Quasilinearization and Invariant Imbedding in Optimization

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The two-point boundary value difficulties have limited the use of the calculus of variations to obtain numerical solutions for optimization problems. Two promising tools to overcome these difficulties are quasilinearization and invariant imbedding.

The quasilinearization technique has been applied to various nonlinear boundary value problems in the literature (*1* to *4*). Rothenberger and Lapidus (*5*) have used a procedure combining quasilinearization and invariant imbedding to solve nonlinear boundary value problems in optimization. This paper shows that the combined procedure is very sensitive to numerical errors of integration. Consequently, the quasilinearization technique, not the combined quasilinearization and invariant imbedding procedure, should be used to solve nonlinear boundary value problems. Nonetheless, the combined procedure is still useful for solving illconditioned problems (*1*).

A SIMPLE OPTIMIZATION PROBLEM

Consider the system of two consecutive reactions

$$A \rightarrow B \rightarrow C \tag{1}$$

which are being carried out in a tubular chemical reactor. Component B is the desired product, the yield of which is to be maximized by the choice of the temperature profile. If x_1 and x_2 are the state variables that represent concentrations of A and B respectively, the kinetics of the reactions are given by

$$\frac{dx_1}{dt} = -k_1 x_1 \tag{2a}$$

$$\frac{dx_2}{dt} = k_1 x_1 - k_2 x_2 \tag{2b}$$

where

$$k_1 = G_1 \exp\left(-\frac{E_1}{R_g T}\right), \quad k_2 = G_2 \exp\left(-\frac{E_2}{R_g T}\right) \tag{3}$$

The initial conditions for Equation (2) are

$$x_1(0) = x_1^0, \quad x_2(0) = x_2^0 \tag{4}$$

This optimization problem has been discussed by various authors (*5* to *9*). Thus a comparison can be made between the present procedures and various others.

The Euler-Lagrange equations are

$$\frac{d\lambda_1}{dt} = k_1\lambda_1 - k_1\lambda_2 \tag{5a}$$

$$\frac{d\lambda_2}{dt} = k_2\lambda_2 \tag{5b}$$

$$x_1 k_1 E_1(\lambda_1 - \lambda_2) + x_2 k_2 E_2 \lambda_2 = 0 \tag{6}$$

From the transversality condition, we have

$$\lambda_1(t_f) = 0, \quad \lambda_2(t_f) = 1 \tag{7}$$

Solving Equation (6) for T, one obtains

$$T = \frac{(E_1 - E_2)/R_g}{\ln \dfrac{x_1 G_1 E_1(\lambda_2 - \lambda_1)}{\lambda_2 x_2 G_2 E_2}} \tag{8}$$

Substituting T into Equation (3), one obtains

$$k_1 = G_1 \exp\left[\frac{E_1}{E_1 - E_2} \ln \frac{\lambda_2 x_2 G_2 E_2}{x_1 G_1 E_1(\lambda_2 - \lambda_1)}\right] = G_1 \exp\left[A_1 \ln(u)\right] \tag{9a}$$

$$k_2 = G_2 \exp\left[\frac{E_2}{E_1 - E_2} \ln(u)\right] = G_2 \exp\left[A_2 \ln(u)\right] \tag{9b}$$

Equations (9) can be further simplified into the following forms

$$k_1 = G_1 u^{A_1} \tag{10a}$$

$$k_2 = G_2 u^{A_2} \tag{10b}$$

Now Equations (2) and (5) become

$$\frac{dx_1}{dt} = -x_1 G_1 u^{A_1} \tag{11a}$$

$$\frac{dx_2}{dt} = x_1 G_1 u^{A_1} - x_2 G_2 u^{A_2} \tag{11b}$$

$$\frac{d\lambda_1}{dt} = (\lambda_1 - \lambda_2) G_1 u^{A_1} \tag{11c}$$

$$\frac{d\lambda_2}{dt} = \lambda_2 G_2 u^{A_2} \tag{11d}$$

with

$$A_1 = \frac{E_1}{E_1 - E_2}, \quad A_2 = \frac{E_2}{E_1 - E_2} \tag{12}$$

$$u = \frac{\lambda_2 x_2 G_2 E_2}{x_1 G_1 E_1(\lambda_2 - \lambda_1)} \tag{13}$$

THE QUASILINEARIZATION APPROACH

Equations (4), (7), and (11) represent a nonlinear two-point boundary value problem. This problem can be solved by the quasilinearization procedure. Consider the system of nonlinear differential equations

$$\frac{dx_i}{dt} = f_i(x_1, x_2, \ldots, x_M, t), \quad i = 1, 2, \ldots, M \tag{14}$$

This equation can be linearized by the generalized Newton-Raphson formula

$$\frac{d\mathbf{x}_{n+1}}{dt} = \mathbf{f}(\mathbf{x}_n, t) + \mathbf{J}(\mathbf{x}_n)(\mathbf{x}_{n+1} - \mathbf{x}_n) \tag{15}$$

where $\mathbf{x}_{n+1}$, $\mathbf{x}_n$, and $\mathbf{f}$ represent M-dimensional vectors with components $x_{1,n+1}, x_{2,n+1}, \ldots, x_{M,n+1}$; $x_{1,n}, x_{2,n}, \ldots, x_{M,n}$; and $f_1, f_2, \ldots, f_M$ respectively. The Jacobi matrix $\mathbf{J}(\mathbf{x}_n)$

$$\mathbf{J}(\mathbf{x}_n) = \begin{bmatrix} \dfrac{\partial f_1}{\partial x_{1,n}} & \dfrac{\partial f_1}{\partial x_{2,n}} & \cdots & \dfrac{\partial f_1}{\partial x_{M,n}} \\ \dfrac{\partial f_2}{\partial x_{1,n}} & \dfrac{\partial f_2}{\partial x_{2,n}} & \cdots & \dfrac{\partial f_2}{\partial x_{M,n}} \\ \dfrac{\partial f_M}{\partial x_{1,n}} & \dfrac{\partial f_M}{\partial x_{2,n}} & \cdots & \dfrac{\partial f_M}{\partial x_{M,n}} \end{bmatrix} \tag{16}$$

If we assume that $\mathbf{x}_n$ is the known value and is obtained from previous calculations and $\mathbf{x}_{n+1}$ is unknown, Equation

(15) will always be linear.

The equations in (11) can be linearized by the recurrence relation, Equation (15):

$$\frac{dx_{1,n+1}}{dt} = -x_1G_1u^{A_1} + (x_{1,n+1} - x_1)[(A_1 - 1)G_1u^{A_1}] + (x_{2,n+1} - x_2)[-x_1G_1A_1u^{A_1}/x_2] + (\lambda_{1,n+1} - \lambda_1)[-x_1G_1A_1u^{A_1}/(\lambda_2 - \lambda_1)] + (\lambda_{2,n+1} - \lambda_2)\, x_1G_1A_1u^{A_1}\frac{\lambda_1}{\lambda_2(\lambda_2 - \lambda_1)} \quad (17a)$$

$$\frac{dx_{2,n+1}}{dt} = x_1G_1u^{A_1} - x_2G_2u^{A_2} + (x_{1,n+1} - x_1)[G_1u^{A_1}(1 - A_1) + x_2G_2A_2u^{A_2}/x_1] + (x_{2,n+1} - x_2)[x_1G_1A_1u^{A_1}/x_2 - G_2u^{A_2}(1 + A_2)] + (\lambda_{1,n+1} - \lambda_1)[(x_1G_1A_1u^{A_1} - x_2G_2A_2u^{A_2})/(\lambda_2 - \lambda_1)] + (\lambda_{2,n+1} - \lambda_2)\left[(-x_1G_1A_1u^{A_1} + x_2G_2A_2u^{A_2})\frac{\lambda_1}{\lambda_2(\lambda_2 - \lambda_1)}\right] \quad (17b)$$

$$\frac{d\lambda_{1,n+1}}{dt} = (\lambda_1 - \lambda_2)G_1u^{A_1} + (x_{1,n+1} - x_1)[-(\lambda_1 - \lambda_2)G_1A_1u^{A_1}/x_1] + (x_{2,n+1} - x_2)[(\lambda_1 - \lambda_2)G_1A_1u^{A_1}/x_2] + (\lambda_{1,n+1} - \lambda_1)[(-A_1 + 1)G_1u^{A_1}] + (\lambda_{2,n+1} - \lambda_2)[(A_1z_1/z_2 - 1)G_1u^{A_1}] \quad (17c)$$

$$\frac{d\lambda_{2,n+1}}{dt} = \lambda_2G_2u^{A_2} + (x_{1,n+1} - x_1)[-\lambda_2G_2A_2u^{A_2}/x_1] + (x_{2,n+1} - x_2)[\lambda_2G_2A_2u^{A_2}/x_2] + (\lambda_{1,n+1} - \lambda_1)[\lambda_2G_2A_2u^{A_2}/(\lambda_2 - \lambda_1)] + (\lambda_{2,n+1} - \lambda_2)\{[1 - A_2\lambda_1/(\lambda_2 - \lambda_1)]G_2u^{A_2}\} \quad (17d)$$

The second subscript n has been omitted from x_1, x_2, λ_1, and λ_2 in the above equations for simplicity. It is understood that the unknown variables are the variables with the second subscript $(n + 1)$. All other variables are known and are calculated from the previous nth iteration. The boundary conditions for Equation (17) are:

$$x_{1,n+1}(0) = x_1^0, \quad x_{2,n+1}(0) = x_2^0 \quad (18a)$$

$$\lambda_{1,n+1}(t_f) = 0, \quad \lambda_{2,n+1}(t_f) = 1 \quad (18b)$$

Since Equations (17) and (18) constitute a linear boundary value problem, they can be solved by the superposition principle (2 to 4). One set of particular and four sets of homogeneous solutions can be obtained by using initial values that are nontrivial and distinct. However, if the initial values listed in Table 1 are used, only two sets of homogeneous solutions are needed.

Table 1. Initial Conditions Used for Obtaining Particular and Homogeneous Solutions

	particular solution	Homogeneous Solutions			
		I	II	III	IV
$x_1(0)$	x_1^0	1	0	0	0
$x_2(0)$	x_2^0	0	1	0	0
$\lambda_1(0)$	0	0	0	1	0
$\lambda_2(0)$	0	0	0	0	1

NUMERICAL RESULTS BY QUASILINEARIZATION

The numerical values for the constants in the Arrhenius expressions are

$$G_1 = 0.535 \times 10^{11}/\text{min.} \qquad E_1 = 18{,}000 \text{ cal./mole}$$
$$G_2 = 0.461 \times 10^{18}/\text{min.} \qquad E_2 = 30{,}000 \text{ cal./mole}$$
$$R_g = 2 \text{ cal./(mole-°K.)} \quad (19)$$

The other numerical values used are

$$t_f = 10 \text{ min}$$
$$x_1^0 = 0.95 \text{ mole/liter}$$
$$x_2^0 = 0.05 \text{ mole/liter} \quad (20)$$
$$\Delta t = 0.025, \quad \text{for } 0 < t < 1.0$$
$$\Delta t = 0.1, \quad \text{for } 1.0 < t < 10.0$$

With the given boundary conditions as the initial approximations

$$x_{1,0}(t_k) = 0.95, \quad x_{2,0}(t_k) = 0.05, \quad \lambda_{1,0}(t_k) = 0.0, \quad \lambda_{2,0}(t_k) = 1.0 \quad (21)$$

and with $k = 0, 1, 2, \ldots, N$, $\Delta t = t_{k+1} - t_k$, no convergence can be obtained for this problem. The particular and homogeneous solutions are obtained using the Runge-Kutta integration formula and Δt is the integration step size. The values listed in Table 1 are used as the initial conditions. In order to obtain convergence, much better initial approximations are needed. Instead of assuming the initial approximation for x and λ, it can be assumed for control variable T. Note that once the values of $T(t)$ are known, Equations (2) and (5) can be solved as two initial value problems. First, Equation (2) can be integrated with the initial condition (4). Then Equation (5) can be integrated backward with (7) as the initial condition. The initial approximations of x and λ are obtained in this fashion with the following assumed temperature profile

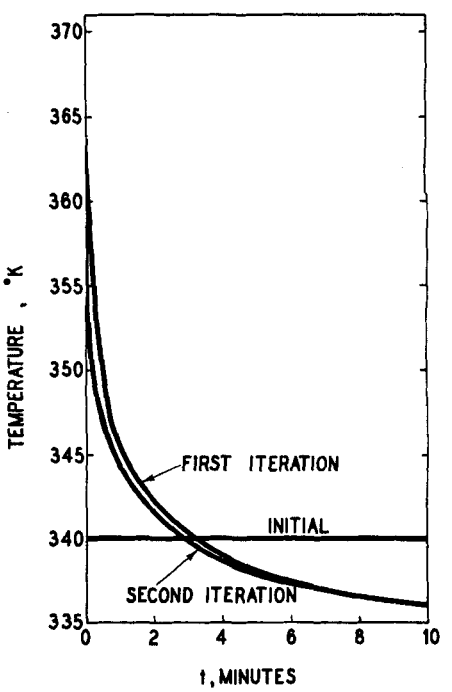

Fig. 1. Convergence rate of temperature.

$$T_0(t_k) = 340°\text{K.}, \quad k = 0, 1, 2, \ldots, N \qquad (22)$$

Part of the results is shown in Figure 1. In spite of the steepness of the temperature profile and the very approximate initial temperature profile used, only two iterations are needed to obtain an accuracy sufficient for the figure. The third iteration can not be distinguished from the second in Figure 1.

This same problem has been solved by the functional gradient (9). With a much better initial approximation for $T(t)$, 45 iterations are still needed as compared to two iterations shown in Figure 1. This problem was also solved on an analog computer by a trial-and-error procedure (8). In order for the procedure to converge, a much better initial approximation than that given in Equation (22) is needed. Even then, 20 to 50 iterations are still needed to obtain the desired accuracy.

QUASILINEARIZATION AND INVARIANT IMBEDDING

Instead of using the superposition principle to solve the linear boundary value problem resulting from quasilinearization, the invariant imbedding procedure can be used to obtain the missing initial conditions. This combined procedure to overcome the ill conditioned problem in the quasilinearization procedure, was originally proposed by Bellman and Kalaba (1). This procedure has been outlined by Rothenberger and Lapidus (5). By using the equations and procedures discussed by these authors, some numerical experiments have been performed. There has been no convergence when the initial approximations are obtained from the assumed temperature profile listed in Equation (22). In fact, even with a better initial temperature profile obtained from Equations (23) and (24), convergence still cannot be obtained.

$$T_0(0) = 345°\text{K.}, \quad T_0(t_f) = 335°\text{K.} \qquad (23)$$

The values of $T_0(t_k)$ for $k = 0, 1, 2, \ldots, N$ are obtained by the following recurrence relation

$$T_0(t_{k+1}) = T_0(t_k) - \frac{T_0(0) - T_0(t_f)}{N}, \qquad k = 0, 1, 2, \ldots, (N-1) \qquad (24)$$

with $T_0(t_0) = T_0(0)$.

To obtain convergence, a smaller integration step size is needed for a more accurate integration. Instead of Equation (20), the following numerical values are used:

$$\begin{aligned} t_f &= 10 \text{ min.} \\ x_1^0 &= 0.95 \text{ mole/liter} \\ x_2^0 &= 0.05 \text{ mole/liter} \\ \Delta t &= 0.01 \end{aligned} \qquad (25)$$

The initially assumed temperature profile is obtained by using Equations (23) and (24); and the initial approximations are obtained from this temperature profile by integration. This problem has been solved by the combined quasilinearization and invariant imbedding procedure, using the reaction rate constants listed in Equation (19). The convergence rates for these two procedures are quite similar. Nevertheless results from the combined procedure have been obtained with a much smaller integration step size than that used in the quasilinearization procedure. The value of $\lambda_1(t_f)$ is 0.23×10^{-3} is obtained by the combined procedure. Since this value should be zero, an accuracy of 0.23×10^{-3} is obtained at this final point. A much higher accuracy has resulted from the quasilinearization procedure even with a much larger integration step size.

DISCUSSION

The combined quasilinearization and invariant imbedding procedure is very sensitive to numerical errors of the integration procedure. This should be expected. The missing initial conditions are obtained by integrating the invariant imbedding equations backward starting with the known final conditions. Then based on these newly obtained missing initial conditions, Equation (17) is solved by integrating (17) forward. Thus, the calculated values of the known final conditions depend upon two integration processes which are performed in series. Consequently, the combined procedure is very sensitive to the accuracy of the integration processes and is not suited when the difficulties in solving the problem lie in the numerical integration process. This procedure should be used, however, when the difficulties in solving the problem is connected with the numerical solution of the algebraic equations. Both the quasilinearization procedure and the combined quasilinearization and invariant imbedding procedure are much more effective than the functional gradient technique and the usual trial-and-error approach.

Rothenberger and Lapidus (5) solved the above problem by the combined procedure under a much less severe reaction condition. The initial values, x_1^0 and x_2^0, used by these authors are approximately equal to the corresponding values at $t = 2$ in Figure 1. Notice the very fast rate of temperature decrease during the first two minutes of the reaction.

The quasilinearization technique also has various disadvantages. A detailed discussion on the advantages and disadvantages of the quasilinearization and the invariant imbedding techniques can be found in the literature (1, 3, 10).

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NOTATION

A_1, A_2 = constants, defined by Equation (12)
E_1, E_2 = activation energies of the reactions
G_1, G_2 = frequency factor constants in the Arrhenius expressions
$\mathbf{J}(\mathbf{x}_n)$ = Jacobi matrix, defined by Equation (16)
k_1, k_2 = reaction rate constants
R_g = gas constant
t = independent variable
T = temperature
t_f = final value of t
Δt = integration step size
x_1, x_2 = concentrations of A and B respectively
λ_1, λ_2 = Lagrange multipliers

Subscripts

n = nth iteration, assumed known
$n+1$ = $(n+1)$st iteration, assumed unknown

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