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Roots of Matrices

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Matrix pth Root

- X is a pth root ($p \in \mathbb{Z}^+$) of $A \in \mathbb{C}^{n\times n}$ $\iff$ $X^p = A$.
- Number of pth roots may be zero, finite or infinite.

Definition

For $A \in \mathbb{C}^{n\times n}$ with no eigenvalues on $\mathbb{R}^- = \{x \in \mathbb{R} : x \le 0\}$ the principal pth root, $A^{1/p}$ is unique pth root X with spectrum in the wedge $|\arg(\lambda(X))| < \pi/p$.

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Definition

For $A \in \mathbb{C}^{n\times n}$ with no eigenvalues on $\mathbb{R}^-$ the principal logarithm, $\log(A)$, is unique solution of $e^X = A$ with $|\operatorname{Im} \lambda(X)| < \pi$.

Arbitrary Power

Definition

For $A \in \mathbb{C}^{n\times n}$ with no eigenvalues on $\mathbb{R}^-$ and $s \in [0,\infty)$, $A^s = e^{s\log A}$, where $\log A$ is the principal logarithm.

$$A^s = \frac{\sin(s\pi)}{s\pi} A \int_0^\infty (t^{1/s} I + A)^{-1}\, dt, \qquad s \in (0,1).$$

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Applications:

- Pricing American options (Berridge & Schumacher, 2004).
- Finite element discretizations of fractional Sobolev spaces (Arioli & Loghin, 2009).
- Computation of geodesic-midpoints in neural networks (Fiori, 2008).

Approximate Diagonalization

If $A = XDX^{-1}$, $D = \mathrm{diag}(d_i)$, then $f(A) = Xf(D)X^{-1}$.
OK numerically if X is well conditioned.

For any A, let $E = \epsilon\,\mathrm{randn}(n)$, $A + E = XDX^{-1}$. Then (Davies, 2007)

$$f(A) \approx Xf(D)X^{-1}.$$

- Especially useful for A^s.
- A Test Problem for Computations of Fractional Powers of Matrices (Davies, 2008).

Root Oddities (1)

- Turnbull (1927): $A_n^3 = I_n$, where

$$A_4 = \begin{bmatrix} -1 & 1 & -1 & 1 \\ -3 & 2 & -1 & 0 \\ -3 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \end{bmatrix}.$$

- $B_n^2 = I_n$, where

$$B_4 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & -1 & -2 & -3 \\ 0 & 0 & 1 & 3 \\ 0 & 0 & 0 & -1 \end{bmatrix}.$$

Arises in BDF solvers for ODEs.

Root Oddities (2)

- Bambaii & Chowla (1946): $B_n^{n+1} = I_n$ where

$$B_4 = \begin{bmatrix} -1 & -1 & -1 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}.$$

- Hill (1932): US patent for involutory matrices in cryptography.
  Bauer (2002): *"since then the value of mathematical methods in cryptology has been unchallenged."*
- Real square roots of $-I$:

$$\begin{bmatrix} a & 1+a^2 \\ -1 & -a \end{bmatrix}^2 = \begin{bmatrix} -1 & 0 \\ 0 & -1 \end{bmatrix}, \quad a \in \mathbb{C}.$$

Markov Models

- Discrete-time Markov process with transition probability matrix P, time unit 1. Unit is 1 **year** in credit risk modelling.
- Transition matrix for fractional time unit α is P^α.
- If P is embeddable, $P = e^Q$ for **generator** Q with $q_{ij} \geq 0$ $(i \neq j)$, $\sum_{j=1}^{n} q_{ij} = 0$. Then $P^\alpha = e^{\alpha Q}$.

Problems:

- P may not be embeddable.
- $P^{1/k}$ may not be a stochastic matrix.
- Is there a stochastic root?

Email from a Power Company

The problem has arisen through proposed methodology on which the company will incur charges for use of an electricity network.

⋮

I have the use of a computer and Microsoft Excel.

⋮

I have an Excel spreadsheet containing the transition matrix of how a company's [Standard & Poor's] credit rating changes from one year to the next. I'd like to be working in eighths of a year, so the aim is to find the ***eighth root of the matrix****.*

- R. B. Israel, J. S. Rosenthal & J. Z. Wei. **Finding generators for Markov chains via empirical transition matrices, with applications to credit ratings.** *Mathematical Finance*, **2001**.
- D. T. Crommelin & E. Vanden-Eijnden. **Fitting timeseries by continuous-time Markov chains: A quadratic programming approach.** *J. Comp. Phys.*, **2006**.
- T. Charitos, P. R. de Waal, & L. C. van der Gaag. **Computing short-interval transition matrices of a discrete-time Markov chain from partially observed data.** *Statistics in Medicine*, **2008**.
- M. Bladt & M. Sørensen. **Efficient estimation of transition rates between credit ratings from observations at discrete time points.** *Quantitative Finance*, **2009**.

HIV to Aids Transition

- Estimated 6-month transition matrix.
- Four AIDS-free states and 1 AIDS state.
- 2077 observations (Charitos et al., 2008).

$$P = \begin{bmatrix} 0.8149 & 0.0738 & 0.0586 & 0.0407 & 0.0120 \\ 0.5622 & 0.1752 & 0.1314 & 0.1169 & 0.0143 \\ 0.3606 & 0.1860 & 0.1521 & 0.2198 & 0.0815 \\ 0.1676 & 0.0636 & 0.1444 & 0.4652 & 0.1592 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}.$$

Want to estimate the **1-month transition matrix**.

$$\Lambda(P) = \{1, 0.9644, 0.4980, 0.1493, -0.0043\}.$$

Toolbox of Matrix Functions

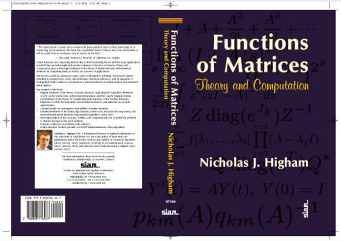
- Want techniques for evaluating interesting f at matrix arguments.
- Example:

$$\frac{d^2y}{dt^2} + Ay = 0, \qquad y(0) = y_0, \quad y'(0) = y_0'$$

$$\Rightarrow \quad y(t) = \cos(\sqrt{A}\,t)y_0 + \left(\sqrt{A}\right)^{-1}\sin(\sqrt{A}\,t)y_0',$$

where $\sqrt{A}$ is any square root of A.

- MATLAB has **`expm`**, **`logm`**, **`sqrtm`**, **`funm`** and ^



Visser Iteration for $A^{1/2}$

$$X_{k+1} = X_k + \alpha(A - X_k^2), \qquad X_0 = (2\alpha)^{-1} I.$$

- Used with $\alpha = 1/2$ by Visser (1932) to show positive operator on Hilbert space has a positive square root.
- Enables proof of existence of $A^{1/2}$ *without using spectral theorem*.
- Likewise in functional analysis texts, e.g. Riesz & Sz.-Nagy (1956).
- Iteration used computationally by Liebl (1965), Babuška, Práger & Vitásek (1966), Späth (1966), Duke (1969), Elsner (1970).
- Elsner proves cgce for $A \in \mathbb{C}^{n\times n}$ with real, positive eigenvalues if $0 < \alpha \le \rho(A)^{-1/2}$.

Visser Convergence

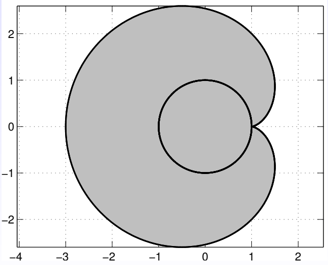
$$X_{k+1} = X_k + \alpha(A - X_k^2), \qquad X_0 = (2\alpha)^{-1} I.$$

Theorem (H, 2008)

Let $A \in \mathbb{C}^{n\times n}$ *and* $\alpha > 0$. *If* $\Lambda(I - 4\alpha^2 A)$ *lies in the cardioid*

$$\mathcal{D} = \{\, 2z - z^2 : z \in \mathbb{C},\ |z| < 1 \,\}$$

then $A^{1/2}$ *exists and* $X_k \to A^{1/2}$ *linearly.*



Iteration for $A^{1/p}$

Rice (1982):

$$X_{k+1} = X_k + \frac{1}{p}(A - X_k^p), \qquad X_0 = 0.$$

For Hermitian pos def A, $0 \le X_k \le X_{k+1}$ for all k and $X_k \to A^{1/p}$.

Existence of pth Roots

Theorem (Psarrakos, 2002)

*$A \in \mathbb{C}^{n\times n}$ has a pth root iff for every integer $\nu \geq 0$ no more than one element of the **ascent sequence**" $d_1, d_2, \dots$ defined by*

$$d_i = \dim(\mathrm{null}(A^i)) - \dim(\mathrm{null}(A^{i-1}))$$

lies strictly between $p\nu$ and $p(\nu + 1)$.

- For $J = J(0) \in \mathbb{C}^{n\times n}$, $\dim(\mathrm{null}(J^k)) = k$, $k = 0\colon n$, $\{d_i\} = \{1, 1, \dots, 1\}$; no pth root for $p \geq 2$.

Existence of Real pth Roots of Real A

Theorem

$A \in \mathbb{R}^{n\times n}$ has a real pth root iff it satisfies the ascent sequence condition and, if p is even, A has an even number of Jordan blocks of each size for every negative eigenvalue.

Block Triangular Case

Lemma

Let

$$A = \begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix} \in \mathbb{C}^{n \times n},$$

where $\Lambda(A_{11}) \cap \Lambda(A_{22}) = \emptyset$*. Then any pth root of A has the form*

$$X = \begin{bmatrix} X_{11} & X_{12} \\ 0 & X_{22} \end{bmatrix},$$

where $X_{ii}^p = A_{ii}$, $i = 1, 2$ *and* X_{12} *is the unique solution of the Sylvester equation* $A_{11}X_{12} - X_{12}A_{22} = X_{11}A_{12} - A_{12}X_{22}$.

- Proof reduces A to $\mathrm{diag}(A_{11}, A_{22})$.

Classification of pth Roots of $A \in \mathbb{C}^{n\times n}$

Jordan canonical form $Z^{-1}AZ = J = \mathrm{diag}(J_0, J_1)$.
All pth roots of A are given by $A = Z\mathrm{diag}(X_0, X_1)Z^{-1}$, where

- $X_1^p = J_1$ (have characterization),
- $X_0^p = J_0$ (no nice characterization).

History:

- Cayley (1858, 1872).
- Sylvester (1882, 1883).
- Gantmacher (1959).
- Higham (1987).

Stochastic Matrices

$A \in \mathbb{R}^{n \times n}$, $A \geq 0$, $Ae = e$.

Theorem

Let $A \in \mathbb{R}^{n \times n}$ be stochastic. Then

- $\rho(A) = 1$;
- 1 *is a semisimple eigenvalue of A with eigenvector e;*
- *if A is irreducible, then* 1 *is a simple eigenvalue of A.*

Nonneg Root may not be Stochastic

$X^p = A$ and $X \geq 0$ imply that $\rho(X) = \rho(A)^{1/p} = 1$ is an ei'val with ei'vec $v \geq 0$ (Perron–Frobenius) but *not* that $v = e$:

$$A = \begin{bmatrix} 1/2 & 1/2 & 0 \\ 1/2 & 1/2 & 0 \\ 0 & 0 & 1 \end{bmatrix}, \qquad \Lambda(A) = \{1, 1, 0\}.$$

$A = X^{2k}$ for

$$X = \begin{bmatrix} 0 & 0 & 2^{-1/2} \\ 0 & 0 & 2^{-1/2} \\ 2^{-1/2} & 2^{-1/2} & 0 \end{bmatrix}, \qquad \Lambda(X) = \{1, 0, -1\}.$$

. . . but OK for Irreducible

Lemma

Let $A \in \mathbb{R}^{n\times n}$ *be an irreducible stochastic matrix. Then for any nonnegative* X *with* $X^p = A$, $Xe = e$.

... but OK for Irreducible

Lemma

Let $A \in \mathbb{R}^{n\times n}$ be an irreducible stochastic matrix. Then for any nonnegative X with $X^p = A$, $Xe = e$.

In fact ...

Theorem

Let $C \geq 0$ be irreducible with e'vec $x > 0$ corr. to $\rho(C)$. Then $A = \rho(C)^{-1}D^{-1}CD$ is stochastic, where $D = \mathrm{diag}(x)$. Moreover, if $C = Y^p$ with Y nonnegative then $A = X^p$, where $X = \rho(C)^{-1/p}D^{-1}YD$ is stochastic.

M-Matrix Connection

Definition of Nonsingular M-matrix $A \in \mathbb{R}^{n\times n}$

$A = sI - B$ with $B \geq 0$ and $s > \rho(B)$.

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Theorem

If the stochastic matrix $A \in \mathbb{R}^{n\times n}$ is the inverse of an M-matrix then $A^{1/p}$ exists and is stochastic for all p.

Proof

- Since $M = A^{-1}$ is "M", $\operatorname{Re} \lambda_i(M) > 0$ so $M^{1/p}$ exists.
- $M^{1/p}$ is an M-matrix for all p (Fiedler & Schneider, 1983)
- Thus $A^{1/p} = (M^{1/p})^{-1} \geq 0$ for all p, and $A^{1/p}e = e$ (shown via JCF arguments), so $A^{1/p}$ is stochastic.

Example 1

$$A = \begin{bmatrix} 1 & & & \\ \frac{1}{2} & \frac{1}{2} & & \\ \vdots & \vdots & \ddots & \\ \frac{1}{n} & \frac{1}{n} & \cdots & \frac{1}{n} \end{bmatrix}.$$

$$A^{-1} = \begin{bmatrix} 1 & & & & \\ -1 & 2 & & & \\ 0 & -2 & 3 & & \\ \vdots & \vdots & \ddots & \ddots & \\ 0 & 0 & \cdots & -(n-1) & n \end{bmatrix}.$$

A^{-1} is an M-matrix so $A^{1/p}$ is stochastic for all $p > 0$.

Example 2

$$Y^2 = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}^2 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 2 & 2 \\ 1 & 2 & 3 & 3 \\ 1 & 2 & 3 & 4 \end{bmatrix} = M.$$

$\lambda_k(M) = \frac{1}{4}\sec(k\pi/(2n+1))^2$, $k = 1: n$.
Positive e'vec x for $\rho(M)$.

- $A = \rho(M)^{-1}D^{-1}MD$ is stochastic, where $D = \mathrm{diag}(x)$, has stochastic sq. root $X = \rho(M)^{-1/2}D^{-1}YD$.
- Note: X is **indefinite.**
- But A has another stochastic sq. root: $A^{1/2}$, by previous theorem!

Example 2 cont.

For $n = 4$:

$$\begin{bmatrix} 0.1206 & 0.2267 & 0.3054 & 0.3473 \\ 0.0642 & 0.2412 & 0.3250 & 0.3696 \\ 0.0476 & 0.1790 & 0.3618 & 0.4115 \\ 0.0419 & 0.1575 & 0.3182 & 0.4825 \end{bmatrix}$$

$$= \begin{bmatrix} 0 & 0 & 0 & 1.0000 \\ 0 & 0 & 0.4679 & 0.5321 \\ 0 & 0.2578 & 0.3473 & 0.3949 \\ 0.1206 & 0.2267 & 0.3054 & 0.3473 \end{bmatrix}^2$$

$$= \begin{bmatrix} 0.2994 & 0.2397 & 0.2315 & 0.2294 \\ 0.0679 & 0.3908 & 0.2792 & 0.2621 \\ 0.0361 & 0.1538 & 0.4705 & 0.3396 \\ 0.0277 & 0.1117 & 0.2626 & 0.5980 \end{bmatrix}^2 .$$

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- *A stochastic matrix may have a stochastic principal pth root as well as a stochastic nonprimary pth root.*
- *A stochastic matrix may have a stochastic principal pth root but no other stochastic pth root.*
- *The principal pth root of a stochastic matrix with distinct, real, positive eigenvalues is not necessarily stochastic.*

Facts cont.

- *A (row) diagonally dominant stochastic matrix may not have a stochastic principal pth root.*

$$A = \begin{bmatrix} 9.9005 \times 10^{-1} & 9.9005 \times 10^{-7} & 9.9500 \times 10^{-3} \\ 9.9005 \times 10^{-7} & 9.9005 \times 10^{-1} & 9.9500 \times 10^{-3} \\ 4.9750 \times 10^{-3} & 4.9750 \times 10^{-3} & 9.9005 \times 10^{-1} \end{bmatrix}.$$

None of the 8 square roots of A is nonnegative.

Facts cont.

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None of the 8 square roots of A is nonnegative.

- *A stochastic matrix whose principal pth root is not stochastic may still have a primary stochastic pth root.*

$$A = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}^2 = X^2.$$

$$\Lambda(A) = \Lambda(X) = \{e^{\pm 2\pi/3}, 1\}.$$

Embeddability Problem

When can nonsingular stochastic A be written $A = e^Q$ with $q_{ij} \geq 0$ for $i \neq j$ and $\sum_j q_{ij} = 0$, $i = 1\colon n$?

Kingman (1962): holds iff for every positive integer p there exists some stochastic X such that $A = X^p$.
Conditions (e.g.)

- $\det(A) > 0$
- $\det(A) \leq \prod_i a_{ii}$

are **necessary for embeddability** of a stochastic A but *not necessary for existence of a stochastic pth root for a particular p.*

New classes of embeddable matrices.

Inverse Eigenvalue Approach

Karpelevič (1951) determined
$\Theta_n = \{\, \lambda : \lambda \in \Lambda(A),\ A \in \mathbb{R}^{n\times n} \text{ stochastic} \,\}$.

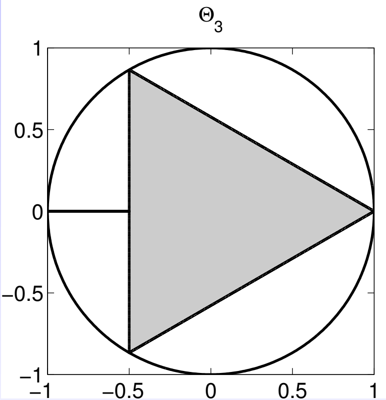
Theorem

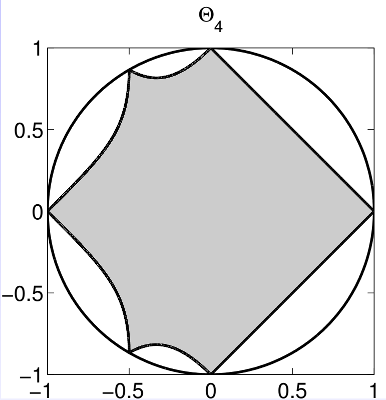
$\Theta_n \subseteq$ unit disk and intersects unit circle at $e^{2i\pi a/b}$, all a, b s.t. $0 \le a < b \le n$. Boundary of Θ_n is curvilinear arcs defined by

$$\begin{aligned} \lambda^q(\lambda^s - t)^r &= (1-t)^r, \\ (\lambda^b - t)^d &= (1-t)^d \lambda^q, \end{aligned}$$

where $0 \le t \le 1$, and $b, d, q, s, r \in \mathbb{Z}^+$ determined from certain specific rules.

$n = 3, 4$



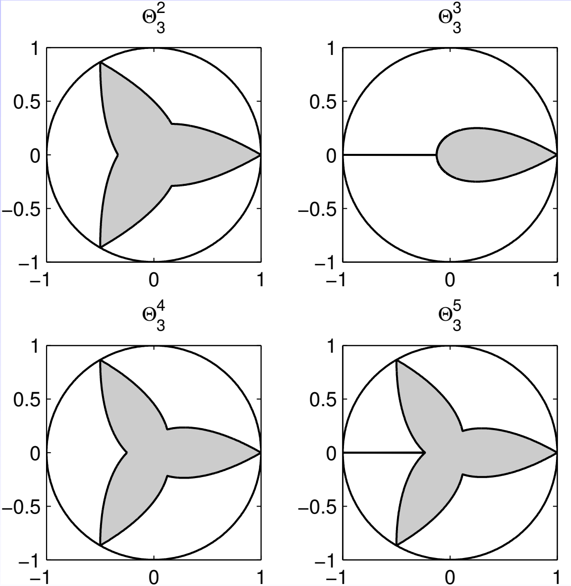


Necessary Condition

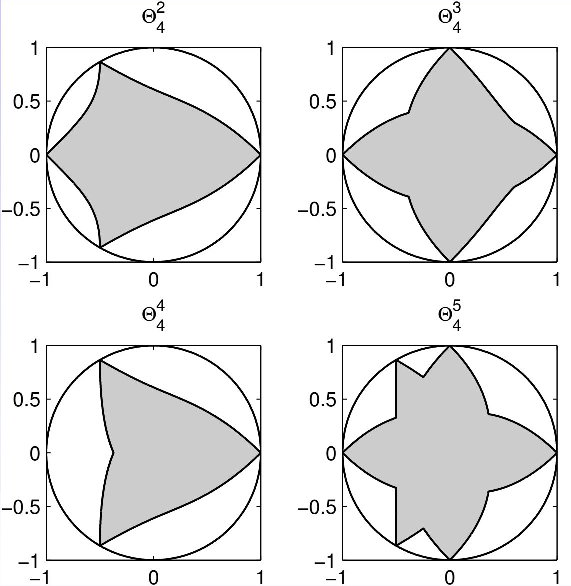
If A and X are stochastic and $X^p = A$ then it is necessary that

$$\lambda_i(A) \in \Theta_n^p := \{\lambda^p : \lambda \in \Theta_n\} \quad \text{for all } i.$$

Powers 2, 3, 4, 5 for $n = 3$

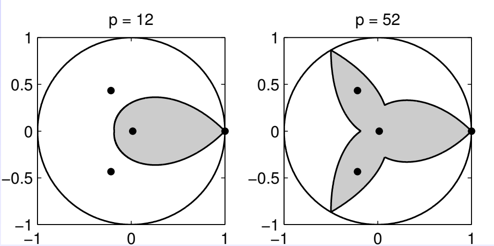


Powers 2, 3, 4, 5 for $n = 4$



Example

$$A = \begin{bmatrix} 1/3 & 1/3 & 0 & 1/3 \\ 1/2 & 0 & 1/2 & 0 \\ 10/11 & 0 & 0 & 1/11 \\ 1/4 & 1/4 & 1/4 & 1/4 \end{bmatrix}.$$



A cannot have a stochastic 12th root, but may have a stochastic 52nd root. None of the 52nd roots is stochastic; $A^{1/12}$ and $A^{1/52}$ both have negative elements.

Dependence on n

- $\Theta_3 \subseteq \Theta_4 \subseteq \Theta_5 \subseteq \dots$.
- # points at which Θ_n intersects unit circle increases rapidly with n: 23 intersection points for Θ_8 and 80 for Θ_{16}.
- As n increases the region Θ_n and its powers tend to fill the unit circle.

Practicalities

- HIV-Aids matrix has spectrum

$$\Lambda(P) = \{1, 0.9644, 0.4980, 0.1493, -0.0043\}.$$

  No real pth root for **even** p.
- Practitioners **regularize** the principal pth root—several approaches.
- Practitioners probably unaware of existence of a non-principal stochastic root.

Conclusions

- Literature on roots of stochastic matrices emphasizes computational aspects over theory.
- Identified two classes of stochastic matrices for which $A^{1/p}$ is stochastic for all p.
- Wide variety of possibilities for existence and uniqueness, in particular re. primary versus nonprimary roots.
- Gave some necessary spectral conditions for existence.
- More work needed on theory and algorithms.

N. J. Higham and L. Lin. On pth roots of stochastic matrices. MIMS EPrint 2009.21, March 2009.

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