ψ = stream function

Subscripts

i = at interface

δ = at edge of thick boundary layer

LITERATURE CITED

Bowman, C. W., D. M. Ward, A. I. Johnson, and D. Trass, "Mass Transfer from Fluid and Solid Spheres at Low Reynolds Numbers," *Can. J. Chem. Eng.*, **39**, 9 (1961).

Friedlander, S. K., "Mass and Heat Transfer to Single Spheres and Cylinders at Low Reynolds Numbers", *AIChE J.*, **3**, 43 (1957).

Gal-Or, B., "On Motion of Bubbles or Drops", *Can. J. Chem. Eng.*, **48**, 526 (1970).

———, and S. Waslo, "Hydrodynamics of an Ensemble of Drops or Bubbles in the Presence or Absence of Surfactants", *Chem. Eng. Sci.*, **23**, 1431 (1968).

Waslo, S., and B. Gal-Or, "Boundary Layer Theory for Mass and Heat Transfer in Clouds of Moving Drops, Bubbles or Solid Particles," *ibid.*, **26**, 829 (1971).

Yaron, I., and B. Gal-Or, "Convective Mass or Heat Transfer from Size-Distributed Drops, Bubbles or Solid Particles", *Intern. J. Heat Mass Transfer*, **14**, 727 (1971).

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A Modified Maximum Principle

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While the maximum principle of Pontryagin remains as the standard theoretical development for optimal control, the implementation of the theory to even modestly realistic systems remains a most difficult problem. This is because of the generation of two-point-boundary value (TPBV) equations which are, when combined with special instability features, almost impossible to solve except in trivial cases.

In this note we wish to point out a modified form of the maximum principle as detailed by Chuprun (1967) which removes the instability feature. As such, it opens the door further for the use of the maximum principle in optimal control problems.

THEORY

In one form of the maximum principle (Lapidus and Luus, 1967) the optimal control problem consists of a state equation and initial condition

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

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

a final value index

$$S = cx(t_f) \tag{3}$$

and the object is to select the control $u(t)$ such that S is minimized while satisfying the constraints of (1) and (2). t_f is the final time of control and these equations can be visualized in scalar or vector-matrix form depending on the various dimensions.

The maximum principle proceeds by introduction of a scalar Hamiltonian function

$$H = f\lambda \tag{4}$$

with the resulting conditions for optimality

$$\begin{aligned} \dot{x} &= H_\lambda = f & x(0) &= b \\ \dot{\lambda} &= -H_x = -f_x\lambda & \lambda(t_f) &= -c \end{aligned} \tag{5}$$

$$H_u = 0 \tag{6}$$

Here $\lambda(t)$ is a new variable (the adjoint variable) which has been introduced and the condition of a stationary value of H (given by $\partial H/\partial u = H_u = 0$) yields the optimal control $u^0(t)$. In the regular problem (6) yields $u^0(t)$ in terms of $x(t)$ and $\lambda(t)$; in the singular problem (6) does not yield $u^0(t)$ and further information must be obtained. We here only consider the regular problem in which case the TPBV of (5) must be solved in order to remove the dependence of $x(t)$ and $\lambda(t)$ in $u^0(t)$.

In solving (5) it is frequently found that when $x(t)$ is stable in a positive time direction $\lambda(t)$ is unstable in the same direction (and vice-versa). It is important to realize however, that it is the direction of the adjoint equations as vectors in coordinate space and not their actual magnitude which is of importance. As indicated by Sagan (1969) $\lambda(t)$ need only be determined but for a multiplicative constant. This property will be used to advantage shortly.

Chuprun's method consists of replacing the adjoint variable $\lambda(t)$ with a new variable $\rho(t)$ such that

$$H = f\rho \tag{7}$$

and

$$\rho = -f_x\rho + e(\rho, t)\rho \tag{8}$$

where $e(\rho, t)$ is a scalar function (in general, nonlinear). He then proves that (8) and the second equation in (5) have identical directions for all times t and thus can be used interchangeably without altering the results of the standard maximum principle. Further he shows that as long as $e(\rho, t)$ is chosen carefully, the solution of (8) must remain on a sphere of constant radius, and (8) can be made stable or bounded in the positive time direction. In simple geometric terms, the introduction of $e(\rho, t)$ means that the normal velocity component of the representative point in phase space varies while the tangential component remains constant. It is also apparent that the

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condition on ρ at $t = t_f$ is the same as $\lambda(t_f)$ except for an arbitrary multiplicative constant.

The only question left is to choose the explicit form for $e(\rho, t)$. Chuprun presents five such forms of which we merely quote

$$e(\rho, t) = \frac{\sum_{p=0}^{n} \sum_{s=0}^{n} -\left(\frac{\partial f_s}{\partial x_p} \right) \rho_s \rho_p}{\sum_{j=0}^{n} \rho_j^2} \tag{9}$$

where $n + 1$ is the total number of states used in any augmented system equation. In the form (9) the sum of squares of the coordinates of any solution of $\rho(t)$ is invariant with time, that is,

$$\sum_{i=0}^{n} \rho_i^2(t) = \text{constant} \tag{10}$$

The constant may be obtained from the boundary conditions $\rho(t_f)$ as illustrated shortly.

NUMERICAL EXAMPLES

To indicate the computational feasibility of the present approach we consider two problems. The first is given by Lapidus and Luus (1967) on pages 94 to 96 for the effluent tracer flow from a CSTR; the pertinent equations are

$$\begin{aligned}
&\dot{x}_0(t) = \frac{1}{2}[x_1^2 + u^2] = f_0 && x_0(0) = 0 \\
&\dot{x}_1(t) = -x_1 + u = f_1 && x_1(0) = \text{given} \\
&S = x_0(t_f) && \\
&\dot{\lambda}_0(t) = 0;\ \lambda_0(t) = 1.0 && \lambda_0(t_f) = 1.0 \\
&\dot{\lambda}_1(t) = -\lambda_0 x_1 + \lambda_1 && \lambda_1(t_f) = 0
\end{aligned} \tag{11}$$

The second problem is the optimal temperature profile in a plug flow tubular reactor with first-order consecutive reactions as detailed by many workers, including Rothenberger and Lapidus (1967); the pertinent equations are

$$\begin{aligned}
&A \xrightarrow{k_1} B \xrightarrow{k_2} C && k_i = k_{i0} e^{-E_i/RT} \\
&\dot{x}_1(t) = -k_1 x_1 && x_1(0) = \text{given} \\
&\dot{x}_2(t) = k_1 x_1 - k_2 x_2 && x_2(0) = \text{given} \\
&S = x_2(t_f) && \\
&\dot{\lambda}_1(t) = k_1 \lambda_1 - k_2 \lambda_2 && \lambda_1(t_f) = 0 \\
&\dot{\lambda}_2(t) = k_2 \lambda_2 && \lambda_2(t_f) = 1.0
\end{aligned} \tag{12}$$

All of the derivations and parameters for these two problems are given in the references indicated and will not be repeated here.

Problem 1

This problem is a relatively simple one which involves two state variables $x_0(t)$ and $x_1(t)$ and a single control variable $u(t)$. As shown by Lapidus and Luus the solution for $u^0(t)$ can be obtained in analytical terms since the canonical equations are linear. In the use of Chuprun's method Bertucci (1971) has shown that for $e(\rho,t)$ chosen as in (9) such that explicitly

$$e(\rho, t) = -\frac{\rho_1^2 - x_1 \rho_0 \rho_1}{\rho_0^2 + \rho_1^2} \tag{13}$$

there results (using $u^0(t) = -\rho_1/\rho_0$ as obtained from $H_u = 0$)

$$\begin{aligned}
&\dot{x}_1(t) = -x_1 - \rho_1/\rho_0 && x_1(0) = \text{given} \\
&\dot{\rho}_0(t) = e(\rho, t)\rho_0 && \rho_0(t_f) = \text{an arbitrary constant} \\
&\dot{\rho}_1(t) = \rho_0 x_1 + \rho_1 + e(\rho, t)\rho_1 && \rho_1(t_f) = 0
\end{aligned} \tag{14}$$

In this case (14) contains three nonlinear canonical equations instead of the two linear canonical equations resulting from (11). Obviously a numerical solution must be obtained rather than an analytical one. However, this is not important since in a more complex problem no analytical solution will ever be possible.

To carry out the numerical solution a simple forward time marching procedure was used. Note that from (10) only one initial condition need be determined as initial boundary conditions. The results obtained by Bertucci completely confirm the stability of the modified adjoint equations in the forward time direction and the attainment of exact optimal control (conversely $\lambda_1(t)$ is completely unstable in the forward time direction).

Problem 2

Here the problem is again a two-state variable system with one control variable. The system equations are however nonlinear as contrasted to those of Problem 1. As shown by Bertucci once again the use of Chuprun's method yields identical numerical results as those obtained by other authors but by using a direct forward time integration of the canonical equations. Further, the computation time seems much shorter by the present procedure than by the alternate direction methods of the reference.

SUMMARY

This communication has pointed out that by the use of Chuprun's modified maximum principle it is possible to remove the stability problem usually associated with the adjoint equations in optimal control systems. Implementation of these modifications is quite simple and suggests that the method has much promise. The extension to constraints in the state and control variables would seem a natural next step.

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LITERATURE CITED

Bertucci, J. A., "The Solution of Optimal Control Problems Using a Modified Maximum Principle," Master's thesis, Princeton Univ., N. J. (1971).

Chuprun, B. E., "Solution of Optimization Problems by the Maximum Principle," *Auto. Remote Control,* **11,** 126 (1967).

Lapidus, L., and R. Luus, *Optimal Control of Engineering Processes,* Blaisdell (1971).

Rothenberger, B. F., and L. Lapidus, "The Control of Nonlinear Systems III: Invariant Imbedding and Quasilinearization," *AIChE J.,* 13, 114 (1967).

Sagan, H., *Introduction to the Calculus of Variations,* McGraw-Hill, N. Y. (1969).

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