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Manchester Numerical Analysis

The University of Manchester

The Matrix Logarithm: from Theory to Computation

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Outline

1. Properties, Formulas & Applications

2. Computation

Matrix Logarithm

A logarithm of $A \in \mathbb{C}^{n \times n}$ is any matrix X such that $e^X = A$.

- Existence.
- Representation, classification.
- Computation.
- Conditioning.

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- Exists iff A nonsingular.
- Not unique.

Logarithm Example

Find a *real* log of $A = -I_{2n}$, i.e., real solution of $e^X = A$.

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$\{-1, -1\} \to \{(2k+1)\pi i, -(2k+1)\pi i\}$.

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Let $H = \pi \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$. Then $e^H = -I_2$.

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Let $H = \pi \left[\begin{smallmatrix} 0 & 1 \\ -1 & 0 \end{smallmatrix}\right]$. Then $e^H = -I_2$. All solutions are

$$X = U \operatorname{diag}\big((2k_1+1)H, (2k_2+1)H, \dots, (2k_n+1)H\big) U^{-1},$$

for real nonsingular U. Thus, e.g., $k_1 = 0$, $k_2 = 1$, integer U,

$$e^X = -I_4 \quad \text{for} \quad X = \pi \begin{bmatrix} 39 & 20 & 12 & 6 \\ -55 & -28 & -15 & -10 \\ 7 & 3 & 0 & 4 \\ -71 & -36 & -24 & -11 \end{bmatrix}.$$

Markov Models (1)

- Time-homogeneous continuous-time Markov process with transition probability matrix $P(t) \in \mathbb{R}^{n \times n}$.
- **Transition intensity matrix** Q: $q_{ij} \geq 0$ $(i \neq j)$, $\sum_{j=1}^{n} q_{ij} = 0$, $P(t) = e^{Qt}$.

For discrete-time Markov processes:

Embeddability problem

When does a given **stochastic** P have a real logarithm Q that is an **intensity matrix**?

NP-hard (Cubitt, Eisert & Wolf, 2012).

Markov Models (2)—Example

With $x = -e^{-2\sqrt{3}\pi} \approx -1.9 \times 10^{-5}$,

$$P = \frac{1}{3}\begin{bmatrix} 1+2x & 1-x & 1-x \\ 1-x & 1+2x & 1-x \\ 1-x & 1-x & 1+2x \end{bmatrix}.$$

- P diagonalizable, $\Lambda(P) = \{1, x, x\}$.
- Every primary log complex (can't have complex conjugate ei'vals).
- Yet a generator is the non-primary log

$$Q = 2\sqrt{3}\pi \begin{bmatrix} -2/3 & 1/2 & 1/6 \\ 1/6 & -2/3 & 1/2 \\ 1/2 & 1/6 & -2/3 \end{bmatrix}.$$

Markov Models (3)–Practicalities

- Let P be transition probability matrix for discrete-time Markov process.
- If P is transition matrix for 1 year, $P(1/12) = P^{1/12} = e^{\frac{1}{12}\log P}$ is matrix for 1 month.
- **Problem**: $\log P$, $P^{1/k}$ may have wrong sign patterns $\Rightarrow$ "regularize".
- In credit risk, P is **strictly diagonally dominant**, which implies at most one generator.

Principal Logarithm and pth Root

Let $A \in \mathbb{C}^{n\times n}$ have no eigenvalues on $\mathbb{R}^-$.

Principal log

$X = \log(A)$ denote unique X such that

- $e^X = A$.
- $-\pi < \operatorname{Im}\big(\lambda(X)\big) < \pi$.

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Principal power

For $s \in \mathbb{R}$, $A^s = e^{s\log A}$.

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Principal power

For $s \in \mathbb{R}$, $A^s = e^{s \log A}$.

- On next few slides relax to arbitrary nonsingular A and $-\pi < \operatorname{Im}\big(\lambda(X)\big) \le \pi$.

Matrix Unwinding Function

Definition (Aprahamian & H, 2014)

$$\mathcal{U}(A) = \frac{A - \log e^A}{2\pi i}, \qquad A \in \mathbb{C}^{n\times n}.$$

Corless, Hare & Jeffrey (1996): $\mathcal{U}(z) = \left\lceil \frac{\operatorname{Im} z - \pi}{2\pi} \right\rceil \in \mathbb{Z}$.

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Jordan form: for $Z^{-1}AZ = \operatorname{diag}(J_k(\lambda_k))$,

$$U(A) = Z\operatorname{diag}(U(\lambda_k)I_{m_k})Z^{-1}.$$

$U(A)$ is diagonalizable and has integer ei'vals.

When is $\log e^A = A$?

Theorem

For $A \in \mathbb{C}^{n\times n}$, $\mathcal{U}(A) = 0$ iff $\operatorname{Im} \lambda(A_j) \in (-\pi, \pi]$ for all j.

Proof: Immediate from JCF formula and scalar case.

Thus $\log e^A = A$ for

- Hermitian
- unitary
- idempotent
- stochastic

as $|\lambda| \le 1$ in every case.

Logarithm of a Fractional Matrix Power (1)

Lemma

For $A \in \mathbb{C}^{n\times n}$ *and* $\alpha \in \mathbb{C}$*,*

$$\log A^{\alpha} = \alpha \log A - 2\pi i \mathcal{U}(\alpha \log A).$$

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Proof.

$$\begin{aligned} \log A^{\alpha} &= \log e^{\alpha \log A} \\ &= \alpha \log A - 2\pi i \mathcal{U}(\alpha \log A). \end{aligned}$$

Logarithm of a Fractional Matrix Power (2)

Corollary

For $A \in \mathbb{C}^{n \times n}$

$$\log(A^\alpha) = \alpha \log A$$

for $\alpha \in (-1, 1]$ *and for* $\alpha = -1$ *if* A *has no eigenvalues on* $\mathbb{R}^-$.

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For $A \in \mathbb{C}^{n\times n}$

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Special cases: $\log A^{-1} = -\log A, \quad \log A^{1/2} = \frac{1}{2}\log A.$

Function of 2×2 Triangular Matrix

$$f\left(\begin{bmatrix} \lambda_1 & t_{12} \\ 0 & \lambda_2 \end{bmatrix}\right) = \begin{cases} \begin{bmatrix} f(\lambda_1) & t_{12}\dfrac{f(\lambda_2)-f(\lambda_1)}{\lambda_2-\lambda_1} \\ 0 & f(\lambda_2) \end{bmatrix}, & \lambda_1 \neq \lambda_2, \\ \begin{bmatrix} f(\lambda) & t_{12}f'(\lambda) \\ 0 & f(\lambda) \end{bmatrix}, & \lambda_1 = \lambda_2 = \lambda. \end{cases}$$

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- (1,2) element given by $t_{12} f[\lambda_2, \lambda_1]$ always.
- **Inaccurate** if $\lambda_1 \approx \lambda_2$.

Log of 2×2 Triangular Matrix

$$\begin{aligned}\log\lambda_2 - \log\lambda_1 &= \log\left(\frac{\lambda_2}{\lambda_1}\right) + 2\pi i\,\mathcal{U}(\log\lambda_2 - \log\lambda_1)\\ &= \log\left(\frac{1+z}{1-z}\right) + 2\pi i\,\mathcal{U}(\log\lambda_2 - \log\lambda_1),\end{aligned}$$

where $\quad z = (\lambda_2 - \lambda_1)/(\lambda_2 + \lambda_1)$.

$$\operatorname{atanh} z := \frac{1}{2}\log\left(\frac{1+z}{1-z}\right),$$

Log of 2 × 2 Triangular Matrix

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where $z = (\lambda_2 - \lambda_1)/(\lambda_2 + \lambda_1)$.

$$\operatorname{atanh} z := \frac{1}{2}\log\left(\frac{1+z}{1-z}\right),$$

$$f_{12} = t_{12}\,\frac{2\operatorname{atanh} z + 2\pi i\,\mathcal{U}(\log\lambda_2 - \log\lambda_1)}{\lambda_2 - \lambda_1}.$$

The Average Eye

First order character of optical system characterized by **transference matrix**

$$T = \begin{bmatrix} S & \delta \\ 0 & 1 \end{bmatrix} \in \mathbb{R}^{5\times 5},$$

where $S \in \mathbb{R}^{4\times 4}$ is **symplectic**:

$$S^T J S = J = \begin{bmatrix} 0 & I_2 \\ -I_2 & 0 \end{bmatrix}.$$

Average $m^{-1}\sum_{i=1}^{m} T_i$ is not a transference matrix.

Harris (2005) proposes the average $\exp(m^{-1}\sum_{i=1}^{m} \log T_i)$.

Other Applications

- Patch modeling-based skin detection (Hu, Zuo, Wu, Chen, Zhang & Suter, 2011).
- In-betweening in computer animations (Rossignac & Vinacua, 2011).
- Mueller matrix $M \in \mathbb{R}^{4\times 4}$ in optics—associated with an element that alters the polarization of light (Chipman, 2010).

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Henry Briggs (1561–1630)

- **Arithmetica Logarithmica** (1624)
- Logarithms to base 10 of 1–20,000 and 90,000–100,000 to **14 decimal places**.

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Briggs must be viewed as one of the great figures in numerical analysis.

—Herman H. Goldstine,
A History of Numerical Analysis (1977)

ARITHMETICA

LOGARITHMICA

SIVE

LOGARITHMORVM CHILIADES TRIGINTA, PRO

numeris naturali ſerie creſcentibus ab vnitate ad 20,000: et a 90,000 ad 100,000. Quorum ope multa perficiuntur Arithmetica problemata et Geometrica.

HOS NVMEROS PRIMVS INVENIT CLARISSIMVS VIR IOHANNES NEPERVS Baro Merchiſtonij: eos autem ex eiuſdem ſententia mutavit, eorumque ortum et vſum illuſtravit HENRICVS BRIGGIVS, in celeberrima Academia Oxonienſi Geometriæ profeſſor SAVILIANVS.

DEVS NOBIS VSVRAM VITÆ DEDIT ET INGENII, TANQVAM PECVNIÆ, NVLLA PRÆSTITVTA DIE.

LONDINI,
Excudebat GVLIELMVS IONES. 1624.

	Numeri continue Medij inter Denarium & Unitatem.	Logarithmi Rationales.
	10	1,000
1	31622,77660,16837,93319,98893,54	0,50
2	17782,79410,03892,28011,97304,13	0,25
3	13335,21432,16332,40256,65389,308	0,125
4	11547,81984,68945,81796,61918,213	0,0625
5	10746,07828,32131,74972,13817,6538	0,03125
6	10366,32928,43769,79972,90627,3131	0,01562,5
7	10181,51721,71818,18414,73723,8144	0,00781,25
8	10090,35044,84144,74377,59005,1391	0,00390,625
9	10045,07364,25446,25156,64670,6113	0,00195,3125
10	10022,51148,29291,29154,65611,7367	0,00097,65625
11	10011,24941,39987,98759,85395,51805	0,00048,82812,5
12	10005,62312,60220,86366,18495,91839	0,00024,41406,25
13	10002,81116,78778,01323,99249,64325	0,00012,20703,125
14	10001,40548,51694,72581,62767,32715	0,00006,10351,5625
15	10000,70271,78941,14355,38811,70845	0,00003,05175,78125
16	10000,35135,27746,18565,08581,37077	0,00001,52587,89062,5
17	10000,17567,48442,26738,33846,78274	0,00000,76293,94531,25
18	10000,08783,70363,46121,46574,07431	0,00000,38146,97265,625
19	10000,04391,84217,31672,36281,88083	0,00000,19073,48632,8125
20	10000,02195,91867,55542,03317,07719	0,00000,09536,74316,40625
21	10000,01097,95873,50204,09754,72940	0,00000,04768,37158,20312,5
22	10000,00548,97921,68211,14626,60250,4	0,00000,02384,18579,10156,25
23	10000,00274,48957,07382,95091,25449,9	0,00000,01192,09289,55078,125
24	10000,00137,24477,59510,83282,69572,5	0,00000,00596,04644,77539,0625
25	10000,00068,62238,56210,25737,18748,2	0,00000,00298,02322,38769,53125
26	10000,00034,31119,22218,83912,75020,8	0,00000,00149,01161,19384,76562,5
27	10000,00017,15559,59637,84719,93879,1	0,00000,00074,50580,59692,38281,25
28	10000,00008,57779,79451,03051,17588,8	0,00000,00037,25290,29846,19140,625
29	10000,00004,28889,89633,54198,42901,3	0,00000,00018,62645,14923,09570,3125
30	10000,00002,14444,94793,77767,42970,4	0,00000,00009,31322,57461,54785,15625
31	10000,00001,07222,47391,14050,76926,8	0,00000,00004,65661,28730,77392,57812,5
32	10000,00000,53611,23594,13317,14831,4	0,00000,00002,32830,64365,38696,28906,25
33	10000,00000,26805,61846,70731,51508,7	0,00000,00001,16415,32182,69348,14453,125
34	10000,00000,13402,80923,26383,99277,7	0,00000,00000,58207,66091,34674,07226,5625
35	10000,00000,06701,40461,60946,55519,6	0,00000,00000,29103,83045,67337,03613,28125
36	10000,00000,03350,70230,79911,91730,0	0,00000,00000,14551,91522,83668,51806,64062,5
37	10000,00000,01675,35115,39815,61857,6	0,00000,00000,07275,95761,41834,25903,32031,25
38	10000,00000,00837,67557,69872,72426,9	0,00000,00000,03637,97880,70917,12951,66015,625
39	10000,00000,00418,83778,84927,59087,9	0,00000,00000,01818,98940,35458,56475,83007,8125
40	10000,00000,00209,41889,42461,60262,5	0,00000,00000,00909,49470,17729,28237,91503,90625
41	10000,00000,00104,70944,71230,25311,0	0,00000,00000,00454,74735,08864,64118,95751,95312

Briggs' Log Method (1617)

$$\log(ab) = \log a + \log b \quad \Rightarrow \quad \log a = 2\log a^{1/2}.$$

Use repeatedly:

$$\log a = 2^k \log a^{1/2^k}.$$

Write $a^{1/2^k} = 1 + x$ and note $\log(1+x) \approx x$. Briggs worked to base 10 and used

$$\log_{10} a \approx 2^k \cdot \log_{10} e \cdot (a^{1/2^k} - 1).$$

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Assume A has no ei'vals on $\mathbb{R}^-$. From *matrix unwinding result*,

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Use Briggs' idea: $\log A = 2^k \log\left(A^{1/2^k}\right).$

Kenney & Laub's (1989) **inverse scaling and squaring** method:

- Bring A close to I by repeated square roots.
- Approximate $\log A^{1/2^k}$ using an $[m/m]$ Padé approximant $r_m(x) \approx \log(1+x)$.
- Rescale to find $\log A$.

Choice of Parameters s, m

Must have $\|I - A^{1/2^s}\| < 1$. Recall $r_m(x) \approx \log(1 + x)$.

- Larger Padé degree m means smaller s.

Let $h_{2m+1}(X) = e^{r_m(X)} - X - I$.
Assume $\rho(r_m(X)) < \pi$, so $\log(e^{r_m(X)}) = r_m(X)$. Then

$$r_m(X) = \log(I + X + \underbrace{h_{2m+1}(X)}_{\Delta X})$$

where

$$h_{2m+1}(X) = \sum_{k=2m+1}^{\infty} c_k X^k.$$

Bounding the Backward Error

Want to bound norm of $h_{2m+1}(X) = \sum_{k=2m+1}^{\infty} c_k X^k$.

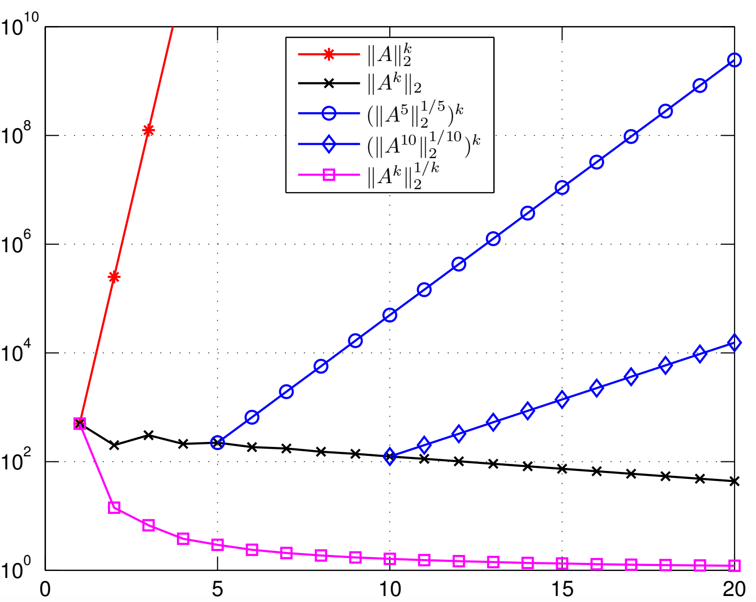
- Non-normality implies $\rho(A) \ll \|A\|$.
- Note that

$$\rho(A) \le \|A^k\|^{1/k} \le \|A\|, \qquad k = 1\colon \infty.$$

  and $\lim_{k\to\infty} \|A^k\|^{1/k} = \rho(A)$.

- Use $\|A^k\|^{1/k}$ instead of $\|A\|$ in the truncation bounds.

$$A = \begin{bmatrix} 0.9 & 500 \\ 0 & -0.5 \end{bmatrix}.$$



Algorithm of Al-Mohy & H (2012)

- Truncation bounds use $\|A^k\|^{1/k}$ rather than $\|A\|$, leading to major benefits in speed and accuracy.
  Matrix norms not such a blunt tool!
- Use *estimates* of $\|A^k\|$ (alg of H & Tisseur (2000)).
- Choose s and m to achieve double precision backward error at minimal cost.
- Initial Schur decomposition: $A = QTQ^*$.
- Directly and accurately compute certain elements of $T^{1/2^s} - I$ and $\log T$. Use

$$a^{1/2^s} - 1 = \frac{a-1}{\prod_{i=1}^{s}(1 + a^{1/2^i})}.$$

Algorithm of Al-Mohy & H (2012) Cont.

- Use above formula for log of 2×2 blocks.
- For real Schur decomposition 2×2 diagonal blocks

$$B = \begin{bmatrix} a & b \\ c & a \end{bmatrix},$$

where $bc < 0$. Ei'vals $\lambda_\pm = a \pm i(-bc)^{1/2}$.
Let $\theta = \arg(\lambda_+) \in (-\pi, \pi)$. Have

$$\log(B) = \begin{bmatrix} \log(a^2 - bc)/2 & \theta b(-bc)^{-1/2} \\ \theta c(-bc)^{-1/2} & \log(a^2 - bc)/2 \end{bmatrix}.$$

Frechét Derivative of Logarithm

$$f(A+E) - f(A) - L_f(A,E) = o(\|E\|).$$

- Integral formula

$$L_f(A,E) = \int_0^1 \bigl(t(A-I)+I\bigr)^{-1} E \bigl(t(A-I)+I\bigr)^{-1} \, dt.$$

- Method based on

$$f\left(\begin{bmatrix} X & E \\ 0 & X \end{bmatrix}\right) = \begin{bmatrix} f(X) & L_f(X,E) \\ 0 & f(X) \end{bmatrix}.$$

- Kenney & Laub (1998): Kronecker–Sylvester alg, Padé of $\tanh(x)/x$. Requires complex arithmetic.

Algorithm of Al-Mohy, H & Relton (2013)

Fréchet differentiate the ISS algorithm!

$E_0 = E$
for $i = 1\colon s$
  Compute $A^{1/2^i}$.
  Solve the Sylvester eqn $A^{1/2^i} E_i + E_i A^{1/2^i} = E_{i-1}$.
end
$\log(A) \approx 2^s r_m(A^{1/2^s} - I)$
$L_{\log}(A, E) \approx 2^s L_{r_m}(A^{1/2^s} - I, E_s)$

Backward Error Result

$$r_m(X) = \log(I + X + \Delta X),$$
$$L_{r_m}(X, E) = L_{\log}(I + X + \Delta X, E + \Delta E).$$

Knowledge Transfer Partnership

- University of Manchester and NAG (2010–2013) funded by EPSRC, NAG and TSB.
- Developed suite of 40 NAG Library codes for matrix functions.
- Extensive set of new codes included in Mark 23 (2012) onwards.
- Improvements to existing state of the art: **faster and more accurate**.

WEDNESDAY, 16 JANUARY 2013

Matrix Functions in Parallel

Last year I wrote a blog post about NAG's work on parallelising the computation of the matrix square root. More recently, as part of our Matrix Functions Knowledge Transfer Partnership with the University of Manchester, we've been investigating parallel implementations of the Schur-Parlett algorithm [1].

Most algorithms for computing functions of matrices are tailored for a specific function, such as the matrix exponential or the matrix square root. The Schur-Parlett algorithm is much more general; it will work for any "well behaved" function (this general term can be given a more mathematically precise meaning). For a function such as

$$f(A) = e^A + \sin 2A - \cosh 4A,$$

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- HPC Technology Consulting
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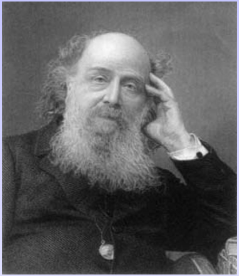
- Training
- Partner Program
- Research & Development

Availability of Algorithms

	MATLAB built-in	MATLAB Third party	NAG Library	SciPy
e^A	$\times$	$\surd$	$\surd$	$\surd$
$\log A$	$\times$	$\surd$	$\surd$	$\surd$
$A^{1/2}$	$\surd$	$\surd$	$\surd$	$\surd$
$f(A)$	$\surd$	$-$	$\surd$	$\times$
A^t	$\times$	$\surd$	$\surd$	$\surd$
$\mathrm{cond}(f, A)$	$\times$	$\surd$	$\surd$	$\times$
$e^A b$	$\times$	$\surd$	$\surd$	$\surd$
$L_{\exp}$	$\times$	$\surd$	$\surd$	$\surd$
$L_{\log}$	$\times$	$\surd$	$\surd$	$\times$
L_{x^t}	$\times$	$\surd$	$\surd$	$\times$

A Catalogue of Software for Matrix Functions (Deadman & H, 2014).

Connections



- **James Joseph Sylvester** (September 3, 1814–March 15, 1897), FRS. Gave first general $f(A)$ formula in 1883:

$$f(A) = \sum_{i=1}^{n} f(\lambda_i) \prod_{j \neq i} \frac{A - \lambda_j I}{\lambda_i - \lambda_j}.$$

  Savilian Professor of Geometry, Oxford: Briggs (1619–1631), Sylvester (1883–1894).

- **Lambert *W* function**: $We^W = A$ (Corless, Gonnet, Hare, Jeffrey & Knuth, 1996).

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