Eigenvalues of Graphs and Their Applications: Survey and New Results

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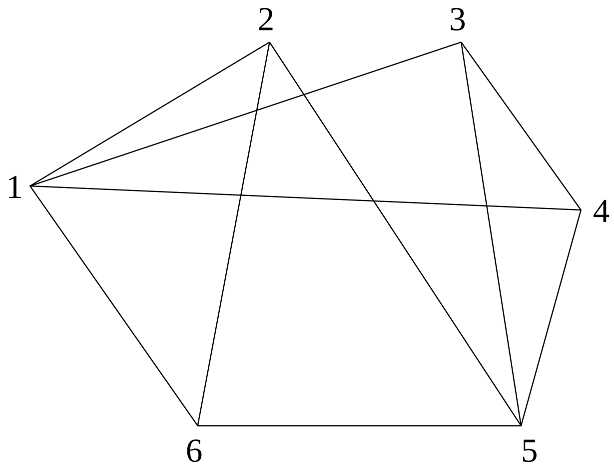
1. Introduction and Definitions

All graphs or digraphs considered here are simple unless otherwise specified. (This is just for simplicity, we may allow them to contain multiple edges or arcs).

Definition 1.1. Let $G = (V, E)$ be a graph with vertex set $V = \{v_1, v_2, \cdots, v_n\}$ and edge set $E = \{(v_i, v_j)|i, j = 1, 2, \cdots, n; i \neq j\}$.
Its adjacency matrix $A(G)$ is an $n \times n$ $(0, 1)$-matrix (a_{ij}), where

$$a_{ij} = \begin{cases} 1, & \text{if } (v_i, v_j) \in E \text{ ;} \\ 0, & \text{otherwise.} \end{cases}$$

Example 1.1. A graph G and its adjacency matrix



$$A(G) = \begin{pmatrix} 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 0 & 1 & 0 \end{pmatrix}$$

Note that, if G is a graph with n vertices, $A(G)$ is an $n \times n$ symmetric $(0, 1)$-matrix with zero diagonal entries.

Definition 1.2. The eigenvalues of a graph G are defined to be the eigenvalues of its adjacency matrix $A(G)$. Collection of the eigenvalues of G is called the spectrum of G .

Note 1: Since $A(G)$ is real symmetric, the eigenvalues of G, $\lambda_i(G)$, $i = 1, 2, \ldots, n$, are real numbers. We therefore may let

$$\lambda_1(G) \geq \lambda_2(G) \geq \cdots \geq \lambda_k(G) \geq \lambda_{k+1}(G) \geq \cdots \geq \lambda_n(G).$$

If $D = diag(d_1, \ldots, d_n)$ is the diagonal matrix where d_j is the degree of vertex v_j. The eigenvalues of $D - A(G)$ are called the Laplacian eigenvalues of G [e.g., Chung, 1997].

Definition 1.3. Given $G_1 = (V_1, E_1)$, $G_2 = (V_2, E_2)$ is the *complement* of G_1 if $V_1 = V_2$ and an edge $e \in E_2$ iff $e \notin E_1$. The *complement* of G is written as G^c.

Outline of the Presentation

- **Definitions and Applications**
- **Some Recent Results**
- **Spectra of Graphs with** $\lambda_3(G) < 0$
- **Graphs Characterized by** $\lambda_{n-2}(G)$
- **Open Problems**

1.1. Why Eigenvalues of Graphs?

(1) Eigenvalues of graphs appear in mathematics, physics, chemistry and computer science etc.. e.g.,

http://www.cs.yale.edu/homes/spielman/
Graduate Course of CS Dept. at Yale and MIT (2004 –) - graph algorithms, NP-problems

(2) The spectral technique is useful in graph theory, combinatorics and the related areas in applied sciences.

(3) An Open Problem, recently paid much attention:

$$Which\ graphs\ have\ distinct\ eigenvalues?$$

(Harary and Schwenk in 1974).

Representatives: [Cvetkovic et al., 95], [Biggs, 95], [Chung, 97], [Wilf et al., 98], [Golin et al., 04], [Wilf, 06]....

The eigenvalues of a graph characterize the topological structure of the graph

Examples :

(1) if $\lambda_1(G) = -\lambda_n(G)$, then G is bipartite;

(2) if $\lambda_2(G) = 0$, then G is complete multi-partite;

(3) if $\lambda_2(G) = -1$, then G is a complete graph;

(4) ...

Representatives: [Cvetkovic et al., 95], [Biggs, 95], [Wilf et al., 98], [Yong, 99], [Wilf, 06] ....

Why Eigenvalues of Graphs? (more specifically)

The technique is often efficient in counting structures, e.g., acyclic digraphs, spanning trees, Hamiltonian cycles, independent sets, Eulerian orientations, cycle covers, k-colorings etc.. [Golin et al., 05], [Wilf, 06].

For a recursive graph (a graph that can be constructed recursively), it is possible to apply its eigenvalues to derive recurrence formulas for counting the number of structures. Therefore, counting structures can be algorithmic for certain graphs.

Many graphs in applied sciences have recursive properties. [Stanley, 73], [Yong et al., 02], [Golin et al., 05],....

1.3 The Eigenvalues in Applied Sciences

1.3 (a) In Information Theory

In Shannon information theory, the channel capacity, which characterizes the maximum amount of information that is transmitted over a channel or stored into a storage medium per bit, can be expressed in terms of the eigenvalues of its channel graph [Wilf, 98], [Cohn, 95].

Combinatorically, the capacity can be discussed by counting the number of closed walks of length k in the channel graph G and then by letting the k tend to infinity.

Construction of encoder/decoder for a given code is based on the largest eigenvalue of its channel graph. (The information transmission rate must be less than, but be expected to be very close to, the largest eigenvalue) [Cohn, 95], [Immink, 99].

1.3 (b) In Coding Theory

In coding theory, the minimum *Hamming distance* of a linear code can be represented by the second largest eigenvalue of a regular graph. (*Hamming distance* is the number of entries in which two codewords differ.)

A code with minimum Hamming distance d allows the correction of $\lfloor d/2 \rfloor$ errors during the transmission over a noisy channel. [Spielman, 96]

Interested in regular graphs having smaller second largest eigenvalues — expanders.

1.3 (c) In Quantum Chemistry

In quantum chemistry, the skeleton of a non-saturated hydrocarbon is represented by a graph. The energy levels of the electrons in such a molecule are the eigenvalues of the graph. The stability of molecules is closely related to the spectrum of its graph. [Cvetkovic et al., 95].

Correspondences :

$$\begin{aligned} vertex &\quad - \quad carbon\ atom \\ edge &\quad - \quad bond \\ vertex\ degree &\quad - \quad valency \\ adjacency\ matrix &\quad - \quad topological\ matrix - Huckel\ matrix\ .... \end{aligned}$$

1.3 (d) In Geographic Studies

In geographic studies, the eigenvalues and eigenvectors of a transportation network provide information about its connectedness. It is proven that the more highly connected in a transportation network G is, the larger is the largest eigenvalue $\lambda_1(G)$. [Tinkler, 72], [Roberts, 78].

Given the numbers of vertices and edges, how to design a graph with larger $\lambda_1(G)$? – very interesting

Only one paper is found, which arranges for trees according to the values of their largest eigenvalues [Zhang, 2002].

1.3 (e) In Social Sciences

Social networks have been studied actively in social sciences, where the general feature is that the networks are viewed as static graphs whose vertices are ‘individuals’ and whose edges are the social interactions between these ‘individuals’.

The problem is to analyze the topology and dynamics of (given) data sets which have relationships between themselves in the network.

Interested in analyzing degree sequences and shortest connecting paths – they can be represented by the eigenvalues.

Representatives: [Roberts, 78], [Wasserman et al., 94], [Kochen, 89].

1.3 (f) In Finite Dynamical Systems

A finite dynamical system is a time-discrete dynamical system on a finite state set, where the important thing is to link the structure of the system with its dynamics (e.g., Boolean networks used in computational biology) [Albert et al., 03], [Celada et al., 92], ...

Where the number of state transitions usually has *exponential size* in the number of model variables, so analyzing the dynamics of the models without calculating the state transitions is important.[Omar et al., 04]

In the case of linear systems, this can be attacked by examining the primitivity of a graph — algebraically, by checking if its largest eigenvalue is simple and strictly dominant. [Berman et al., 94]

1.3 (g) In Epidemiology

In epidemiology, an epidemic threshold (a notion of prediction introduced recently) is a critical state beyond which infections become endemic. [Wang et al., 2003]

The epidemic threshold depends fundamentally on the structure of the graph, where the challenge is to capture the structure in as few parameters as possible. Wang et al. presented, recently, a model that can predict the epidemic threshold with the largest eigenvalue.

Again, bounding the largest eigenvalue!

1.3.8. In Game Theory

There are many papers that develop network models for large-population game theory and economics. e.g., [Kearns, 05].

In those models, each player/organization is represented by a vertex of a graph, and the payoffs and transactions are restricted to obey the topology of the graph. This allows a detailed specification of its rich structure (social, organizational, political etc.) in strategic and economic systems.

Eigenvalues of a graph specify the topological structure of it.[Farkas, 02]

1.4. The Tools for Attacking the Problems

(More applications ....)

In attacking the problems addressed above, to the best of our knowledge, the main tool is combination of the techniques from algebraic graph theory, combinatorics and advanced matrix analysis (intrinsic to random graphs).

Many of them can be modified to consider the number of walks of length k in their graphs – which can be represented by the eigenvalues of the graphs involved.

1.5. Difficulties of Attacking the Problems

(1) Getting better bounds of the eigenvalues requires getting more information on their eigenspaces.

(2) The sizes of graphs are usually very large, so direct computation of eigenvalues is usually unacceptable.

(3) The dominant roots (especially, the second, the third largest) of a polynomial are not easy to evaluate (even if we derive the characteristic polynomial of a graph)

2. Some Recent Results on Graph Spectra

Given G, the largest eigenvalue $\lambda_1(G)$ has been studied extensively in the past decades. Recently, its second largest eigenvalue $\lambda_2(G)$ has also been considered by several authors.

For the third largest eigenvalue $\lambda_3(G)$, it is known that: (1) $\lambda_3(G) = -1$ iff G^c is isomorphic to the union of a complete bipartite graph and some isolated vertices, (2) there exist no graphs such that $-1 < \lambda_3(G) < -\frac{\sqrt{5}-1}{2} = -0.618...$.

[Cvetkovic et al., 95], [Neumaier et al., 83], [Pertrovic, 91], [Cao, 98], etc.

...

Some Recent Results on Graph Spectra (Cont'd)

For the least eigenvalue $\lambda_n(G)$, it is known that [Yong, 99]

$$-\frac{n}{2} \leq \lambda_n(G) \leq -\frac{1+\sqrt{1+4\frac{n-3}{n-1}}}{2} = -1.618....$$

Motivated by the *Open Problem* by Harary et al.:

$$Which\ graphs\ have\ distinct\ eigenvalues?$$

There has been research on the graphs with multiple eigenvalues, e.g., introducing *star sets* of eigenvalues, e.g., [Pertrovic, 98].

2.1. Some New Results

(I) Strengthened a classical theorem on graphs with multiple eigenvalues (for a regular graph, its eigenvalues can be simple).

(II) Found two classes of graphs with multiple eigenvalues:

- graphs with negative third largest eigenvalues;
- graphs characterized by $\lambda_{n-2}(G)$.

2.2. Conventions

K_r is the *clique* of order r.

$K_{i,j}$ is the complete bipartite graph with the partition numbers i, j.

Let $a_{-n+1}, a_{-n+2}, \ldots, a_{n-1}$ be a sequence of numbers. Then $A = (a_{ij})$ is called a *Toeplitz matrix* if $a_{ij} = a_{i-j}$ for all $i, j = 1, 2, \ldots, n$.

2.3. Some Definitions

Definition 2.1. Let $A = (a_{i-j})$ be a symmetric Toeplitz matrix. If $a_{i-j} \neq 0$ for all $1 \leq |i-j| \leq k$, then A is a symmetric Toeplitz matrix with *width* k. A graph G with its adjacency matrix having this property is called a *Toeplitz graph* with width k.

Definition 2.2. ([Berman et al., 94]). An $n \times n$ matrix A is *cogredient* to a matrix B if, for some permutation matrix P, we have $PAP^t = B$.

Two graphs are isomorphic iff their adjacency matrices are *cogredient*.

2.4. A General Result

Theorem 2.1. Let A be an $n \times n$ real symmetric matrix. Then A has n distinct eigenvalues iff, $\forall\ P \in S = \{X|AX = XA, X\ is\ a\ real\ matrix\}$, P is symmetric.

Corollary 2.1. For the adjacency matrix A of G. If there is a non-symmetric permutation matrix P such that $AP = PA$ then G has multiple eigenvalues.

Theorem 2.1 generalizes [Cvetkovic et al., Theorem 5.1]. Corollary 2.1 provides information about a graph that has multiple eigenvalues. For example, if A is the adjacency matrix of a circulant graph C, and P the adjacency matrix of a *directed* Hamiltonian cycle with the same vertices, then $AP = PA$ and so C has multiple eigenvalues. This is a known result [Biggs, 93, p.16].

2.5. Spectra of graphs with multiple eigenvalues

Theorem 2.2. If G has $t+1$ eigenvalues equal to α:

$$\lambda_k(G) = \lambda_{k+1}(G) = \cdots = \lambda_{k+t}(G) = \alpha,$$

then (1) G^c has at least t eigenvalues equal to $-\alpha - 1$ and

$$\lambda_{n-(k+t)+2}(G^c) = \lambda_{n-(k+t)+3}(G^c) = \lambda_{n-k+1}(G^c) = -\alpha - 1;$$

(2) G and G^c share a common eigenspace with dimension at least t.

This theorem reveals the relationships between the eigenvalues, the eigenspaces of G and of G^c. In particular, when $\alpha = 0$ it characterizes graphs having eigenvalues equal to 0. Graphs without 0 eigenvalues are considered in [Bell, 93] etc.

Spectra of graphs with multiple eigenvalues (cont'd)

Corollary 2.4. If a regular graph G with n vertices has t eigenvalues equal to α and

$$\lambda_k(G) = \lambda_{k+1}(G) = \cdots = \lambda_{k+t-1}(G) = \alpha,$$

then G^c has t eigenvalues equal to $-\alpha - 1$, and

$$\lambda_{n-(k+t)+2}(G^c) = \lambda_{n-(k+t)+3}(G^c) = \lambda_{n-k+1}(G^c) = -\alpha - 1,$$

and G and G^c share the same eigenspace for each eigenvalue.

Combining all above, we see that a non-zero vector is an eigenvector of a regular graph G iff it is an eigenvector of its complement G^c. (This is known.)

Spectra of graphs with multiple eigenvalues - Example

Example. Let G be a graph with n vertices. If G^c is complete $k-$partite, then G has $n-k-1$ eigenvalues equal to -1, and

$$\lambda_{k+1}(G) = \lambda_{k+2}(G) = \cdots = \lambda_{n-1}(G) = -1.$$

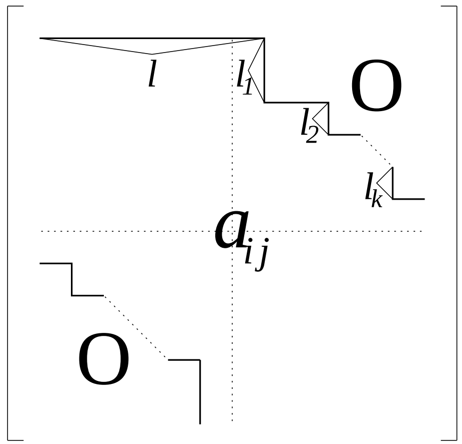
In fact, If G^c is complete $k-$partite, then [Yong, 97]

$$\lambda_2(G^c) = \lambda_3(G^c) = \cdots = \lambda_{n-k+1}(G^c) = 0.$$

Hence the assertion follows directly from Theorem 2.2.

3. Spectra of the graphs with $\lambda_3(G) < 0$

Lemma 3.1. Let G be a connected graph with n vertices, and $\lambda_3(G) < 0$. Then there exists a permutation matrix P such that $PA(G)P^t$ has the following form



where $a_{ij} = 1$ if $i \neq j$, and $l_1 + l_2 + \ldots + l_k \leq l$.

Spectra of graphs with $\lambda_3(G) < 0$ (cont'd)

Theorem 3.4. Let G be a connected graph with n vertices, and $\lambda_3(G) < 0$. Then

(1) -1 is an eigenvalue of G except the case that $A(G)$ is cogredient to the symmetric Toeplitz matrix with width $\lfloor \frac{n-1}{2} \rfloor$.

(2) Let V_r, V_{n-r} be the vertex sets of the disjoint cliques K_r, K_{n-r}, respectively. Then G has $n - \kappa - \sigma$ eigenvalues equal to -1, where κ is the number of distinct degrees in V and $\sigma = 1$ if there are 2 vertices with degree $n - 1$ and one of which is in V_r and the other in V_{n-r}, and 0, otherwise.

Spectra of graphs with $\lambda_3(G) < 0$ (cont'd)

Theorem 3.5. Let G be a connected graph with n vertices and $\lambda_3(G) < 0$. Let $2r$ be the rank of $A(G^c)$. Then (1) if $r < \frac{n}{2}$, we have

$$-1 \le \lambda_j(G) < 0, \quad j = 3, 4, \cdots, r+1,$$
$$\lambda_j(G) = -1, \quad j = r+2, \cdots, n-r;$$

(2) if $r = \frac{n}{2}$, then

$$-1 \le \lambda_j(G) < 0,\ j = 3, 4, \cdots, \frac{n}{2}; \quad \lambda_{\frac{n}{2}+1}(G) \ge -2.$$

Corollary 3.6. Let G be a connected graph with n vertices and $\lambda_3(G) < 0$. If there exists an index k, $2 \le k \le \lfloor \frac{n}{2} \rfloor$ such that $\lambda_k(G) = -1$, then

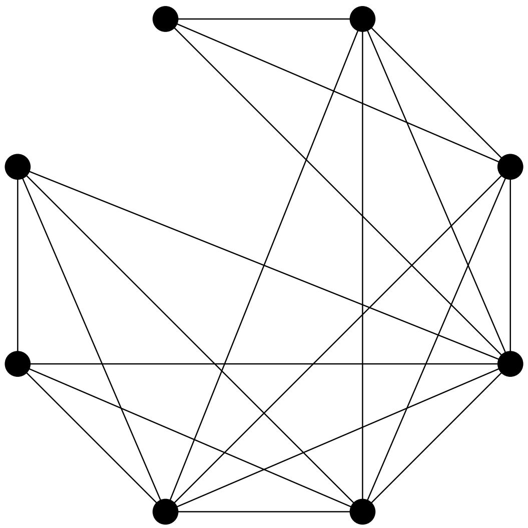
$$\lambda_j(G) = -1, \quad j = k, k+1, \ldots, n-r,$$

where $2r$ is the rank of $A(G^c)$ and $r \le k-1$.

Spectra of graphs with $\lambda_3(G) < 0$ — Example

The following example indicates that the relation $r = k - 1$ in Corollary 3.6 does not always hold. [Yong, 99].

Example. Let G and its adjacency matrix $A(G)$ be given by



$$\begin{bmatrix} 0 & 1 & 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 0 & 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 & 0 & 1 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 \\ 0 & 0 & 0 & 1 & 1 & 1 & 1 & 0 \end{bmatrix}$$

Spectra of graphs with $\lambda_3(G) < 0$ — Example (cont'd)

By Maple we obtain that

$$\begin{aligned}
\lambda_1(G) &= 5.24384, \lambda_2(G) = 1.60317,\ \lambda_3(G) = -0.182062, \\
\lambda_4(G) &= -1, \quad \lambda_5(G) = -1, \quad \lambda_6(G) = -1, \\
\lambda_7(G) &= -1.53035, \quad \lambda_8(G) = -2.1346.
\end{aligned}$$

The rank of $A(G^c)$ is 4, so $r = 2$. From the above theorem

$$\lambda_4(G) = \lambda_5(G) = \lambda_6(G) = -1.$$

Comparing this with Corollary 3.6, we see that this is the case that $r = 2, k = 4, n = 8$.

Spectra of graphs with $\lambda_3(G) < 0$ (cont'd)

Two special cases:

Corollary 3.7. Let G be a connected graph with n vertices. Then

(1) $\lambda_3(G) = -1$ iff G^c is the union of a complete bipartite graph and some isolated vertices.

(2) $\lambda_3(G) = -1$ implies that $\lambda_j(G) = -1$, $j = 3, 4, \ldots, n-1$.

This corollary generalizes the corresponding results obtained in [Cao, 95] and in [Cvetkovic et al., 95].

4. Graphs characterized by $\lambda_{n-2}(G)$

A graph has multiple eigenvalues equal to -1 if the third least eigenvalue of its complement is zero.

Lemma 4.1. Given G with at least seven vertices, we have $\lambda_4(G) \geq -1$. Moreover, If G^c is not 3-partite, then $\lambda_4(G) \geq \frac{1-\sqrt{5}}{2}$.

Corollary 4.2. Let G be a graph with at least seven vertices. If $\lambda_4(G^c) < \frac{1-\sqrt{5}}{2}$, then the chromatic number of G is 3.

Spectra of graphs characterized by $\lambda_{n-2}(G)$ (cont'd)

Theorem 4.3. Let G be a graph with $n \geq 7$ vertices. Then

(1) $\lambda_{n-2}(G) \leq 0$; and $\lambda_{n-2}(G) = 0$ implies $\lambda_4(G^c) = -1$ and G is isomorphic to a graph with its adjacency matrix being the following form,

$$A(G) = \begin{pmatrix} 0 & A_{12} & A_{13} \\ A_{12}^t & 0 & A_{23} \\ A_{13}^t & A_{23}^t & 0 \end{pmatrix},$$

and each $B_{ij} = \begin{pmatrix} 0 & A_{ij} \\ A_{ij}^t & 0 \end{pmatrix}$, $1 \leq i,\ j \leq 3$, is cogredient to

$$\begin{pmatrix} 0 & \begin{pmatrix} J_1 & J_2 & J_3 \\ J_4 & J_4 & J_6 \end{pmatrix} \\ * & 0 \end{pmatrix},$$

where J_i are either all 1's matrices of appropriate sizes or the 0 matrices, for each $i = 1, 2, ..., 6$;

(2) $\lambda_{n-2}(G) = 0$ implies $\lambda_{n-\lceil \frac{n}{3} \rceil+2}(G) = \lambda_{n-\lceil \frac{n}{3} \rceil+3}(G) = \cdots = \lambda_{n-2}(G) = 0$;

(3) $\lambda_{n-2}(G) = 0$ implies $\lambda_1(G) \leq -2\lambda_n(G)$.

5. Two Conjectures

There are many *open problems or conjectures*. In the following are two of them:

Conjecture 1. Given G of n vertices, if k is the smallest index that satisfies (1) $k \leq \lceil \frac{n}{2} \rceil$ (2) $\lambda_k(G^c) < \frac{1-\sqrt{5}}{2}$, (3) $\lambda_1(G) + (k-3)\lambda_n(G) > 0$, then $k-1$ is the chromatic number of G.

The Four-Color Theorem could be re-proven from here, if the conjecture would be true.

The conjecture is true for $k = 2,\ 3,\ 4.$ If the conjecture would be true in general, then $(-v+3)\lambda_n(G) \leq \lambda_1(G) \leq (-v+1)\lambda_n(G)$, where v is the chromatic number.

Two Conjectures (Cont'd)

Conjecture 2. Let A be an $n \times n$ $(0,1)$-matrix with its graph G being irregular. Then

$$|det(A)| \leq F_n$$

where F_n is the Fibonacci number: $F_n = F_{n-1} + F_{n-2}$, with $F_0 = 0$, $F_1 = 1$.

There are a number of rough bounds on $|det(A)|$. The conjecture is true for many $(0,1)$-matrices and the equality holds for a class of Hessenberg matrices.

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