$$\lambda = \frac{\epsilon_b v}{2D_A}\left[1 - \sqrt{1 + \frac{4D_A}{\epsilon_b v^2}\left[s + \frac{1-\epsilon_b}{\epsilon_b}\int_0^\infty \frac{3}{R}\, k_m \frac{\alpha R - \tanh \alpha R}{\alpha R + (k_m R/D_i - 1)\tanh \alpha R} f(R)\, dR\right]}\right]$$

μ'_1 = first absolute moment of chromatographic output response, s
μ_2 = second central moment of chromatographic output response, s^2
ρ_p = particle density, g/cm^3
ν = fluid kinematic viscosity, cm^2/s

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Relationship of the Two-Level Optimization Procedure to the Discrete Maximum Principle

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We propose to show the relationship between the Discrete Maximum Principle (*1*) and the Two-Level Optimization Procedure (*2* to *5*) as applied to static or discrete time optimization problems. This will indicate the basis on which the Two-Level Optimization Procedure has been developed and will show that it is another method for solving the necessary conditions of the Discrete Maximum Principle. The immediate consequence of this is that the shortcomings of Two-Level Optimization are those of the Discrete Maximum Principle and of all problem solving techniques in which the decision variables appear linearly.

Consider, as a basis for the development of the comparison, the optimal control of sequential, unconstrained problems. (Constraints and recycle do not change the resulting relationship, and we wish to keep the development here as simple as possible.) The problem is to minimize the performance index

$$I[\mathbf{x}(0), N] = \mathbf{C}'\mathbf{x}(N) + \sum_{k=1}^{N} J[\mathbf{x}(k-1), (\mathbf{u}(k-1)] \tag{1}$$

subject to the state equation

$$\mathbf{x}(k) = \mathbf{f}(k) = \mathbf{f}[\mathbf{x}(k-1), \mathbf{u}(k-1)]$$
$$\mathbf{x}(0) \text{ given}; k = 1, \ldots, N \tag{2}$$

by means of appropriately choosing the unconstrained control policy $\mathbf{u}(0), \mathbf{u}(1), \ldots, \mathbf{u}(N-1)$.

The Two-Level Optimization approach requires the decomposition of the performance index as

$$I[\mathbf{x}(0), N] = \sum_{k=1}^{N+1} J(k) \tag{3}$$

where

$$J(k) = J[\mathbf{x}(k-1), \mathbf{u}(k-1)];\ k = 1, \ldots, N$$
$$J(N+1) = \mathbf{C}'\mathbf{x}(N)$$

and the formulation of the Lagrangian function

$$L = \sum_{k=1}^{N+1} J(k) + \sum_{k=1}^{N} \mathbf{p}'(k)\,[\mathbf{f}(k) - \mathbf{x}(k)] \tag{4}$$

The subsequent independent subproblems consist of minimization of the subLagrangians $L(k)$ defined as

$$L(k) = J(k) + \mathbf{p}'(k)\mathbf{f}(k) - \mathbf{p}'(k-1)\mathbf{x}(k-1) \tag{5}$$
$$k = 1, \ldots, N+1$$

with

$$\mathbf{p}(0) = \mathbf{p}(N+1) = \mathbf{f}(N+1) = \mathbf{0}$$

The first level of optimization involves minimizing the subLagrangians of Equation (5) for given values of the decomposition vectors $\mathbf{p}(k)$, $k = 1, \ldots, N$. Necessary conditions for these minima are the following stationary conditions

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$$\frac{\partial L(k)}{\partial \mathbf{x}(k-1)} = \frac{\partial J(k)}{\partial \mathbf{x}(k-1)} + \frac{\partial \mathbf{f}'(k)}{\partial \mathbf{x}(k-1)}\mathbf{p}(k) - \mathbf{p}(k-1) = \mathbf{0} \quad (6)$$

$$k = 2, \ldots, N+1$$

$$\frac{\partial L(k)}{\partial \mathbf{u}(k-1)} = \frac{\partial J(k)}{\partial \mathbf{u}(k-1)} + \frac{\partial \mathbf{f}'(k)}{\partial \mathbf{u}(k-1)}\mathbf{p}(k) = \mathbf{0} \quad (7)$$

$$k = 1, \ldots, N$$

The second level of optimization requires that the state equation be satisfied, that is,

$$\frac{\partial L}{\partial \mathbf{p}(k)} = \mathbf{f}(k) - \mathbf{x}(k) = \mathbf{0} \quad (8)$$

$$k = 1, \ldots, N$$

which gives us Equation (2).

The procedure used in finding the problem solution involves relaxing the equality to zero in Equation (8) and iterating on the decomposition vectors $\mathbf{p}(k)$, $k = 1, \ldots, N$ until some convergence criterion is satisfied.

When the Maximum Principle is used, the performance index of Equation (1) is first put into the Mayer form by defining the new state variable $x_0(k)$ as

$$x_0(k) = f_0(k) = J(k) + x_0(k-1) \quad (9)$$

$$x_0(0) = 0;\ k = 1, \ldots, N$$

With this definition, the performance index may be written as

$$I^*[\mathbf{x}(0), N] = x_0(N) + \mathbf{C}'\mathbf{x}(N) = \mathbf{C}^{*\prime}\mathbf{x}^*(N) \quad (10)$$

where

$$C^{*\prime} = [1, C_1, \ldots, C_n]$$

$$\mathbf{x}^{*\prime} = [x_0, x_1, \ldots, x_n]$$

The Hamiltonian is formed as

$$H^*(k) = \mathbf{z}^{*\prime}(k)\,\mathbf{f}^*(k) \quad (11)$$

where

$$\mathbf{z}^{*\prime}(k) = [z_0(k), z_1(k), \ldots, z_n(k)]$$

$$\mathbf{f}^{*\prime}(k) = [f_0(k), f_1(k), \ldots, f_n(k)]$$

The resulting equations, which are instrumental in the solution of the problem posed, are the definition of the adjoint vector

$$\mathbf{z}^*(k\text{-}1) = \frac{\partial H^*(k)}{\partial \mathbf{x}^*(k\text{-}1)} = \frac{\partial \mathbf{f}^{*\prime}(k)}{\partial \mathbf{x}^*(k\text{-}1)}\mathbf{z}^*(k)\ k = 2, \ldots, N$$

with the final condition

$$\mathbf{z}^*(N) = \frac{\partial I^*}{\partial \mathbf{x}^*(N)} = \mathbf{C}^* \quad (12)$$

and the stationary condition for the Hamiltonian

$$\frac{\partial H^*(k)}{\partial \mathbf{u}(k\text{-}1)} = \frac{\partial \mathbf{f}^{*\prime}(k)}{\partial \mathbf{u}(k\text{-}1)}\mathbf{z}^*(k) = \mathbf{0};\ k = 1, \ldots, N \quad (13)$$

By realizing that $z_0(N)$ is 1 and that $f_0(k) \equiv J(k) + x_0(k\text{-}1)$, we may rewrite Equation (12) as

$$\frac{\partial J(k)}{\partial \mathbf{x}(k\text{-}1)} + \frac{\partial \mathbf{f}'(k)}{\partial \mathbf{x}(k\text{-}1)}\mathbf{z}(k) - \mathbf{z}(k\text{-}1) = \mathbf{0} \quad (14)$$

$$k = 2, \ldots, N$$

and

$$\mathbf{z}(N) = \mathbf{C}$$

Comparing this result with Equation (6), we see that the two equations are identical if $\mathbf{z}$ is replaced by $\mathbf{p}$. Similarly Equations (7) and (13) are identical. From this, it is clear that the Two-Level Optimization Procedure is another technique for solving the necessary conditions of the Discrete Maximum Principle.

The Two-Level Optimization Procedure is most closely related to control vector iteration techniques, and this similarity indicates some of the present difficulties researchers are having in determining an efficient method for updating the decomposition vectors during iteration.

As recently pointed out by Avery and Foss (*6*), not all problems may be solved by Two-Level Optimization, and also decomposition into subproblems requires great care. That considerable care must be taken has also been shown by others (*4, 8, 9*). Similarly the weaknesses of the Discrete Maximum Principle as shown by Horn and Jackson (*7*) and others are inherent also in Two-Level Optimization.

The major advantage of Two-Level Optimization is that, at the first level of solution problems of reduced dimension are solved. This provides strong encouragement for continued research in the area of linear decision variable problems. In addition, the drawbacks of Two-Level Optimization make up only a small class of problems compared to those for which it is applicable, so as to be of only minor consequence.

NOTATION

$\mathbf{C}$ = constant vector ($n \times 1$)
$\mathbf{C}^*$ = $[1, \mathbf{C}']'$ = constant vector ($(n+1) \times 1$)
$\mathbf{f}(k)$ = vector function defining stage k ($n \times 1$)
$\mathbf{f}^*(k)$ = $[f_0(k), \mathbf{f}'(k)]'$ = vector function ($(n+1) \times 1$)
$H^*(k)$ = Hamiltonian
I = performance index
I^* = augmented performance index
$J(k)$ = performance function related to stage k
L = overall Lagrangian function
$L(k)$ = Lagrangian for subproblem k
N = total number of stages
$\mathbf{p}(k)$ = decomposition vector associated with stage k ($n \times 1$)
$\mathbf{u}(k)$ = control vector associated with stage $k+1$ ($r \times 1$)
$\mathbf{x}(k)$ = input state vector to stage $k+1$ ($n \times 1$)
$\mathbf{x}^*(k)$ = $[x_0(k), \mathbf{x}'(k)]'$ = state vector ($(n+1) \times 1$)
$\mathbf{z}(k)$ = adjoint vector of stage k ($n \times 1$)
$\mathbf{z}^*(k)$ = $[z_0(k), \mathbf{z}'(k)]'$ = adjoint vector ($(n+1) \times 1$)

Superscripts

* = augmented quantity
$'$ = transpose

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