On Nonnegative Factorization of Matrices

M. Kaykobad
School of Mathematical Sciences
Flinders University
Bedford Park, S.A. 5042, Australia

Submitted by Thomas J. Laffey

ABSTRACT

It is shown that a sufficient condition for a nonnegative real symmetric matrix to be completely positive is that the matrix is diagonally dominant.

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1. INTRODUCTION

A number of authors have discussed the problem of deriving conditions for a given matrix to be completely positive [3,4,7]. The purpose of this paper is to establish a set of "easily verifiable" sufficient conditions for a given matrix to be completely positive and provide an algorithm for factorization of such matrices.

A real $n \times n$ symmetric matrix A is called completely positive if A can be factored as BB^t for some $n \times m$ nonnegative real matrix B for $m < \infty$ (here t denotes transpose). Results of Diananda [1] and Hall and Newman [3] on quadratic forms show that a nonnegative factorization of a nonnegative positive semidefinite $n \times n$ matrix is possible when $n \leq 4$. Furthermore, for any completely positive matrix, a nonnegative factorization with $m \leq 2^n$ was constructed by Hall and Newman [3]. Hannah and Laffey [4] have found a better bound for m. They have shown that there exists a factorization with $m \leq \frac{1}{2}k(k+1) - N$, where $2N$ is the maximal number of off-diagonal entries which equal zero in a nonsingular principal submatrix of A, and k is the rank of the matrix A. In general for $n \geq 5$, it was shown by Horn (see [1]) and Gray and Wilson [2] that such a nonnegative factorization does not exist.

Interest in work on nonnegative factorization came from the theory of inequalities, the study of block designs in combinatorics, and the context of

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association in random vectors. Gray and Wilson [2] studied a mathematical model of energy demand for certain sectors of the U.S. economy, wherein $A = B^tB$, and elements of B are parameters and should satisfy nonnegativity constraints because of their physical interpretation.

Hannah and Laffey [4] remarked that no general necessary and sufficient conditions for A to be completely positive are known. Some special results in this respect were obtained by Markham [7] and Lau and Markham [6]. In our work we will present a set of easily verifiable sufficient conditions for nonnegative positive semidefinite symmetric matrices to be completely positive. Also we will give an algorithm for constructing the factorization, associating the given matrix with a graph.

2. PRELIMINARIES

An $n \times m$ matrix B is said to be a vertex-edge incidence matrix if there exists a graph G such that

$$b_{i(i,j)} = \begin{cases} 1 & \text{if vertex } i \text{ is incident at edge } (i, j) \text{ in } G, \\ 0 & \text{otherwise.} \end{cases}$$

We refer to Harary [5] for definitions of graphical terminology.

BB^t is a nonnegative positive semidefinite symmetric matrix. In fact, $A - D(A)$ is an adjacency matrix of the graph G, where $D(A)$ is a diagonal matrix with the diagonal entries of A. The diagonal entries a_{ii} are the node degrees of vertex i, $i = 1, \dots, n$. If the entries of B are any nonnegative numbers, then B is said to be a weighted vertex-edge incidence matrix, and $b_{i(i,j)}$ is referred to as the length of edge (i, j). $A = BB^t$ implies the existence of column vectors $\beta_k \geq 0$, $k = 1, \dots, m$, such that $A = \sum_{k=1}^{m} \beta_k \beta_k^t$.

3. THE MAIN RESULT

A square matrix $P = (p_{ij})$ is called diagonally dominant if $p_{ii} \geq \sum_{j \neq i}^{n} |p_{ij}|$. Our main result is formulated as follows:

THEOREM 1. *Let A be a nonnegative diagonally dominant symmetric matrix. Then A is completely positive.*

Proof. We prove this theorem by constructing a factorization of an arbitrary diagonally dominant symmetric matrix A. We relate a multigraph $G=(V,E)$ to the matrix in the following way: Row i and column i of the matrix A correspond to vertex $i \in V$. Vertex i is connected to vertex j if $a_{ij}>0$, $i \neq j$. Vertex i is connected to itself by a loop if $a_i = a_{ii} - \sum_{j \neq i} a_{ij} > 0$. For each positive a_{ij} there is an edge $(i,j) \in E$. The set E also includes loops. To each edge (i,j) we associate a number $b_{i(i,j)} = \sqrt{a_{ij}}$ if $i \neq j$; otherwise $b_{i(i,i)} = \sqrt{a_i}$. Now construct the weighted vertex-edge incidence matrix B (vertex corresponds to row, and edge corresponds to column) of the graph G. Clearly, we will have exactly two positive entries in each column corresponding to edges which are not loops. For loops we have a single entry, since a loop is incident at a a single vertex. Then we have

$$(BB^t)_{ij} = \sum_{k\,(i,k) \in E} b_{i(i,k)} b_{j(i,k)}.$$

Now $b_{j(i,k)}$ is positive only if edge (i,k) is incident on vertex j, that is, either $i=j$ or $k=j$. Thus

$$(BB^t)_{ij} = b_{i(i,j)} b_{j(i,j)} = a_{ij} \qquad \text{for} \quad i \neq j$$

$$(BB^t)_{ii} = \sum_{i\,|\,(i,k) \in E} b_{i(i,k)} b_{i(i,k)} = \sum_{j \neq i} a_{ij} + a_i$$

$$= \sum_{j \neq i} a_{ij} + a_{ii} - \sum_{j \neq i} a_{ij} = a_{ii} \qquad \text{for} \quad i \in V.$$

This proves that $BB^t = A$. ∎

This result can obviously be generalized as in the following theorem:

THEOREM 2. *Let $C = PAP^t$ with $P \geq 0$, and A be a nonnegative diagonally dominant symmetric matrix. Then C is completely positive.*

Proof. Since A is completely positive by virtue of Theorem 1, we have

$$C = PAP^t = PBB^tP^t = (PB)(PB)^t.$$

As both P and B are nonnegative, so is $\overline{B} = PB$. So C is factorizable as $C = \overline{B}\overline{B}^t$, and the result follows. ∎

The dimension of the constructed matrix B is $n \times m$, where $m = \frac{1}{2}n(n+1) - N - l$, $2N$ is the number of off-diagonal entries which equal zero, and l is the number of rows the diagonal entry of which is equal to the sum of the off-diagonal entries.

In the following we provide an algorithm which will find a factorization with a better bound for m. The algorithm is described as follows:

ALGORITHM 1.

Step 0. Mark all vertices as unlabeled.
Step 1. Choose any spanning tree T of G.
Step 2. Mark all vertices without loops as labeled.
Step 3. If there is no more than one unlabeled vertex, Go to Step 6. Otherwise, choose an unlabeled vertex i such that there exists a partition

$$T = T^1 \cup T^2, \qquad i \in T^1 \cap T^2, \quad T^1 = (V^1, E^1), \quad T^2 = (V^2, E^2).$$

Here all vertices of T^1 are labeled except vertex i. Label vertex i.
Step 4. Remove the loop on vertex i.
Step 5. Adjust the length of row vector i by putting $b_{i(i,i)} = 0$, $b_{i(i,j)} = \sqrt{a_{ij} + a_i}$ for some $(i,j) \in E^2$. To adjust inner products assign $b_{j(j,i)} = a_{ij}/\sqrt{a_{ij} + a_i}$. In order to adjust the length of the vector b_j, increase $b_{j(j,j)}$ accordingly. If $b_{j(j,j)} > 0$ then unlabel vertex j. Go to step 3.
Step 6. Stop.

Note that since T is a spanning tree, there can be at most one unlabeled vertex with a loop when the algorithm stops. The solution will correspond to a graph $G_1 = (V, E_1)$ with at most a single loop, and if we assume that G has a loop around each vertex, then $|E_1| = |E| - (n-1)$.

4. A NUMERICAL EXAMPLE

In this section we will take a matrix that satisfies the conditions in Theorem 1 and find the required factors by the algorithm described in the

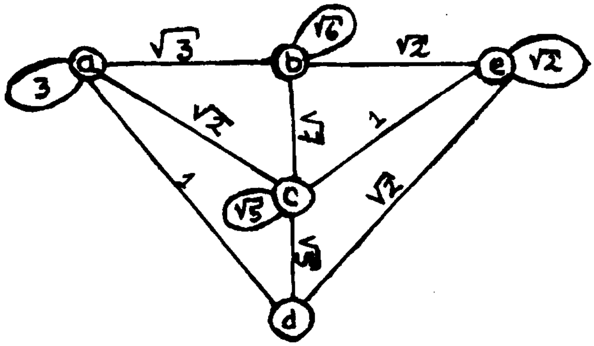

FIG. 1.

previous section. We have taken a 5×5 matrix, since matrices of smaller size are amenable to even square factorization with a diagonal-dominance condition [2]. Let

$$A=\begin{array}{c} \\ a\\ b\\ c\\ d\\ e\end{array}\begin{array}{c}\begin{array}{ccccc} a & b & c & d & e\end{array}\\ \begin{pmatrix} 15 & 3 & 2 & 1 & 0\\ 3 & 18 & 7 & 0 & 2\\ 2 & 7 & 20 & 6 & 1\\ 1 & 0 & 6 & 9 & 2\\ 0 & 2 & 1 & 2 & 7\end{pmatrix}\end{array}$$

That the matrix is diagonally dominant is easily verifiable. Let the rows and columns of A be labeled by a,b,c,d,e [vertices in the graph $G=(V,E)$ below]. Weights are assigned to the edges as shown in Figure 1. It is easy to check that the value of m corresponding to G is

$$13=\frac{5\times 6}{2}-2=\frac{n\times(n+1)}{2}-N.$$

Now using Algorithm 1, we get a reduced matrix B with nine columns as shown below:

$$B = \begin{array}{c} \\ a \\ b \\ c \\ d \\ e \end{array} \begin{array}{c} \begin{array}{ccccccccc} ab & ac & ad & bc & be & cd & ce & de & cc \end{array} \\ \begin{pmatrix} \sqrt{12} & \sqrt{2} & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ \sqrt{\frac{3}{4}} & 0 & 0 & \sqrt{\frac{191}{12}} & \sqrt{\frac{4}{3}} & 0 & 0 & 0 & 0 \\ 0 & \sqrt{2} & 0 & \sqrt{\frac{568}{191}} & 0 & \sqrt{\frac{25}{6}} & 1 & 0 & \sqrt{\frac{11179}{1146}} \\ 0 & 0 & 1 & 0 & 0 & \sqrt{6} & 0 & \sqrt{2} & 0 \\ 0 & 0 & 0 & 0 & \sqrt{3} & 0 & 1 & \sqrt{2} & 0 \end{pmatrix} \end{array}$$

In B there is just one column corresponding to a loop, and the value of m is $9 = n(n+1)/2 - N - (n-1)$.

5. CONCLUSIONS

Using Section 4, we have the following result:

THEOREM 3. *If A is a diagonally dominant nonnegative symmetric matrix, then A can be factored as BB^t, where B is an $n \times m$ matrix, $m \leq \frac{1}{2}n(n+1) - N - (n-\mu)$, $2N$ is the number of zeros in off-diagonal positions of A, and μ is the number of connected components of the graph G.*

We observe that given any nonnegative diagonally dominant symmetric integer matrix A, one can find a 0, 1 matrix B by replacing edge (i, j) with a_{ij} multiple edges, and then B will correspond to the vertex-edge incidence matrix of the corresponding multigraph. The dimension of B in this case will be increased, and the value of m will be $\sum_{i \in V} a_{ii}$. If we restrict to an integer matrix B, then the following theorem gives a better bound for m:

THEOREM 4. *If A is a diagonally dominant symmetric nonnegative integer matrix, then A can be factored as BB^t, where B is an $n \times m$ integer matrix, $m \leq 2(n^2 + n - 2N)$.*

This theorem can be deduced from a theorem of Lagrange [8, p.82] which asserts that every positive integer is the sum of four or fewer squares of positive integers. If we restrict to integer B, then the value of m for our example of Section 4 is 25, compared to 69 when B is a 0, 1 matrix. The problem of obtaining an easily verifiable set of necessary and sufficient conditions for a matrix to be completely positive remains unsolved.

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