A Matrix Method for Location of Cycles of a Directed Graph

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A matrix method is given for determining the nests of cycles of a directed graph. This has been applied to determining the recycle loops of a chemical process flow diagram.

The problem of finding the nests of cycles in a directed graph arose in developing a generalized heat and material balancing program (*6*). This connection will be illustrated in the example at the end of the paper.

The method developed here uses the matrix associated with a graph (*1*). It has been programmed and incorporated into the input and initiation phase of the generalized heat and material balancing program.

A directed graph consists of nodes denoted by $1, \ldots, n$ and directed arcs joining certain pairs of nodes. Define the matrix $A = (a_{ij})$ associated with a directed graph as follows: $a_{ij} = 1$ if there exists an arc going from node i to node j; otherwise $a_{ij} = 0$. Thus, the network of Figure 1 gives rise to the associated matrix A shown in Figure 2.

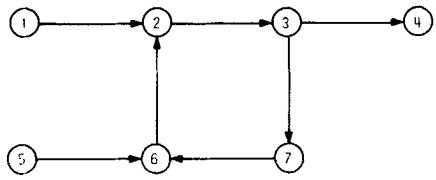

Fig. 1. A directed graph *G*.

A is used by Prosser (*5*) and Marimont (*4*) to examine the connectivity and "reactability" of parts of a computer program logical flow sheet. Harary (*3*) gives to A the name "adjacency matrix" and shows its usefulness in matrix inversion. A recent article by Chen (*2*) deals with the same subject.

The rule for matrix multiplications results in a useful property of the matrix A. It is stated here as a theorem. A proof has been given by Berge (*1*, p. 127, Corollary 1).

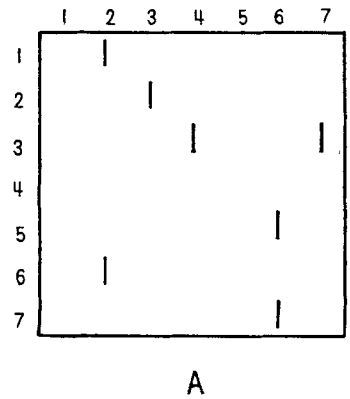

Fig. 2. Matrix *A* associated with graph *G*.

THEOREM

If A is the matrix associated with a directed graph, then the coefficient h_{ij} of the matrix $H = A^{\lambda}$ is equal to the number of distinct paths involving $(\lambda + 1)$ nodes going from node i to node j.

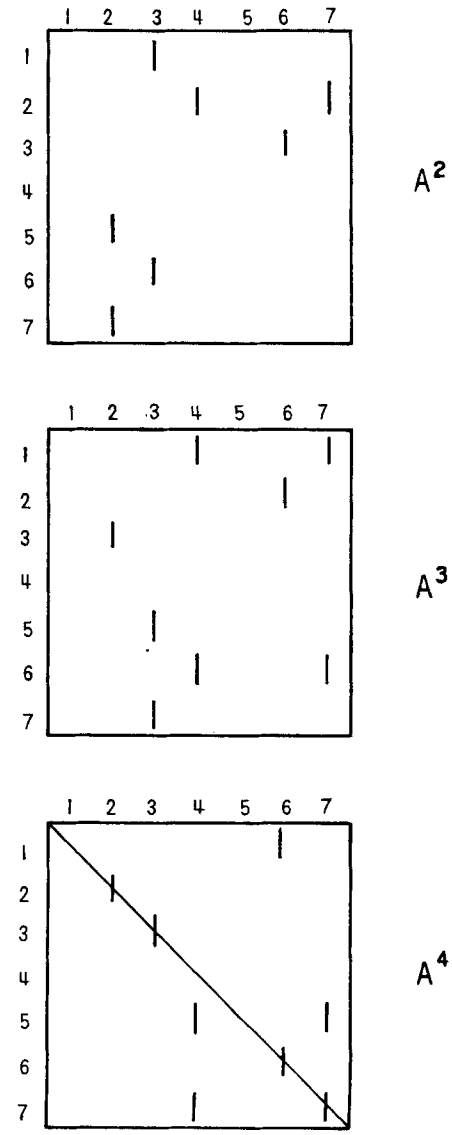

Fig. 3. Successive powers of associated matrix of graph *G*.

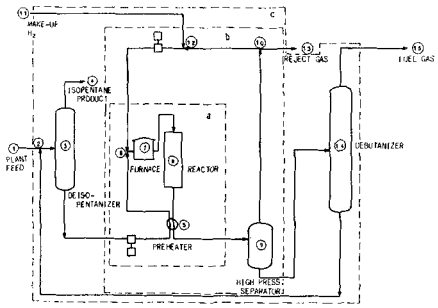

Fig. 4. Simplified flow sheet of a pentane isomerization plant.

PROOF

If it is true that in matrix $G = A^{\lambda-1}$, g_{kj} is the number of λ-node paths going from k to j, then the product $a_{ik} \cdot g_{kj}$ indicates the number of $(\lambda + 1)$-node paths going from i to j which start with an arc from i to k. Summing overall possible intermediate nodes k gives the total of all $(\lambda + 1)$-node paths going from i to j:

$$\sum_{k=1}^{n} a_{ik} \cdot g_{kj}$$

This is the general coefficient h_{ij} of the matrix $H = A \cdot G = A^{\lambda}$.

For $\lambda = 1$, the statement is true by the definition of A. From the above, if it is true for $\lambda - 1$, then it is also true for λ; thus, by induction, the theorem is shown to be true for $\lambda > 0$.

APPLICATION OF THEOREM

If one now forms the successive powers of the matrix A of Figure 2, one can observe the practical results of the theorem. Note, for example, that in A^2 of Figure 3 the element with $i = 1$, $j = 3$, is a 1. This indicates a three-node path going from node 1 to node 3. This may be observed in Figure 1.

A^3 contains information about all four-node paths in the network; A^4 contains information about all five-node paths. There are elements on the major diagonal of A^4 at positions 2, 3, 6, and 7. This indicates that five-node paths go from each of the indicated nodes to itself or a cycle. Each element of the diagonal of A^4 is a member of the cycle shown in the network of Figure 1.

MULTIPLE LOOP NETWORKS

When a cycle has been located, it can be replaced by a pseudo node. One is interested only in the relation of the cycle as a whole with the rest of the network. Thus, change the basic matrix A to remove all reference to the individual members of the cycle. In place of the rows and columns corresponding to these nodes, insert one row and one column corresponding to the cycle, and in these place all information concerning connections between nodes external to the cycle and nodes in the cycle.

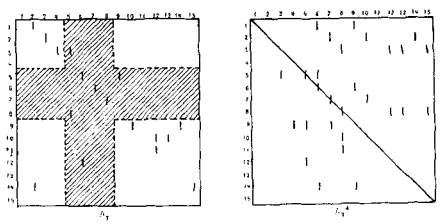

Fig. 5. First associated matrix of pentane isomerization plant graph.

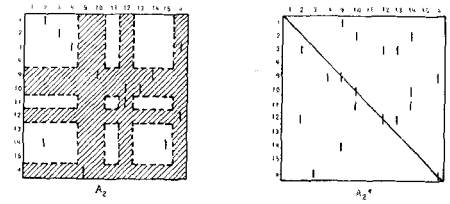

Fig. 6. Second associated matrix of pentane isomerization plant graph.

If this modification is not performed, cycles corresponding to multiple passage around the cycle will appear. For example, if a three-member cycle appears, it will, if not contracted to a node, give rise to six-member cycle, a nine-member cycle, etc.

Since there is a finite number of nodes in the network, this process will terminate with a zero matrix when all cycles will have been removed and $\lambda - 1$ is equal to the number of nodes in the longest path left in the network.

MULTIPLE LOOPS OF THE SAME SIZE

Several cycles of the same size may exist in a given network. This will occur during the procedure if and only if the sum of the diagonal elements of A^{λ} is greater than the power λ (in fact, the sum will be a multiple of λ).

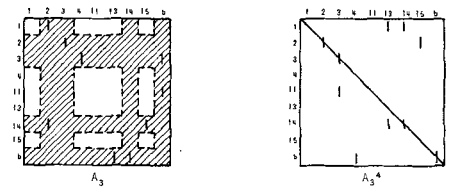

Fig. 7. Third associated matrix of pentane isomerization plant graph.

If any diagonal elements are greater than 1, it means that the corresponding nodes are involved in more than one cycle.

The procedure used to sort out the cycles is as follows: The base matrix A is searched for an $a_{ij} = 1$ such that A^{λ} has positive elements at positions i and j on the diagonal. Matrix B is constructed identical to A but with this $a_{ij} = 0$. The matrix B^{λ} is computed, and the diagonal elements are then substracted from those of A^{λ}. The difference will be a set of positive entries in the locations referring to the members of any cycles which were destroyed by removal of the arc. If there are more than two cycles, the process is repeated on B or else on A with a different element removed. This procedure is repeated until all cycles have been identified.

AN EXAMPLE

Figure 4 is the simplified flow sheet of a pentane isomerization plant. In Figure 5, the base case matrix A_1 is constructed to describe the two-node paths in the flow sheet. From A_1^4, a cycle consisting of nodes 5, 6, 7, and 8

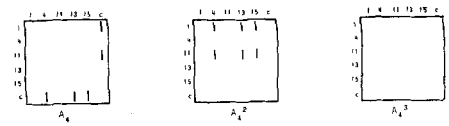

Fig. 8. Final associated matrix of pentane isomerization plant graph.

is located. A_1 is partitioned as shown by the cross hatching and modified to produce the second base case A_2 of Figure 6. The cycle is now pseudo node a indicated in Figure 4.

Operations are continued up to A_2^4 when another cycle is located consisting of nodes 9, 10, 12, and pseudo node a. A_2 is partitioned and modified to produce the next base case matrix A_3 of Figure 7. The new cycle is now pseudo node b shown again in Figure 4.

Powers of A_3 are computed until with A_3^4 another cycle is found consisting of nodes 2, 3, 14, and pseudo node b. The matrix is changed again to produce A_4 of Figure 8.

As before, the matrix multiplications are carried out until the zero matrix A_4^3 appears. This indicates that there are no paths involving four or more modules left in the simplified scheme and, therefore, no possibility of additional cycles. This terminates the procedure.

ACKNOWLEDGMENT

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The Effect of Concentration on Diffusion Coefficient in Polymer Solutions

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A microinterferometric method was used to measure the diffusion coefficient as a function of concentration in the system dimethylformamide-polyacrylonitrile at 25°C. The diffusion coefficient increases with increasing polymer concentration up to the maximum employed, 17.72% by weight. The theoretical basis for this type of behavior is explained. The diffusion coefficient in the limit as the polymer concentration approaches zero was calculated from theory to be 0.30×10^{-6} sq.cm./sec. This value is consistent with the diffusion coefficients obtained experimentally.

Mass transfer operations involving polymer solutions are often controlled by molecular diffusion. However, values of the diffusion coefficient are usually lacking. Furthermore, since diffusion coefficients in polymeric systems are frequently very concentration dependent, it is important to include this dependence in mathematical representations of diffusional processes.

In a solution of flexible chain molecules so dilute that interactions between the macromolecules may be neglected, it has been shown that the diffusing polymer molecule may be represented by an equivalent hydrodynamic sphere. It has furthermore been established that the effective diameter of this sphere is proportional to the root-mean-square distance between chain ends for linear molecules. This model has permitted diffusion coefficients at infinite dilution to be calculated from the molecular weight of the polymer, the intrinsic viscosity of the polymer-solvent system, and the viscosity of the solvent (*11*).

A statistical treatment of dilute polymer solutions (*8*) has led to the development of an equation representing the concentration dependence of the diffusion coefficient when the domains of the polymer molecules do not overlap (*10*). As the volume in space occupied by a polymer molecule may be several hundred times its molecular volume (*7*), appreciable entanglement and overlapping can occur at polymer concentrations as low as a few tenths of 1%.

Since diffusion in polymer solutions exhibiting extensive overlapping of adjacent, mobile, polymer molecules has received very little attention, the present study was initiated.

EXPERIMENTAL METHOD, APPARATUS, AND PROCEDURE

Diffusion coefficients for the system dimethylformamide-polyacrylonitrile were determined at 25°C. by a microinterferometric method. The procedure was adapted from methods used for studying concentration profiles around growing crystals (*1, 2*), for measurement of local viscosities (*13*), and for studies of diffusion (*5, 14, 16*). The experimental apparatus is shown in Figure 1. Light from a sodium lamp is passed through a collimating lens and a filter, which isolates the D line (589 mμ). The monochromatic light passes upward through the diffusion cell and into the objective lens of a microscope. The diffusion cell consists of two partially metallized, plate glass microscope slides separated by a spacer at one end to form a wedge. The slides (3 × 1 × ⅛ in.) were coated on one side with aluminum by vacuum evaporation so that they were partly transmitting and partly reflecting to light. The light passing through the wedge produces interference fringes that may be viewed through the eyepiece of the microscope.