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Nonnegative square roots of matrices

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ABSTRACT

By the square root of a (square) matrix A we mean a matrix B that satisfies $B^2 = A$. In this paper, we begin a study of the (entrywise) nonnegative square roots of nonnegative matrices, adopting mainly a graph-theoretic approach. To start with, we settle completely the question of existence and uniqueness of nonnegative square roots for 2-by-2 nonnegative matrices. By the square of a digraph H, denoted by H^2, we mean the digraph with the same vertex set as H such that (i, j) is an arc if there is a vertex k such that (i, k) and (k, j) are both arcs in H. We call a digraph H a square root of a digraph G if $H^2 = G$. It is observed that a necessary condition for a nonnegative matrix to have a nonnegative square root is that its digraph has a square root, and also that a digraph G has a square root if and only if there exists a nonnegative matrix A with digraph G such that A has a nonnegative square root. We consider when or whether certain kinds of digraphs (including digraphs that are disjoint union of directed paths and circuits, permutation digraphs or a special kind of bigraphs) have square roots. We also consider when certain kinds of nonnegative matrices (including monomial matrices, rank-one matrices and nilpotent matrices with index two) have nonnegative square roots. A known characterization of loopless digraphs to have square roots, due to F. Escalantge, L. Montejano, and T. Rojano,

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is extended (and amended) to digraphs possibly with loops. Some natural open questions are also posed.

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1. Introduction

By a square root of a (square) matrix A we mean a matrix B that satisfies $B^2 = A$. The study of square roots or pth roots of a general (real or complex) matrix can be traced back to the early works of Cayley [7,8], Sylvester [26], Frobenius [12] in the 19th century, followed by the works of Kreis [19] and Cecioni [9] in the early 20th century. For more recent works on the pth roots or square roots of matrices, refer to the reference list of [14].

Motivated by the use of stochastic matrices in the theory of Markov chain models in finance and healthcare, in [14] by exploiting the theory of functions, Higham and Lin have considered the question of under what conditions a given stochastic matrix has stochastic pth roots. Except for this and some isolated results on doubly stochastic matrices or on M-matrices, and hence on inverse M-matrices (see [21, Theorem 2], [1, Theorem 4]), there is not much literature addressed to (entrywise) nonnegative square roots or pth roots of a nonnegative matrix. In this paper we offer an initial study of the nonnegative square root problem, adopting mainly a graph-theoretic approach.

This paper is organized as follows. In Section 2 after introducing the necessary definitions and notations, we give the known characterizations for a complex (respectively, real) matrix to have a square root (respectively, real square root). We also collect some known necessary conditions for a multi-set to be the spectrum of a nonnegative matrix that have arisen from studies of the Nonnegative Inverse Eigenvalue Problem.

In Section 3 we treat the nonnegative square root problem for the 2-by-2 case. It is proved that a 2×2 nonnegative matrix A has a nonnegative square root if and only if all eigenvalues of A are nonnegative and A is not a positive multiple of the 2×2 nilpotent elementary Jordan block $J_2(0)$ or its transpose. We also show that the result no longer holds for nonnegative matrices of higher order.

In Section 4 we connect the study of nonnegative square roots of a nonnegative matrix with the study of square roots of a digraph. It is found that a necessary condition for a nonnegative (respectively, symmetric nonnegative) matrix to have a nonnegative (respectively, symmetric nonnegative) square root is that its digraph has a square root (respectively, symmetric square root), and also a digraph (or symmetric digraph) G has a square root (or symmetric square root) if and only if there exists a nonnegative (respectively, symmetric nonnegative) matrix A with G as its digraph such that A has a nonnegative (respectively, symmetric nonnegative) square root.

In Section 5 we provide an example which shows that even if a nonnegative matrix is completely positive and satisfies the graph-theoretic and spectral necessary conditions for having a nonnegative square root, it need not have a nonnegative square root.

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