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Sufficiency Conditions For Constrained Optima

Ju-Chang Huang
Missouri University of Science and Technology

Robert M. Wellek
Missouri University of Science and Technology

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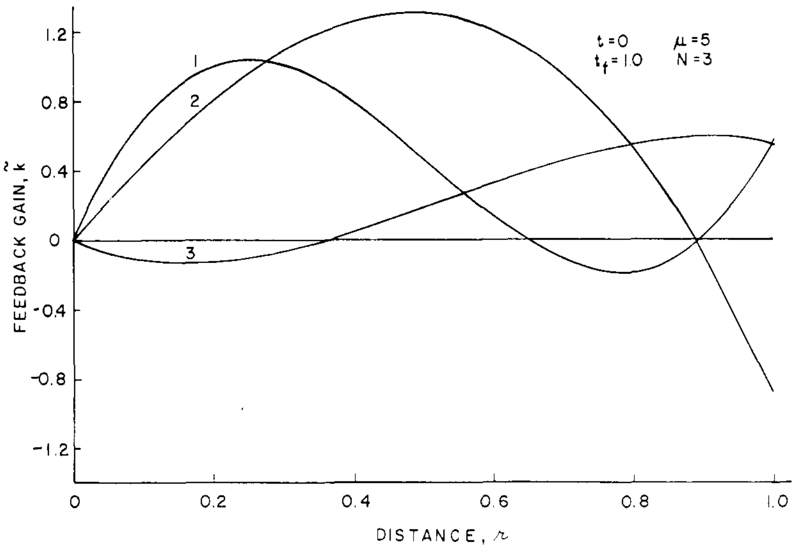

Figure 4. Near-optimal feedback gains for $N = 3$ at $t = 0$

Still another advantage of trajectory approximation when applied to linear distributed systems is that a near-optimal feedback law is obtained, which is expressed in terms of values of the state variable x at N arbitrary probe locations. As can be seen in Figures 1 and 2, three or four probes are sufficient to achieve almost complete optimality. This also demonstrates the rapid convergence of the trajectory approximation algorithm. In practice, a value of N could be selected to provide a near-optimal control in keeping with the accuracy of the model.

Finally, trajectory approximation extends readily to more complicated systems, such as those in which axial dispersion is important. Then the reduction to a lumped parameter system such as the one that Koppel and Shih (1968) describe would be impossible.

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RAYMOND L. ZAHRADNIK[1]
LEROY L. LYNN[2]

Carnegie-Mellon University
Pittsburgh, Pa. 15213

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[1] To whom correspondence should be sent.
[2] Present address, Esso Mathematics & Systems, Inc., Florham Park, N.J.

Sufficiency Conditions for Constrained Optima

Sufficiency conditions for constrained optimization problems were derived by the use of constrained second total derivatives. The results are in a simpler form than the Schechter and Beveridge relation. The sufficiency conditions of Phipps were corrected.

The sufficiency conditions for constrained optimization problems are derived through an alternate approach and result in a simpler form than in the recent work of Schechter and Beveridge (1966). The relations presented in this note can be used with equality and/or inequality constraints. The sufficiency conditions of Phipps (1952), which have been quoted for years in the literature, were corrected in this work.

Definition of Problem

The constrained optimization problem is defined in this work as to determine the optimum of an objective function the form

$$S = f(X_1, X_2, \ldots, X_n) \tag{1}$$

which is subject to m independent equality constraints

$$g^k(X_1, X_2, \ldots X_n) = 0, k = 1,2, \ldots, m \tag{2}$$

where $m < n$ and both f and g^k are continuous functions and possess partial derivatives at least through second order.

This problem can be generalized to handle problems with inequality constraints by introducing slack variables.

Methodology

The sufficiency conditions for an optimum of the problem defined above have been derived by Phipps (1952) and independently by Schechter and Beveridge (1966). These two independent works result in two different forms of sufficiency tests, the former being simpler than the latter.

This paper presents a third approach to derive the sufficiency conditions (Huang, 1968). The methodological framework of the approach can be described as follows:

Since the problem has $n - m$ degrees of freedom, we choose for convenience the first m variables, $X_1, X_2, \ldots, X_m$, as dependent variables and $X_{m+1}, X_{m+2}, \ldots, Xn$ as independent variables. From Equation 2 one obtains

$$dg^k = \sum_{l=1}^{N} g_l{}^k dX_l = 0 \qquad k = 1,2, \ldots, m \tag{3}$$

From Equation 3 we can solve dX_k, ($k = 1,2, \ldots, m$), in terms of dX_j, ($j = m + 1, m + 2, \ldots, n$), and we call the results the "constraint relations." Substituting the constraint relations into the first total derivative of the objective function, (dS), we obtain the constrained first total derivative, $(dS)_g$, and once again substituting the constraint relations into the expression of $d[(dS)_g]$ we obtain the constrained second total derivative, $(d^2S)_g$.

The above described mathematical manipulation is made possible by use of the Lagrangian function, L, defined as

$$L = f + \sum_{k=1}^{m} \lambda^k g^k \tag{4}$$

where λ^k, ($k = 1,2, \ldots, m$) are Lagrange multipliers.

Sufficiency Test

Let

$$B_p = \frac{(-1)^m}{(J^0)^2} \begin{vmatrix} 0 & \cdots & 0 & g_1{}^1 & \cdots & g^1_{m+p} \\ \vdots & & \vdots & \vdots & & \\ 0 & \cdots & 0 & g_1{}^m & \cdots & g^m_{m+p} \\ g_1{}^1 & \cdots & g_1{}^m & L_{11} & \cdots & L_{1,\, m+p} \\ \vdots & & \vdots & \vdots & & \vdots \\ g_{m+p}{}^1 & \cdots & g_{m+p}{}^m & L_{m+p,\,1} & \cdots & L_{m+p,\, m+p} \end{vmatrix} \tag{5}$$

$p = 1,2, \ldots, n - m$

where

$$L_{nl} = \frac{\partial^2 L}{\partial X_l \partial X_n}; \qquad g_l{}^k = \frac{\partial g^k}{\partial X_l}$$

$n,l = 1,2, \ldots, n \qquad k = 1,2, \ldots, m$

and

$$J^0 = J\left(\frac{g^1, g^2, \ldots g^m)}{X_1, X_2, \ldots, X_m}\right) \neq 0$$

Then the sufficiency test can be described as follows:

For a minimum, all values of B_p should be positive.

For a maximum, the B_p should alternate in sign, B_1 being negative.

If the signs of B_p do not follow either pattern, the point under investigation is not a maximum or a minimum point. If any one of the B_p is equal to zero, the optimality cannot be ascertained by use of this test.

Discussion

The above sufficiency test can be proved to be equivalent to that of Schechter and Beveridge (1966). However, the former is simpler than the latter, in that much less work is required in using the sufficiency test of this study for the formulation of the equations and computer programming, particularly in case of multivariable problems. The sufficiency test of Phipps (1952) is very similar to the results of this work except that Phipps has an error in the range of index t used by him. By comparison with the present work, Phipps' index t should range from $m + 1$ to n instead of from m to n. This error has been quoted in the literature without correction (Wilde and Beightler, 1967).

Example

To show how simple the present sufficiency test is when compared with the test of Schechter and Beveridge, let us compare them by the following example.

Minimize:

$$S = f(X_1, X_2, X_3, X_4) \tag{6}$$

with constraints

$$g_2^1(X_1, X_2, X_3, X_4) = 0 \tag{7}$$

$$g^2(X_1, X_2, X_3, X_4) = 0 \tag{8}$$

$$g^3(X_1, X_2, X_3, X_4) = 0 \tag{9}$$

The Lagrangian function is

$$L = f + \lambda^1 g^1 + \lambda^2 g^2 + \lambda^3 g^3 \tag{10}$$

where λ^1, λ^2, and λ^3 are Lagrange multipliers determined by the stationary points.

Now let us look at the sufficiency tests:

Schechter and Beveridge Sufficiency Test (1966).

Define

$$\begin{aligned}(f_{44})_g = f_{44} &+ f_1 \left(\frac{\partial^2 X_1}{\partial X_4{}^2}\right)_g + 2f_{41}\left(\frac{\partial X_1}{\partial X_4}\right)_g \\ &+ f_2 \left(\frac{\partial^2 X_2}{\partial X_4{}^2}\right)_g + 2f_{42}\left(\frac{\partial X_2}{\partial X_4}\right)_g \\ &+ f_3 \left(\frac{\partial^2 X_3}{\partial X_4{}^2}\right)_g + 2f_{43}\left(\frac{\partial X_3}{\partial X_4}\right)_g \\ &+ f_{11}\left(\frac{\partial X_1}{\partial X_4}\right)_g^2 + 2f_{12}\left(\frac{\partial X_1}{\partial X_4}\right)_g \left(\frac{\partial X_2}{\partial X_4}\right)_g \\ &+ f_{22}\left(\frac{\partial X_2}{\partial X_4}\right)_g^2 + 2f_{23}\left(\frac{\partial X_2}{\partial X_4}\right)_g \left(\frac{\partial X_3}{\partial X_4}\right)_g \\ &+ f_{33}\left(\frac{\partial X_3}{\partial X_4}\right)_g^2 + 2f_{31}\left(\frac{\partial X_3}{\partial X_4}\right)_g \left(\frac{\partial X_1}{\partial X_4}\right)_g\end{aligned}$$

where

$$\left(\frac{\partial X_1}{\partial X_4}\right)_g = -\frac{J^{14}}{J^0};\ \left(\frac{\partial X_2}{\partial X_4}\right)_g = -\frac{J^{24}}{J^0};\ \left(\frac{\partial X_3}{\partial X_4}\right)_g = -\frac{J^{34}}{J^0}$$

$$\left(\frac{\partial^2 X_1}{\partial X_4^2}\right)_g = \frac{1}{J^0}\left[d_1^{44} J\left(\frac{23}{23}\right) - d_2^{44} J\left(\frac{13}{23}\right) + d_3^{44} J\left(\frac{12}{23}\right)\right]$$

$$\left(\frac{\partial^2 \partial X_2}{\partial X_4^2}\right)_g = \frac{1}{J^0}\left[-d_1^{44} J\left(\frac{23}{13}\right) + d_2^{44} J\left(\frac{13}{13}\right) - d_3^{44} J\left(\frac{12}{13}\right)\right]$$

$$\left(\frac{\partial^2 X_3}{\partial X_4^2}\right)_g = \frac{1}{J^0}\left[d_1^{44} J\left(\frac{23}{12}\right) - d_2^{44} J\left(\frac{13}{12}\right) + d_3^{44} J\left(\frac{12}{12}\right)\right]$$

and

$$J^{14} = J\left(\frac{g^1,g^2,g^3}{X_4,X_2,X_3}\right);\ J^{24} = J\left(\frac{g^1,g^2,g^3}{X_1,X_4,X_3}\right);\ J^{34} = J\left(\frac{g^1,g^2,g^3}{X_1,X_2,X_4}\right)$$

$$J\left(\frac{ij}{rs}\right) = J\left(\frac{g^i,g^j}{X_r,X_s}\right), i,j,r,s = 1,2,3$$

$$d_k^{44} = -\left[g_{11}^k\left(\frac{\partial X_1}{\partial X_4}\right)_g + g_{22}^k\left(\frac{\partial X_2}{\partial X_4}\right)_g^2 + g_{33}^k\left(\frac{\partial X_3}{\partial X_4}\right)_g^2 + 2g_{12}^k\left(\frac{\partial X_1}{\partial X_4}\right)_g\left(\frac{\partial X_2}{\partial X_4}\right)_g + 2g_{13}^k\left(\frac{\partial X_1}{\partial X_4}\right)_g\left(\frac{\partial X_3}{\partial X_4}\right)_g + 2g_{23}^k\left(\frac{\partial X_2}{\partial X_4}\right)_g\left(\frac{\partial X_3}{\partial X_4}\right)_g\right] - 2\left[2g_{14}^k\left(\frac{\partial X_1}{\partial X_4}\right)_g + 2g_{24}^k\left(\frac{\partial X_2}{\partial X_4}\right)_g + 2g_{34}^k\left(\frac{\partial X_3}{\partial X_4}\right)_g\right] - g_{44}^k$$

$$k = 1,2,3$$

Now if $J^0 \neq$, then

$$(f_{44})_g > 0 \text{ for a minimum}$$
$$(f_{44})_g < 0 \text{ for a maximum}$$

Present Sufficiency Test.

According to Equation 5,

$$B_1 = \frac{-1}{(J^0)^2}\begin{vmatrix} 0 & 0 & 0 & g_1^1 & g_2^1 & g_3^1 & g_4^1 \\ 0 & 0 & 0 & g_1^2 & g_2^2 & g_3^3 & g_4^4 \\ 0 & 0 & 0 & g_1^3 & g_2^3 & g_3^3 & g_4^3 \\ g_1^1 & g_1^2 & g_1^3 & L_{11} & L_{12} & L_{13} & L_{14} \\ g_2^1 & g_2^2 & g_2^3 & L_{21} & L_{22} & L_{23} & L_{24} \\ g_3^1 & g_3^2 & g_3^3 & L_{31} & L_{32} & L_{33} & L_{34} \\ g_4^1 & g_4^2 & g_4^3 & L_{41} & L_{42} & L_{43} & L_{44} \end{vmatrix}$$

Now if $J^0 \neq 0$, then

$$B_1 > 0 \text{ for a minimum}$$
$$B_1 < 0 \text{ for a maximum}$$

Thus, the present sufficiency test is much simpler and more straightforward than that of Schechter and Beveridge.

It is easily seen from the above that to use the present test all one needs to do is to take derivatives of Equations 7 through 10. Determinant B_1 can be evaluated by use of a simple computer subroutine. Furthermore, in the present test the increased number of variables does not require much extra work, in either the formulation of the equations or the computer programming, as it does in the test of Schechter and Beveridge (1966).

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C. C. HUANG
R. M. WELLEK

University of Missouri—Rolla
Rolla, Mo. 65401

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Asymptotic Expression for the Efficiency of a Staged Reactor

The efficiency for a single reaction of a sequence of equal ideal stirred-tank reactors is exhibited as an asymptotic series in the reciprocal space velocity for a stage, in a form general for any analytical dependence of rate on conversion. The first three terms of the series are given in the expression

$$\frac{S_o}{S} \sim 1 + \frac{1}{2n}\ln\frac{R(x_n)}{R(0)} + \frac{S}{12n^2}\left\{R'(x_n) - R'(0) + \int_0^{x_n}\frac{[R'(x)]^2}{R(x)}dx\right\}$$

where S is the reciprocal space velocity giving conversion x_n in an n-stage reactor, $R(x)$ is the rate of the reaction when the conversion is x, and S_o is the reciprocal space velocity that would give the same conversion in an ideal plug-flow reactor.

If three conditions hold, an asymptotic expression can be derived giving the relationship between the space velocity leading to a certain conversion in a sequence of stirred vessels and the space velocity that would give the same conversion in an ideal plug-flow reactor. The conditions are that all vessels in the sequence have equal volume and temperature, and that only one stoichiometrically independent reaction is going on. The relationship is otherwise completely general, with no restrictions on the kinetics of the reaction.

The expression is derived by a formal summation of the reciprocal space velocities required in a plug-flow reactor to give the actual conversions in the several stages. The