

A pulsed column crystallizer was developed for *p*-xylene purification and showed appreciably higher capacity and efficiency when compared to conventional units (6). In addition the crystallizer was fairly simple and said to be easy to operate. This unit had solid and liquid phases moving countercurrently and had only a single stage.

The application of cycling to fluid bed reactions was reported to have two beneficial effects (5). The first was that the particle size range that could be handled was extended from a ratio of about 5 to 1 to the handling of everything from fine powders to coarse metal chips from machining operations. In addition, flow rates up to 10 times those available in steady flow systems were achieved. The pulses were timed so that the bed settled between pulses to the position it would assume during steady-state flow. A recent report presents laboratory data for the production of butadiene by dehydrogenation (8). By operating the reactor with reactant butenes pulsed into a diluent stream, conversion to butadiene far in excess of equilibrium can be achieved. Furthermore, acceptable conversions were achieved at temperatures where no measurable quantity of butadiene would be produced under conventional steady flow conditions.

The application of cycling to heat transfer was made to welding operations (7) and to film boiling (3). Welding is a particularly complicated heat transfer operation and as such makes an interesting study. The cycling nature of the operation is somewhat different from that described previously. Two power sources were used; one provided background current at a low enough level not to fuse the metal while a second pulsed unit provided current in shots with which the weld was made. The operation is especially suited to joining thin sheets of metal where the problems of maintaining an arc and not burning the metal at the same time are eliminated.

Up to 100% increases in heat transfer rate were observed when cycling was applied to stable film boiling.

There is some information available which indicates that fuel cell performance can be improved by cycling (4). The improvement is primarily an increase in lifetime of the electrodes at high current densities.

Nomenclature

H = holdup
 n = stage number
 t = time
 V = vapor flow rate
 X = mole fraction in liquid
 Y = mole fraction in vapor

Literature Cited

- (1) British Welding Research Association, *Steel* **153**, No. 8, 52 (1964).
- (2) Cannon, M. R., *Ind. Eng. Chem.* **53**, 629 (1961).
- (3) DiCicco, D. A., Schoenhels, R. J., *J. Heat Transfer* **86**, 457 (1964).
- (4) Interagency Advanced Power Group, Project Brief, Contract NAS3-2752, August 1963.
- (5) Levey, R. P., Heidt, H. M., Hamrin, C. M., Jr., 53rd National Meeting, A.I.Ch.E., Pittsburgh, Pa., May 1964.
- (6) Marwil, S. J., Kolner, S. J., *Chem. Eng. Progr.* **59**, No. 2, 60 (1963).
- (7) Robertson, D. C., M. S. thesis, The Pennsylvania State University, University Park, Pa., 1957.
- (8) Semenenko, E. I., Rojinskii, S. Z., *Kinetika i Katiliz* **5**, No. 3, 490 (1964).
- (9) Szabo, T. T., Lloyd, W. A., Cannon, M. R., Speaker, S. S., *Chem. Eng. Progr.* **60**, No. 1, 66 (1964).
- (10) Ziolkowski, Z., Filip, S., *Intern. Chem. Eng.* **3**, 433 (1963).

VERLE N. SCHRODT

Monsanto Co.
 St. Louis, Mo.

RECEIVED for review September 23, 1964
 ACCEPTED December 3, 1964

CORRESPONDENCE

DISCRETE MAXIMUM PRINCIPLE

SIR: The maximum principle of Pontryagin (11) is now a well known method of dealing with a wide class of extremal problems associated with the solution of ordinary differential equations with given initial conditions. In a particularly lucid exposition of this principle, Rozonoer (12) has pointed out that, although one might hypothesize a discrete analog of the maximum principle for difference equations rather than differential equations, such a result is invalid except in certain very special conditions which render it almost trivial. Nevertheless, in three recent papers (8, 9, 10), Katz has presented a proof of a discrete maximum principle around which a significant amount of work—some already published (1, 3, 13, 14) and some still in press—is beginning to build up. However, the purpose of this note is to reaffirm, largely by means of simple counterexamples, Rozonoer's original statement that the discrete maximum principle is invalid, and to show that the "proof" given of it is fallacious.

Firstly, we will briefly recapitulate Katz's results. He considers a system of difference equations of the form

$$x_i^n = F_i^n(x_k^{n-1}, \theta^n); (i = 1, 2, \dots, S); (n = 1, 2, \dots, N) \quad (1)$$

with given initial conditions

$$x_i^0 = a_i; (i = 1, 2, \dots, S) \quad (2)$$

It is customary and convenient to regard each Equation 1 as describing the relation between outputs and inputs for some physical unit, so that the complete set of equations describes the behavior of a sequential chain of units as shown in Figure 1. It is then required to find those values of the variables $\theta^1, \theta^2, \dots, \theta^N$ which minimize (maximize) the value of x_1^N .

The proposed solution makes use of the solutions z_i^n of a set of difference equations adjoined to Equations 1—namely

$$z_i^{n-1} = \sum_{j=1}^S \frac{\partial F_j^n}{\partial x_i^{n-1}} \cdot z_j^n; (i = 1, 2, \dots, S); (n = 1, 2, \dots, N) \quad (3)$$

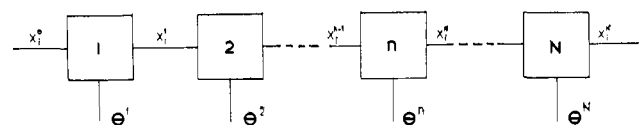


Figure 1. Sequential chain

with the terminal conditions

$$z_i^N = 1; \text{ for } i = 1 \left. \vphantom{\begin{matrix} z_i^N = 1; \text{ for } i = 1 \\ = 0 \text{ otherwise} \end{matrix}} \right\} = 0 \text{ otherwise} \quad (4)$$

It is then asserted that each θ^n should be chosen to minimize (maximize) the corresponding quantity

$$H^n = \sum_{j=1}^S z_j^n F_j^n \quad (5)$$

with the z_j^n regarded as constants from the point of view of the minimization (maximization) process.

In Katz's formulation of the problem, the functions F_j^n are assumed to be the same for each value of n and are written F_j . However, this restriction is not vital to the argument, and Fan and Wang (2, 3) derive the same result without any such assumption. Indeed it has no bearing on the validity or otherwise of the result, as we shall show.

Some doubt may be thrown on the correctness of the above algorithm by the very simple example shown in Figure 2, where the objective is to maximize x^2 . Direct elimination of x^1 shows that

$$x^2 = A - (x^0 + \theta^1)^2 - (\theta^2)^2$$

with a stationary maximum value at $\theta^1 = -x^0$, $\theta^2 = 0$, which also gives the largest value for any choice of θ^1 and θ^2 .

However, F^1 is linear in the adjustable variable θ^1 , so it is not possible to determine a value for θ^1 by the condition that

$$H^1 = \text{const. } x^1$$

should be maximized with respect to θ^1 , as would be required by the computational procedure suggested by Katz (8).

Although this may cast some doubt on the result, it is easy to see that $z^1 = 0$ for the optimal policy, so that H^1 is actually independent of θ^1 and is, in a sense, maximized for any value of θ^1 . To obtain a completely unambiguous counterexample, therefore, one must take $S = 2$, corresponding to a two-dimensional system. Consider, for example, the system shown in Figure 3, where the problem is to minimize x_1^2 with respect to θ^1 and θ^2 . By direct elimination of x_1^1 and x_2^1 , it is easily shown that

$$x_1^2 = 2 + 1/2 (\theta^1)^2 + (\theta^2)^2 \quad (6)$$

with a unique stationary minimum at $\theta^1 = \theta^2 = 0$, which also gives the smallest value of x_1^2 . This is, therefore, the solution of the problem. We now pursue Katz's proposed procedure, solving the adjointed equations backward along the chain, starting from the boundary conditions.

$$z_1^2 = 1, z_2^2 = 0$$

According to Equation 3, we then have

$$z_1^1 = \frac{\partial F_1^2}{\partial x_1^1} \cdot z_1^2 + \frac{\partial F_2^2}{\partial x_1^1} \cdot z_2^2 = 1$$

and

$$z_2^1 = \frac{\partial F_1^2}{\partial x_2^1} \cdot z_1^2 + \frac{\partial F_2^2}{\partial x_2^1} \cdot z_2^2 = 2x_2^1$$

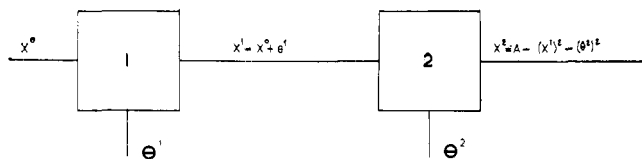


Figure 2. One-dimensional example

H^1 can then be written down by substituting into Equation 5, giving

$$H^1 = z_1^1 \left[1 - 2\theta^1 - \frac{1}{2} (\theta^1)^2 \right] + z_2^1 (1 + \theta^1)$$

where

$$\frac{\partial H^1}{\partial \theta^1} = (z_2^1 - 2z_1^1) - z_1^1 \theta^1 \text{ and } \frac{\partial^2 H^1}{\partial (\theta^1)^2} = -z_1^1 = -1$$

using the value of z_1^1 found above. It is seen that $\partial^2 H^1 / \partial (\theta^1)^2$ is negative for all values of θ^1 , so it follows that H^1 can never be minimized with respect to θ^1 , as would be required by Katz's principle expressed in Equation 5. Indeed the values $\theta^1 = \theta^2 = 0$ and the corresponding solutions $x_1^1 = x_2^1 = 1$, $z_1^1 = 1$, $z_2^1 = 2$, which have been shown by direct calculation (Equation 6) to minimize x_1^2 , actually maximize H^1 in direct contradiction of Katz's algorithm.

In this simple counterexample the functions F_i^n are different for different values of n . It remains to demonstrate the truth of the assertion made above that Katz's result remains invalid even if all the functions F_i^n are the same, as in his original derivation. We shall do this by showing that, from any S dimensional counterexample, it is possible to generate an $(S + 1)$ dimensional counterexample in which all the functions F_i^n are the same.

Consider then an example in S dimensions with state variables

$$x_i^n \quad (i = 1, 2, \dots, S); \quad (n = 1, 2, \dots, N)$$

and recurrence relations $x_i^n = F_i^n(x_k^{n-1}, \theta^n)$, with boundary conditions x_i^0 given, and suppose that this contradicts Katz's result in the same way as the example just quoted, and is therefore a counterexample. Let us call it Example I.

Now introduce a second example (Example II) with $S + 1$ dimensions and recurrence relations

$$x_i^n = G_i(x_k^{n-1}, \theta^n) \quad (7)$$

with the functions G_i independent of n . The functions G_i of any $S + 1$ variables, $\xi_1, \xi_2, \dots, \xi_{S+1}$ are defined by the following relations:

$$\left. \begin{aligned} G_i(\xi_1, \dots, \xi_{S+1}) &= \sum_{m=1}^N \phi_m(\xi_{S+1}) F_i^m(\xi_1, \dots, \xi_S, \theta); \quad (i = 1, \dots, S) \\ G_{S+1}(\xi_1, \dots, \xi_{S+1}) &= \xi_{S+1} + 1 \end{aligned} \right\} \quad (8)$$

where the functions ϕ_m have the following properties

$$\left. \begin{aligned} \text{(i)} \quad \phi_m(x) &= 1 \quad (x = \text{integer} = m) \\ \text{(ii)} \quad \phi_m(x) &= 0 \quad (x = \text{integer} \neq m \text{ and } 1 \leq x \leq N) \\ \text{(iii)} \quad \phi_m(x) &\text{arbitrary for other values of } x. \end{aligned} \right\} \quad (9)$$

There are many such sets of functions—for example,

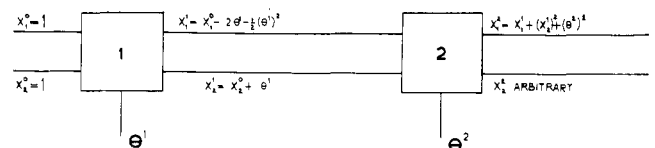


Figure 3. Two-dimensional example

$$\phi_m(x) = \frac{(x-1)(x-2)\dots(x-m+1)(x-m-1)\dots(x-N)}{(m-1)(m-2)\dots(m-m+1)(m-m-1)\dots(m-N)}$$

The boundary conditions for the recurrence relations (Equation 7) are x_i^0 , the same as those given for Example I

$$\text{and} \quad \left. \begin{matrix} (i=1, 2, \dots, S) \\ x_{S+1}^0 = 1 \end{matrix} \right\} \quad (10)$$

Putting $\xi_1 \dots \xi_{S+1}$ equal to $x_1^{n-1}, \dots, x_{S+1}^{n-1}$ in Equations 8 and substituting into Equation 7, it follows on taking account of Equation 9 that only one term in the sum over m retains a nonzero value—namely, the term $m = n$ —so we have

$$\left. \begin{matrix} x_i^n = F_i^n(x_k^{n-1}, \theta^n); (i=1, 2, \dots, S) \\ x_{S+1}^n = x_{S+1}^{n-1} + 1 \end{matrix} \right\} \quad (11)$$

Thus the variables $x_i^n (i=1, \dots, S)$ take the same values in Example II as in Example I. It follows that identical values of $\theta^1, \theta^2, \dots, \theta^N$ in the two examples give identical values of x_1^N , so the same set of values of the θ 's minimizes (maximizes) x_1^N in both cases. Similarly it can be shown that the adjoined variables $z_j^n (j=1, 2, \dots, S)$ are identical in Examples I and II, so the function

$$H_{II}^n = \sum_{j=1}^{S+1} z_j^n G_j = \sum_{j=1}^S z_j^n F_j^n + z_{S+1}^n G_{S+1}$$

for Example II differs from the function

$$H_I^n = \sum_{j=1}^S z_j^n F_j^n$$

for Example I only by the term $z_{S+1}^n G_{S+1}$, which is independent of the adjustable variables $\theta^1, \theta^2, \dots, \theta^N$. Thus, if a set of values of $\theta^1, \dots, \theta^N$ which minimizes x_1^N also maximizes some H^n in Example I, thus contradicting Katz's result, the same will be true in Example II. Example II is therefore a counterexample if Example I is, and furthermore Example II has the same recurrence relations at all stages, thus proving our assertion.

Though Katz's discrete maximum principle is false, as has now been demonstrated, what he refers to as his "weaker algorithm" is true. This states merely that x_1^N takes a stationary value with respect to variations in $\theta^1, \theta^2, \dots, \theta^N$ if and only if each of the functions H^n takes a stationary value, and makes no comment on the relation between the natures of these stationary values. This result was earlier derived and used by the first of the present writers (4). The extension of Katz's results by Fan and Wang (2, 3) to systems topologically more complex than a simple sequential chain is also false, but once again a weaker algorithm relating stationary values is true, and was published by the second of the present writers (6, 7).

The fallacy in the proofs given by Katz and by Fan and Wang lies in the attempt to deduce the natures of stationary values from a consideration of first-order variations only, and the results obtained are simply consequences of a confusion in orders of magnitude of small quantities. The natures of

stationary values of the objective function and of the functions H^n are determined, of course, by Hessian matrices of second derivatives with respect to the variables $\theta^1, \theta^2, \dots, \theta^N$. Indeed, there is no difficulty in writing down the Hessian for variations of x_1^N and hence deducing correctly the nature of a stationary value of x_1^N , as is shown in more detail in another publication (5), in which we also investigate certain special circumstances in which a stronger result is true. Very briefly, we may enumerate these cases here.

In order that x_1^N should take a stationary minimum (maximum) value with respect to variations in $\theta^1, \dots, \theta^N$, it is necessary and sufficient that each function H^n should take a stationary minimum (maximum) value with respect to the same variables in the following circumstances.

A. When the functions $F_i^n(x_k^{n-1}, \theta^n)$ take the special form

$$F_i^n(x_k^{n-1}, \theta^n) = \sum_k \alpha_{ik}^n x_k^{n-1} + f_i^n(\theta^n)$$

where the α_{ik}^n are constants. This is the case quoted by Rozonoer (12).

B. When $S = 1$, in other words when there is only one x -variable at each stage [though there are exceptions in this case, as is discussed elsewhere (5)]. The condition is also necessary, but not sufficient, if the functions F_i^n are linear in the variables x_k^{n-1} , but the coefficients may depend on the θ 's.

These results refer to relations between local minima (maxima) of x_1^N and local minima (maxima) of the functions H^n . Pontryagin's principle is a more powerful result relating the absolute minimum (maximum) of x_1^N with absolute minima (maxima) of the H^n , and this is valid only in the case A above, as was asserted by Rozonoer.

Literature Cited

- (1) Fan, L. T., "Optimization of Multistage Heat Exchanger System by the Discrete Maximum Principle," Kansas State Univ., Eng. Expt. Sta., Spec. Rept., 1964.
- (2) Fan, L. T., Wang, C. S., *J. Electron. Control* **16**, 441 (1964).
- (3) Fan, L. T., Wang, C. S., *J. Soc. Ind. Appl. Math.* **12**, 226 (1964).
- (4) Horn, F., *Chem. Eng. Sci.* **15**, 176 (1961).
- (5) Horn, F., Jackson, R., *J. Electron. Control* (in press).
- (6) Jackson, R., *Chem. Eng. Sci.* **19**, 19 (1964).
- (7) *Ibid.*, p. 253.
- (8) Katz, S., *IND. ENG. CHEM. FUNDAMENTALS* **1**, 226 (1962).
- (9) Katz, S., *J. Electron. Control* **13**, 179 (1962).
- (10) *Ibid.*, **16**, 189 (1964).
- (11) Pontryagin, L. S., *Uspekhi. Mat. Nauk* **14**, 3 (1959).
- (12) Rozonoer, L. I., *Automation & Remote Control* **20**, 1288, 1405, 1517 (1959).
- (13) Wang, C. S., Fan, L. T., *IND. ENG. CHEM. FUNDAMENTALS* **3**, 38 (1964).
- (14) Zahradnik, R. L., Archer, D. H., *Ibid.*, **2**, 238 (1963).

F. Horn

Imperial College of Science & Technology
Prince Consort Rd.
South Kensington, London, England

R. Jackson

University of Edinburgh and Heriot-Watt College
Chambers St.
Edinburgh, Scotland