COMMUNICATIONS TO THE EDITOR

The Discrete Maximum Principle and Complex Process Optimization

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In a recent paper (*1*) Lee discusses the optimization of complex chemical plants by a gradient technique and the use of Lagrange multipliers.

Dynamic programming and the discrete maximum principle are dismissed as suitable only for chemical processes in which the stages are connected in a simple serial form. This is extremely misleading.

As Lee suggests, the use of dynamic programming is limited by the small number of variables that it can conveniently handle.

Neither of these restrictions, however, apply to the use of the discrete maximum principle which can handle both large numbers of variables and complex interconnected topologies (*2*).

It will be argued in this communication that advantage is gained over the method proposed by Lee, not lost as he suggests, by using the discrete maximum principle in the complex case.

Lee's method using classical Lagrange multipliers is to subject the process objective function P to a set of equality constraints, imposed by the necessity of satisfying the state transformation equations describing each stage of the process

$$x_i^n = f_i^n\,(\mathbf{x}^{n-1}, \boldsymbol{\theta}^n) \quad i = 1, 2, \ldots . M \tag{1}$$

The objective function is modified in the classical Lagrange method to include the transformation equations which are constraints in this problem.

$$\phi = P - \sum_{n-1}^{N} \cdot \sum_{i-1}^{M} \lambda_i^n\,(x_i^n - f_i^n) \tag{2}$$

The differential changes in ϕ due to differential changes in the decision variables are

$$d\phi = \sum_{n=1}^{N} \cdot \sum_{i=1}^{M} \frac{\partial \phi}{\partial x_i^n}\,dx_i^n + \sum_{n=1}^{N} \cdot \sum_{j=1}^{S} \frac{\partial \theta}{\partial \theta_j^n}\,d\theta_j^n \tag{3}$$

The Lagrange multipliers are chosen such that the coefficients of dx_i^n are zero. Generally, from Equations (1) and (2)

$$\frac{\partial \phi}{\partial x_i^n} = \frac{\partial P}{\partial x_i^n} - \lambda_i^n + \sum_{i=1}^{M} \lambda_i^{n+1} \frac{\partial f_i^{n+1}}{\partial x_i^n} \qquad \begin{matrix} n = 1, 2, \ldots N \\ i = 1, 2, \ldots M \end{matrix} \tag{4}$$

If

$$\frac{\partial \phi}{\partial x_i^n} = 0$$

$$\lambda_i^n = \frac{\partial P}{\partial x_i^n} + \sum_{i=1}^{M} \lambda_i^{n+1} \frac{\partial f_i^{n+1}}{\partial x_i^n} \qquad \begin{matrix} n = 1, 2, \ldots N \\ i = 1, 2, \ldots M \end{matrix} \tag{5}$$

These equations are precisely those which occur in the discrete maximum principle:

$$Z_i^n = \frac{\partial H^{n+1}}{\partial x_i^n} \qquad \begin{matrix} n = 1, 2, \ldots N \\ i = 1, 2, \ldots M \end{matrix} \tag{6}$$

where

$$H^{n+1} = P + \sum_{i=1}^{M} Z_i^{n+1} f_i^{n+1} \quad n = 1, 2, \ldots N \tag{7}$$

Z_i^{n+1} is the adjoint variable associated with state variable i and stage $n + 1$, corresponding to λ_i^{n+1} in the method of Lagrange multipliers.

P is usually a function only of process output variables, and at these output stages $\partial P/\partial x_i^n$ is nonzero and $\partial f_i^{n+1}/\partial x_i^n$ is zero. Thus $\lambda_i^n = \partial P/\partial x_i^n$. At all the other stages $\partial P/\partial x_i^n$ is zero, to give

$$Z_i^n = \sum_{i=1}^{M} Z_i^{n+1} \frac{\partial f_i^{n+1}}{\partial x_i^n} \quad n = 1, 2, \ldots N \tag{8}$$

This equivalence between Lagrange multipliers and the adjoint variables of the discrete maximum principle is discussed elsewhere (*3*).

The first derivatives of the objective function with respect to each of the decision variables are similarly equivalent to those obtained by differentiating the Hamiltonian function at each stage.

$$\frac{\partial \phi}{\partial \theta_i^n} = \frac{\partial H^n}{\partial \theta_i^n} \qquad \begin{matrix} n = 1, 2, \ldots N \\ i = 1, 2, \ldots S \end{matrix} \tag{9}$$

It is obvious that no extra work is involved by using the discrete maximum principle, since the state transformation equations and the derived adjoint equations are the same as those obtained by Lee, in his Lagrange multiplier approach. The derivatives $\partial H^n/\partial \theta_i^n$ may be used in precisely the same way as Lee describes in the gradient technique, or in other methods of optimization involving first derivatives.

The systematic formulation of the discrete maximum principle does, however, provide an easier method of obtaining the necessary derivatives than the rather extensive, complex objective function and its derivatives that Lee evolves.

The weak version of the discrete maximum principle to which the discussion so far applies, is general to all systems. It states that the Hamiltonian function has a stationary value when the objective function has a stationary value.

The strong version, which does not apply generally to all systems, due to the neglect of second order derivatives, states that the stationary points of both the Hamiltonian and the objective functions are similar in nature. The two versions have been discussed fully in (*4*).

The discrete maximum principle has been applied to the same chemical process as Lee used as an example for his Lagrange multiplier approach. The equations and derivatives obtained were precisely Equations (20) to (36) derived in Lee's paper.

It was revealed that the strong principle could be applied. At each stage the Hamiltonian was maximized independently as a function of only one variable, to give a new decision policy. The complete system was re-evaluated using the new decision policy, to generate a further set of values for the state and adjoint variables. The procedure was repeated until changes in the decision policy became insignificant. The vicinity of the optimum was attained in a few iterations.

An advantage of this method is that the number of complete system evaluations is greatly reduced. This is a major saving in time in the complex case.

It also eliminates the difficulties of applying multivariable optimization techniques using derivatives, which often become exceedingly slow when the number of variables is large. Instead the problem is reduced to several single variable searches to maximize the Hamiltonian at each stage.

It must however be stressed that the strong maximum principle cannot be used in every case. It is perhaps unfortunate that Lee has chosen an example in which it is advantageous to use the discrete maximum principle.

NOTATION

f_i^n = the transformation function of state variable i at stage n
H^n = the Hamiltonian function at stage n
M = number of state variables
N = number of stages
P = objective function
S = number of decision variables at each stage
x_i^n = output state variable i from stage n
$\mathbf{x}^{n+1}$ = input state vector to stage n
Z_i^n = adjoint variable associated with state variable i at stage n
i = indicative of variable
n = indicative of stage

Greek Letters

θ^n = decision variable at stage n
λ_i^n = Lagrange multiplier i at stage n
ϕ = modified objective function

LITERATURE CITED

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SI Units in Chemical Engineering

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EDITOR'S NOTE:

With the adoption of the International System of units by the *Journal* for all new manuscripts submitted after July 1, 1971, we would like to have our readers familiar with developments in other countries, notably in Britain, where the transition to SI is now underway. Therefore, below is a revised and up-dated version of an article published by Professor Mullin four years ago (*1*). The author, who is probably better known for his publications in the area of crystallization, has been actively engaged in the United Kingdom program for the changeover to the metric system. He is a member of several British and International Standards committees concerned with metrication, and played an active part in the drafting of the British Standard Specification on SI units (2).

There is a world-wide trend toward the adoption of a unified system of measurement based on the metric system. The United Kingdom has passed the half-way mark in its 10-year conversion program, and in some sectors of industry the change has already been completed. In the United States of America and Canada there is a growing awareness of the desirability of adopting an internationally rationalized metric system, and the implications of such a change are being studied at the moment.

The metric system we are talking about is the SI, or International System (Système International d'Unités). SI units have been adopted by the International Organisation for Standardization (ISO) and recommended by a large number of national standards organizations. Much has been written about SI units over the past few years, and it is not the present intention to add to that literature. For an ac-