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THE LINEAR-LOGARITHMIC PROGRAMMING PROBLEM

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SANTA MONICA • CALIFORNIA

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PREFACE

The linear-logarithmic programming method documented in this Memorandum was developed to handle chemical equilibrium problems in computer modeling. It forms a part of the continuing program of research at The RAND Corporation in medicine and biology [1,2], and was motivated primarily in conjunction with the work of J. C. DeHaven and E. C. DeLand in modeling biological and physiological processes.

The particular method may also be useful in other modeling applications in which linear and logarithmic terms are present.

SUMMARY

In this Memorandum is developed the algebraic solution of the linear-logarithmic programming problem, derived by means of Lagrange multipliers. Then, two numerical methods for solving the problem are given, one of which is a generalization of a method previously used [3] to solve the chemical equilibrium problem. Convergence has not been proven for either of these methods; however, a number of large chemical equilibrium problems have been solved using one or both of the methods.

THE LINEAR-LOGARITHMIC PROGRAMMING PROBLEM

We wish to consider the problem of minimizing

$$\phi = \sum_{j=1}^{N} x_j (c_j + d_j \log x_j) \qquad (1)$$

while satisfying the constraints

$$\sum_{j=1}^{N} a_{ij} x_j - b_i = 0 \; ; \qquad i = 1,2,3,\ldots,M \quad (2)$$

where a_{ij}, b_i, c_j, d_j, are constants and x_j are unknowns.

If all d_j are zero, we have a linear programming problem--the case that we consider here is when none of the d_j are zero. Using the Lagrange multiplier method of solving the problem, we set

$$L = \phi + \sum_{i=1}^{M} \pi_i \left(\sum_{j=1}^{N} a_{ij} x_j - b_i \right).$$

A local extremum is obtained if

$$\frac{\partial L}{\partial x_j} = 0; \qquad j = 1,2,3,\ldots,N$$

or

$$c_j + d_j \log x_j + d_j + \sum_{i=1}^{M} \pi_i a_{ij} = 0; \qquad (3)$$

$$j = 1,2,3,\ldots,N.$$

Solving (3) we have

$$\log x_j = \frac{-c_j - d_j - \sum_{i=1}^{M} \pi_i a_{ij}}{d_j} ; \qquad (4)$$

$$j = 1,2,3,\ldots,N$$

or,

$$x_j = \exp\left\{ \frac{-c_j - d_j - \sum_{i=1}^{M} \pi_i a_{ij}}{d_j} \right\} ; \qquad (5)$$

$$j = 1,2,3,\ldots,N.$$

Note that for (5) to be a solution of the problem, we must have all $x_j > 0$. Let us thus assume that all $x_j > 0$. The problem then reduces to that of determining M π_i's so that the x_j from (5) satisfy (2). Equivalently, the M + N equations in (2) and (5) must be satisfied simultaneously by proper choice of the N unknown x_j and the M unknown π_i.

Since (5) is non-linear, we cannot solve it directly, but must resort to approximation schemes. We now consider two methods of approximating the solution.

METHOD 1 (Delta-X Method)

Suppose we have an estimate of the x_j which may or may not satisfy (2). Let us denote the estimate by y_j. Then, the Taylor expansion of log x_j about y_j is

$$\log x_j = \log y_j + \frac{1}{y_j}(x_j - y_j) + \text{higher order terms.}$$

Dropping the higher order terms, we have

$$\log x_j \approx \log y_j + \frac{x_j}{y_j} - 1. \tag{6}$$

Substituting (6) in (4), we have

$$\log y_j + \frac{x_j}{y_j} - 1 \approx \frac{-c_j - d_j - \sum_{i=1}^{M} \pi_i a_{ij}}{d_j}$$

or,

$$x_j = -y_j \left[\log y_j + \frac{c_j + \sum_{i=1}^{M} \pi_i a_{ij}}{d_j} \right]. \tag{7}$$

Substituting (7) in (2), we have

$$\sum_{\ell=1}^{M} \left(\sum_{j=1}^{N} \frac{a_{ij} a_{\ell j} y_j}{d_j} \right) \pi_\ell = -b_i - \sum_{j=1}^{N} a_{ij} y_j \left(\log y_j + \frac{c_j}{d_j} \right);$$

$$i = 1, 2, 3, \ldots, M.$$

Letting

$$r_{i\ell} = \sum_{j=1}^{N} \frac{a_{ij}\, a_{\ell j}\, y_j}{d_j}$$

$$S_i = -b_i - \sum_{j=1}^{N} a_{ij}\, y_j \left(\log y_i + \frac{c_j}{d_j} \right),$$

we have

$$\sum_{\ell=1}^{M} r_{i\ell}\pi_\ell = S_i; \qquad i = 1, 2, 3, \ldots, M. \qquad (8)$$

To solve the problem we do the following: Solve (8) for the M unknown π_ℓ and substitute in (7) to get x_j. Then set $y_j = x_j$ and repeat the process. When the change in x_j becomes negligible, we have reached a solution.

METHOD 2 (Delta-π Method)

In this method we assume that we have an approximation to the M π_i's. Substituting these π_i into (5) we get values for x_j. Now, rewrite (2) as

$$g_i = \sum_{j=1}^{N} a_{ij}\, x_j - b_i; \qquad i = 1, 2, 3, \ldots, M. \qquad (9)$$

Substituting the above x_j into (9), we calculate the g_i. If $g_i = 0$, all i, we have a solution.

Since, in general, this will not be the case, we wish to change π_i so that $g_i \longrightarrow 0$. With this in mind, we compute,

$$\frac{\partial g_\ell}{\partial \pi_i} = \frac{\partial}{\partial \pi_i}\left[\sum_{j=1}^{N} a_{\ell j}\; x_j - b_\ell\right] = \sum_{j=1}^{N} a_{\ell j}\; \frac{\partial x_j}{\partial \pi_i}$$

$$= \sum_{j=1}^{N} a_{\ell j}\; \frac{\partial}{\partial \pi_i}\left[\exp\; \frac{-c_j - d_j - \sum_{k=1}^{M} \pi_k\, a_{kj}}{d_j}\right]$$

$$= - \sum_{j=1}^{N} \frac{a_{\ell j}\; x_j\; a_{ij}}{d_j}\;. \tag{10}$$

Denoting the new values of π_i by $\pi_i{}'$ and $P_i = \pi_i{}' - \pi_i$, we may write

$$dg_\ell = \sum_{i=1}^{M} \frac{\partial g_\ell}{\partial \pi_i}\; dP_i\,. \tag{11}$$

Now, approximating dg_ℓ by $-g_\ell$ and letting

$$r_{\ell i} = - \frac{\partial g_\ell}{\partial \pi_i} = \sum_{j=1}^{N} \frac{a_{\ell j}\; x_j\; a_{ij}}{d_j}$$

we have

$$\sum_{i=1}^{M} r_{\ell i} P_i = g_\ell; \qquad \ell = 1,\ldots,M. \tag{12}$$

Here we have M unknown P_i and M equations. The algorithm then is as follows: Substitute the π_ℓ into (5) to get x_j. Substitute these x_j into (9) to get g_i. If these g_i are small, we are done; otherwise, compute $r_{i\ell}$ and solve (12) for P_i. Then change π_i to π_i+P_i and repeat the process.

THE CHEMICAL EQUILIBRIUM PROBLEM

In the chemical equilibrium problem [1], the variables x_j are partitioned into a number of "compartments." For simplicity, let us say that $x_1, x_2, \ldots, x_{n_1}$ are in compartment 1; $x_{n_1+1}, x_{n_1+2}, \ldots, x_{n_2}$ are in compartment 2, $\ldots$; $x_{n_{p-1}+1}, x_{n_{p-2}+2}, \ldots, x_{n_p}$ are in compartment p, where $n_p = n$.

Define $\bar{x}_k = \sum_{j=n_{k-1}+1}^{n_k} x_j$, so $\bar{x}_k$ is the sum of the x_j's in compartment k. Define σ_j so that if j is in the kth compartment, $\sigma_j = \bar{x}_k$. Then the chemical equilibrium problem is to minimize

$$\phi = \sum_{j=1}^{n} x_j \left(c_j + \log \frac{x_j}{\sigma_j} \right) \tag{13}$$

while satisfying

$$\sum_{j=1}^{n} a_{ij} x_j - b_i = 0; \qquad i = 1, 2, 3, \ldots m. \tag{14}$$

To get (13) in the form (1), we add p equations,

$$\sum_{j=n_{k-1}+1}^{n_k} x_j - \bar{x}_k = 0, \text{ where}$$

$\bar{x}_k$ is now the $(n+k)^{th}$ variable and we have a total of $n + p = N$ variables and $m + p = M$ equations. Rewriting (13),

$$\phi = \sum_{j=1}^{n} x_j (c_j + \log \frac{x_j}{\sigma_j})$$

$$= \sum_{j=1}^{n} x_j (c_j + \log x_j) - \sum_{j=1}^{n} x_j \log \sigma_j$$

$$= \sum_{j=1}^{n} x_j (c_j + \log x_j) - \sum_{j=n+1}^{N} x_j \log x_j . \tag{15}$$

Thus, (15) takes the form (1) with $d_j = \pm 1$. Now either Method 1 or Method 2 may be applied to solve the problem. Method 1 turns out to be essentially the method used by White, et al., [3] to solve the problem.

CONVERGENCE

The methods as given above do not, in general, converge. It is necessary that all $x_j > 0$ for either of the methods to work. Furthermore, no x_j may get too close to zero enroute to the solution. At present, we are conducting experiments with the chemical equilibrium model to find ways of assuring convergence. At this point we can only indicate possible areas of difficulty.

In Method 2, if our π_i guesses are not good, the P_i computed by (12) may be large enough so that when the x_j are computed, some x_j is smaller than the smallest number available in the computer and this will cause that x_j to be taken as zero. This may be somewhat alleviated by computing $P_{max} = \max \{P_i\}$ and then dividing P_i by some multiple of P_{max}. This prevents P_i from exceeding some arbitrary value, and hence, prevents x_j from going to zero.

In Method 1, the computed difference $x_j - y_j$ may be large enough (in absolute value) so that some x_j becomes negative. Here again, we may attenuate the distance that we move in one iteration by dividing $x_j - y_j$ by some number that exceeds unity. In either case, there is no assurance that we won't oscillate around a possible solution. Our experience thus far has indicated that Method 1 may be best for starting the solution and that Method 2 works better when we are close to the solution.

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