6. The new value of control is calculated from Equation (41), that is

$$\mathbf{u}^{(j+1)} = \mathbf{u}^{(j)} - [\epsilon\mathbf{T}^{-1}(\mathbf{s} + \mathbf{f}_u\mathbf{q}]^{(j)} - (\mathbf{T}^{-1}\mathbf{R})^{(j)}(\mathbf{x}^{(j+1)} - \mathbf{x}^{(j)})$$

7. Steps 2 to 6 are repeated until no further changes in $\mathbf{u}^{(j+1)}$ occur. Note that $\mathbf{x}^{(j+1)}$ is evaluated at the same time as $\mathbf{u}^{(j+1)}$.

As a side note, if the performance index increases during an iteration step, the parameter ϵ is halved and the procedure continued. In addition, the matrices **P** and **T** must be positive-definite in order to assure convergence to at least a local minimum.

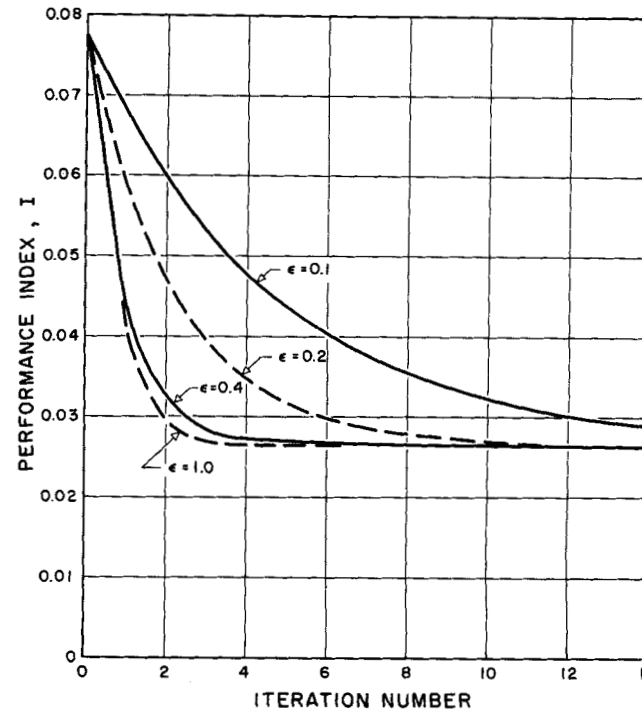

Fig. 1. Effect of size of ϵ on rate of convergence with the second variation.

EXPLICIT CALCULATIONS

Now that we have outlined the second variation equations we shall turn to its specific application to the CSTR problem. First we must evaluate some partial derivatives. From Equation (8) it follows that

$$J_x = \begin{bmatrix} \dfrac{\partial J}{\partial T} \\ \dfrac{\partial J}{\partial C} \end{bmatrix} = \begin{bmatrix} 2T \\ 2C \end{bmatrix} \qquad (42)$$

From Equations (1) and (2)

$$\mathbf{f}_x' = \begin{bmatrix} -2 + (C + 0.5)\dfrac{50}{(T+2)^2}\exp\left(\dfrac{25T}{T+2}\right) - u, & -(C + 0.5)\dfrac{50}{(T+2)^2}\exp\left(\dfrac{25T}{T+2}\right) \\ \exp\left(\dfrac{25T}{T+2}\right), & -1 - \exp\left(\dfrac{25T}{T+2}\right) \end{bmatrix} \qquad (43)$$

Therefore, the adjoint equation may be written as

$$\dot{\mathbf{z}} = \begin{bmatrix} \dot{z}_1 \\ z_2 \end{bmatrix} =$$

$$-\begin{bmatrix} 2T \\ 2C \end{bmatrix} - \begin{bmatrix} -2 + (C + 0.5)\dfrac{50}{(T+2)^2}\exp\left(\dfrac{25T}{T+2}\right) - u, & -(C + 0.5)\dfrac{50}{(T+2)^2}\exp\left(\dfrac{25T}{T+2}\right) \\ \exp\left(\dfrac{25T}{T+2}\right), & -1 - \exp\left(\dfrac{25T}{T+2}\right) \end{bmatrix} \begin{bmatrix} z_1 \\ \dot{z}_2 \end{bmatrix} \qquad (44)$$

Further manipulations of interest are

$$J_{xx} = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} \qquad (45)$$

$$\frac{\partial^2 f_1}{\partial \mathbf{x}^2} = \begin{bmatrix} \dfrac{\partial^2 f_1}{\partial T^2} & \dfrac{\partial^2 f_1}{\partial T \partial C} \\ \dfrac{\partial^2 f_1}{\partial C \partial T} & \dfrac{\partial^2 f_1}{\partial C^2} \end{bmatrix} = -\frac{\partial^2 f_2}{\partial \mathbf{x}^2}$$

$$= \begin{bmatrix} (C + 0.5)\left(\dfrac{2500}{(T+2)^4} - \dfrac{100}{(T+2)^3}\right)\exp\left(\dfrac{25T}{T+2}\right), & \dfrac{50}{(T+2)^2}\exp\left(\dfrac{25T}{T+2}\right) \\ \dfrac{50}{(T+2)^2}\exp\left(\dfrac{25T}{T+2}\right), & 0 \end{bmatrix} \qquad (46)$$

Equation (25) thus becomes

$$\mathbf{R} = [-(T + 0.25)\, P_{11} - z_1,\ -(T + 0.25)\, P_{12}] \quad (47)$$

and Equation (27) gives

$$\mathbf{T} = 2r, \text{ a scalar} \quad (48)$$

From this information we can evaluate the differential equation [Equation (23)]

$$\dot{\mathbf{P}} = \begin{bmatrix} \dot{P}_{11} & \dot{P}_{12} \\ \dot{P}_{21} & \dot{P}_{22} \end{bmatrix} = -\begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix} + (z_2 - z_1)\frac{\partial^2 f_1}{\partial \mathbf{x}^2} - \{\mathbf{P}\ \mathbf{f}_x + \mathbf{f}_x'\ \mathbf{P}\} + \frac{1}{2r}\mathbf{R}'\ \mathbf{R} \quad (49)$$

Also, in this example, s as defined by Equation (28) is

$$\mathbf{s} = 2ru - z_1(T + 0.25) = s = \text{scalar} \quad (50)$$

and with the above, we can evaluate Equation (39)

$$\dot{\mathbf{q}} = \begin{bmatrix} \dot{q}_1 \\ \dot{q}_2 \end{bmatrix} = \frac{s}{2r}\begin{bmatrix} R_{11} \\ R_{12} \end{bmatrix} + \frac{1}{2r}\begin{bmatrix} R_{11} \\ R_{12} \end{bmatrix} [-(T + 0.25), 0] \begin{bmatrix} q_1 \\ q_2 \end{bmatrix} - \mathbf{f}_x \begin{bmatrix} q_1 \\ q_2 \end{bmatrix} \quad (51)$$

The final conditions are $t_f = 0.78$, $\mathbf{z}(0.78) = \mathbf{0}$, $\mathbf{P}(0.78) = \mathbf{0}$, and $\mathbf{q}(0.78) = \mathbf{0}$.

Now we are in a position to perform a calculation on the CSTR. Equations (44), (50), and (51) are to be integrated backward from $t_f = 0.78$ with known values of T, C, and u. The values of T and C are obtained by a forward integration (from $t = 0$) of Equations (1) and (2), and u is obtained by the iteration formula

$$u^{(j+1)} = u^{(j)} - \left[\frac{\epsilon}{2r}\ (s + \mathbf{f}_u'\mathbf{q})\right]^{(j)} - \frac{\mathbf{R}}{2r}[\mathbf{x}^{(j+1)} - \mathbf{x}^{(j)}] \quad (52)$$

All that is needed is an initial guess for the control $\mathbf{u}^{(0)}$ to start the iterations. This initial guess should be as good as possible, that is, close enough to the optimal values; otherwise the iterations may not converge and instability might be encountered.

As an illustration of a careful selection of an initial policy, we shall choose the bang-bang control as obtained for time optimal control of the CSTR when u_1 is bounded above by 2.0 (9). This is not the correct optimal control policy to the current problem but it is close enough to ensure convergence of the iterations. We thus choose $u = 1.0$ for the time interval (0, 0.47), $u = -1.0$ for the time interval (0.47, 0.76), and $u = 0.0$ for the time interval (0.76, 0.78). In addition, we select $r = 0.1$.

An interesting parameter in the computation is the step size factor ϵ, which determines the magnitude of the step taken in each iteration stage j. Thus we have selected a series of values of ϵ and carried out an equivalent set of computations for each value of ϵ. With $\epsilon = 1.0$ the second variation iterations converged from a starting value of the performance index of $I^{(0)} = 0.0782$ to the minimum value of $I^o = 0.0266$ in only four iterations; with $\epsilon = 0.5$, five iterations were required and with $\epsilon = 0.25$ twelve iterations were required. The step size for integration of the various differential equations was taken as 0.0025 for all these cases. It is apparent that in the present case there is no overstepping of the control during the iterations and thus the full allowable control correction ($\epsilon = 1.0$) is best to use.

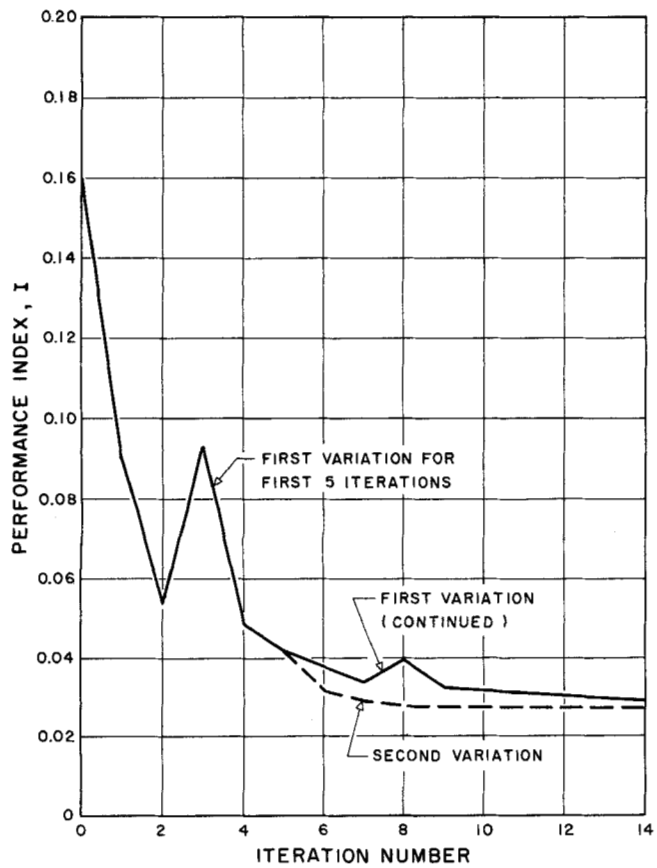

Fig. 2. First and second variation iterations. Initial policy: $u(t) = 0.5$ for $(t = 0, 0.76)$ and $u(t) = 0$ for $(t = 0.76, 0.78)$.

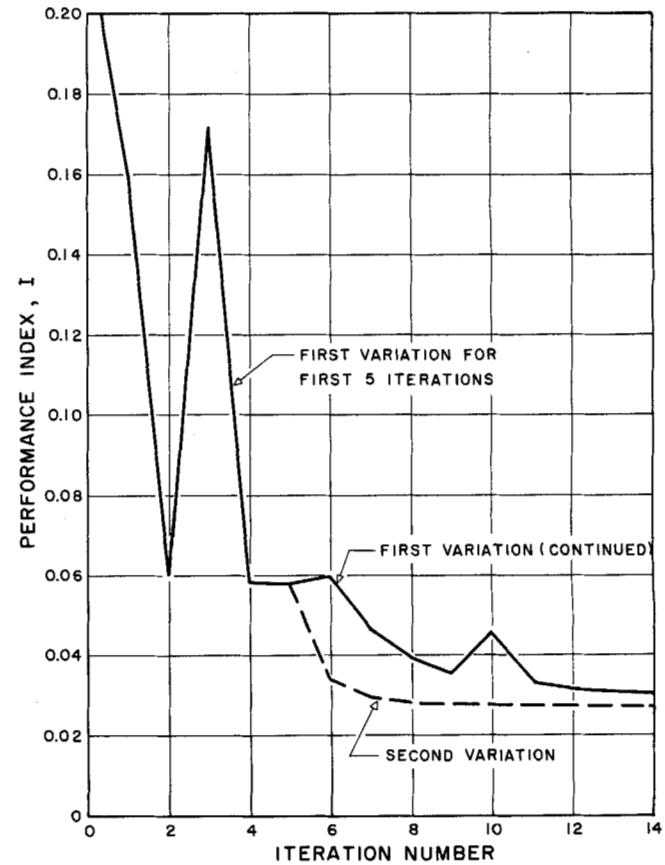

Fig. 3. First and second variation iterations. Initial policy: $u(t) = 0$ for $(t = 0, 0.78)$.

Similar results were also obtained for a larger step size in integration of the various differential equations (0.01 instead of 0.0025) and the values of the performance index I are plotted in Figure 1 to give a visual picture of the rate of convergence. Once again $\epsilon = 1.0$ yields fastest convergence rate as compared to any other ϵ used. Also, the number of iterations for an integration interval of 0.0025 and 0.01 is approximately the same. Thus, in all subsequent computations 0.01 is used to minimize computer time.

COMBINATION OF FIRST AND SECOND VARIATION METHODS

The above results were obtained with the carefully chosen initial control policy which ensured convergence. When, however, other initial policies were used, the iteration scheme as outlined diverged, because certain of the matrices in the iterations do not have the correct characteristics; that is **T** is not positive definite. Therefore, we turn to the combined use of the first and second variation methods to try to remove this initial policy defect.

Since the first variation method itself has been detailed extensively in the literature (*9, 14*) we shall not attempt here to describe its formulation. However, it is important to repeat that it has the feature of going quickly from almost any initial policy *to the neighborhood* of the optimum. It thus seems intuitively apparent that one may use the first variation method to bring the trajectory *close* to the optimal and then switch over to the second variation method to obtain convergence to the optimum. This feature is shown for two different initial policies in Figures 2 and 3. The first variation method is used for the first five iterations and then the second variation method is used until convergence results. The solid curves show the result of a complete application of the first variation method and it can be seen that even after fourteen iterations there is still a considerable deviation from the optimum. If the initial policies are used immediately for the second variation method, divergence results. The combined method, however, ensures rapid convergence.

This example effectively illustrates the versatility and importance associated with the combined use of the first and second variations. Although the time per iteration is greater for the combined method than the first method alone, 2.4 vs. 1.5 sec. on the IBM 7094, this is not a serious restriction. Of further importance is the fact that after even fifty iterations of the first variation alone, convergence is not reached. By contrast, fewer than ten iterations of the combined method yields complete convergence. This can most easily be seen in Figure 4. Therefore, there is an overall saving of computer time in the use of the combined methods.

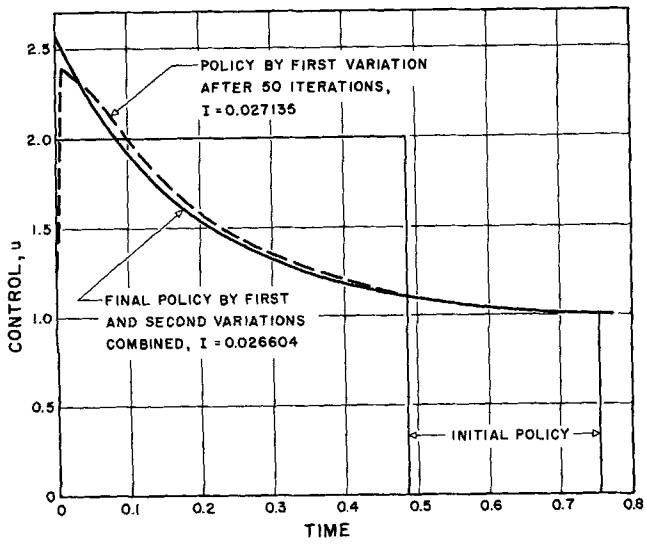

Fig. 4. Comparison of final policy achieved by first and second variations.

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NOTATION

- C = deviation from steady state concentration
- $\mathbf{f}$ = nonlinear vector function of state and control ($n \times 1$)
- H = Hamiltonian
- I = performance index
- I^* = augmented performance index
- J = integrand for the performance index
- $\mathbf{K}$ = variational matrix ($n \times r$)
- $\mathbf{P}$ = variational matrix ($n \times n$)
- q = scalar function of t
- $\mathbf{q}$ = vector function of t ($n \times 1$)
- $\mathbf{Q}$ = matrix function of t ($n \times n$)
- r = weighting factor
- $\mathbf{R}$ = variational matrix ($r \times n$)
- $\mathbf{s}$ = variational vector ($r \times 1$)
- t = time
- t_f = final time
- T = deviation from steady state temperature
- $\mathbf{T}$ = variational matrix ($r \times r$)
- u = normalized control action
- u_1 = control action
- $\mathbf{u}, u$ = control vector ($r \times 1$)
- V = integral expression to be minimized
- $\mathbf{x}, x$ = state vector ($n \times 1$)
- $\mathbf{z}$ = vector of Lagrange multipliers ($n \times 1$)
- ϵ = step size parameter

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