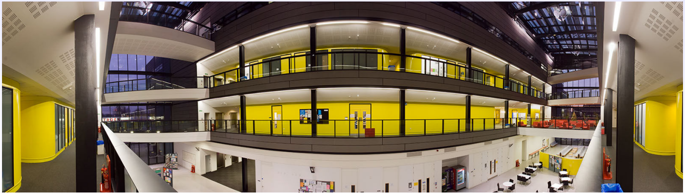
How and How Not to Compute the Exponential of a Matrix

Nick Higham
School of Mathematics
The University of Manchester

higham@ma.man.ac.uk
http://www.ma.man.ac.uk/~higham/

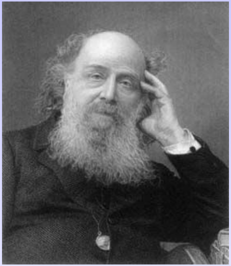


Outline

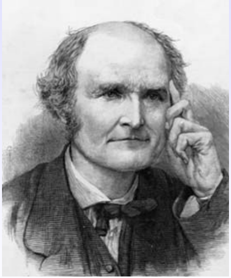
1. History & Properties
2. Applications
3. Methods

Cayley and Sylvester

- Term **"matrix"** coined in 1850 by James Joseph Sylvester, FRS (1814–1897).



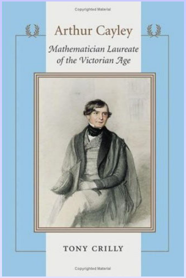
- **Matrix algebra** developed by Arthur Cayley, FRS (1821–1895).
  Memoir on the Theory of Matrices (1858).



Cayley and Sylvester on Matrix Functions

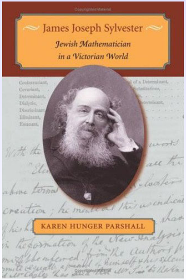
- Cayley considered matrix square roots in his 1858 memoir.

  Tony Crilly, *Arthur Cayley: Mathematician Laureate of the Victorian Age*, 2006.



- Sylvester (1883) gave first definition of $f(A)$ for general f.

  Karen Hunger Parshall, *James Joseph Sylvester. Jewish Mathematician in a Victorian World*, 2006.



Laguerre (1867):

En particulier, si nous définissons e^{X}, X étant un système d'ordre quelconque, comme étant la somme de la série

$$\Omega + \mathrm{X} + \frac{\mathrm{X}^2}{1.2} + \frac{\mathrm{X}^3}{1.2.3} + \ldots,$$

e^{X} sera une fonction de la variable X; mais il est à remarquer qu'en général on n'aura pas

$$e^{\mathrm{X}}.e^{\mathrm{Y}} = e^{\mathrm{X}+\mathrm{Y}}.$$

Peano (1888):

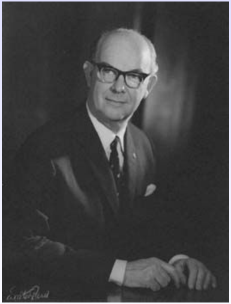
$$\mathbf{x} = \left[1 + \mathbf{R}t + \frac{1}{2!}(\mathbf{R}t)^2 + \cdots\right]\mathbf{a},$$

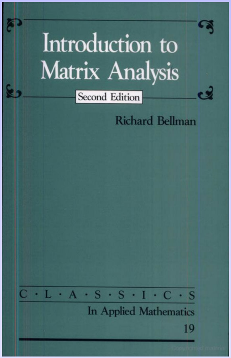
ou, en posant $e^{\mathbf{R}} = 1 + \mathbf{R} + \frac{1}{2!}\mathbf{R}^2 + \cdots,$

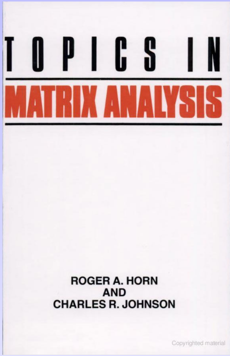
$$\mathbf{x} = e^{\mathbf{R}t}\,\mathbf{a}.$$

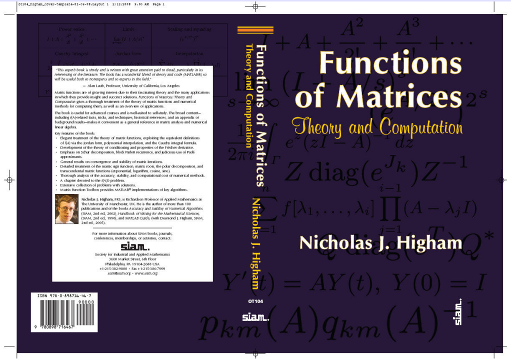
Matrices in Applied Mathematics

- Frazer, Duncan & Collar, Aerodynamics Division of NPL: aircraft flutter, matrix structural analysis.
- **Elementary Matrices & Some Applications to Dynamics and Differential Equations, 1938**. Emphasizes importance of e^A.
- Arthur Roderick Collar, FRS (1908–1986): *"First book to treat matrices as a branch of applied mathematics".*




Introduction to
Matrix Analysis
Second Edition
Richard Bellman
C·L·A·S·S·I·C·S
In Applied Mathematics
19


TOPICS IN
MATRIX ANALYSIS
ROGER A. HORN
AND
CHARLES R. JOHNSON


Functions
of Matrices
Theory and Computation
Nicholas J. Higham
OT104
siam

Formulae

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

Power series $I + A + \frac{A^2}{2!} + \frac{A^3}{3!} + \cdots$	**Limit** $\lim_{s\to\infty} (I + A/s)^s$	**Scaling and squaring** $(e^{A/2^s})^{2^s}$
Cauchy integral $\frac{1}{2\pi i}\int_\Gamma e^z (zI - A)^{-1}\, dz$	**Jordan form** $Z\mathrm{diag}(e^{J_k})Z^{-1}$	**Interpolation** $\sum_{i=1}^{n} f[\lambda_1, \ldots, \lambda_i] \prod_{j=1}^{i-1} (A - \lambda_j I)$
Differential system $Y'(t) = AY(t), \;\; Y(0) = I$	**Schur form** $Q\mathrm{diag}(e^T)Q^*$	**Padé approximation** $p_{km}(A)q_{km}(A)^{-1}$

Properties (1)

Theorem

For $A, B \in \mathbb{C}^{n\times n}$, $e^{(A+B)t} = e^{At}e^{Bt}$ *for all* t *if and only if* $AB = BA$.

Theorem (Wermuth)

Let $A, B \in \mathbb{C}^{n\times n}$ *have algebraic elements and let* $n \geq 2$. *Then* $e^A e^B = e^B e^A$ *if and only if* $AB = BA$.

Properties (1)

Theorem

For $A, B \in \mathbb{C}^{n\times n}$, $e^{(A+B)t} = e^{At}e^{Bt}$ for all t if and only if $AB = BA$.

Theorem (Wermuth)

Let $A, B \in \mathbb{C}^{n\times n}$ have algebraic elements and let $n \ge 2$. Then $e^A e^B = e^B e^A$ if and only if $AB = BA$.

Theorem

Let $A \in \mathbb{C}^{n\times n}$ and $B \in \mathbb{C}^{m\times m}$. Then $e^{A\oplus B} = e^A \otimes e^B$, where $A \oplus B = A \otimes I_m + I_n \otimes B$.

Properties (2)

Theorem (Suzuki)

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

$$T_{r,s} = \left[\sum_{i=0}^{r} \frac{1}{i!}\left(\frac{A}{s}\right)^i\right]^s.$$

Then

$$\|e^A - T_{r,s}\| \le \frac{\|A\|^{r+1}}{s^r(r+1)!} e^{\|A\|}$$

and $\lim_{r\to\infty} T_{r,s}(A) = \lim_{s\to\infty} T_{r,s}(A) = e^A$.

Outline

Application: Control Theory

Convert **continuous-time system**

$$\begin{aligned} \frac{dx}{dt} &= Fx(t) + Gu(t), \\ y &= Hx(t) + Ju(t), \end{aligned}$$

to **discrete-time state-space system**

$$\begin{aligned} x_{k+1} &= Ax_k + Bu_k, \\ y_k &= Hx_k + Ju_k. \end{aligned}$$

Have

$$A = e^{F\tau}, \qquad B = \left(\int_0^\tau e^{Ft} dt \right) G,$$

where τ is the sampling period.
MATLAB Control System Toolbox: **`c2d`** and **`d2c`**.

Psi Functions: Definition

$$\psi_0(z) = e^z, \quad \psi_1(z) = \frac{e^z - 1}{z}, \quad \psi_2(z) = \frac{e^z - 1 - z}{z^2}, \ldots$$

$$\psi_{k+1}(z) = \frac{\psi_k(z) - 1/k!}{z}.$$

$$\boxed{\psi_k(z) = \sum_{j=0}^{\infty} \frac{z^j}{(j+k)!}.}$$

Psi Functions: Solving DEs

$y \in \mathbb{C}^n$, $A \in \mathbb{C}^{n\times n}$.

$$\frac{dy}{dt} = Ay, \quad y(0) = y_0 \quad \Rightarrow \quad y(t) = e^{At} y_0.$$

Psi Functions: Solving DEs

$y \in \mathbb{C}^n$, $A \in \mathbb{C}^{n\times n}$.

$$\frac{dy}{dt} = Ay, \quad y(0) = y_0 \quad \Rightarrow \quad y(t) = e^{At}y_0.$$

$$\frac{dy}{dt} = Ay + b, \quad y(0) = 0 \quad \Rightarrow \quad y(t) = t\,\psi_1(tA)b.$$

Psi Functions: Solving DEs

$y \in \mathbb{C}^n$, $A \in \mathbb{C}^{n\times n}$.

$$\frac{dy}{dt} = Ay, \quad y(0) = y_0 \quad \Rightarrow \quad y(t) = e^{At}y_0.$$

$$\frac{dy}{dt} = Ay + b, \quad y(0) = 0 \quad \Rightarrow \quad y(t) = t\,\psi_1(tA)b.$$

$$\frac{dy}{dt} = Ay + ct, \quad y(0) = 0 \quad \Rightarrow \quad y(t) = t^2\,\psi_2(tA)c.$$

$$\vdots$$

Exponential Integrators

Consider

$$y' = Ly + N(y).$$

$N(y(t)) \approx N(y(0))$ implies

$$y(t) \approx e^{tL} y_0 + t\psi_1(tL) N(y(0)).$$

Exponential Euler method:

$$\boxed{y_{n+1} = e^{hL} y_n + h\psi_1(hL) N(y_n).}$$

Lawson (1967); recent resurgence.

The Average Eye

First order character of optical system characterized by transference matrix $T = \left[\begin{smallmatrix} S & \delta \\ 0 & 1 \end{smallmatrix}\right] \in \mathbb{R}^{5\times 5}$, where $S \in \mathbb{R}^{4\times 4}$ is symplectic: $S^T J S = J$, where $J = \left[\begin{smallmatrix} 0 & I_2 \\ -I_2 & 0 \end{smallmatrix}\right]$.

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

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

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

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

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

For Hermitian pos def A and B, Arsigny et al. (2007) define the log-Euclidean mean

$$E(A, B) = \exp(\tfrac{1}{2}(\log(A) + \log(B))).$$

Beyond Matrices

- GluCat library: generic library of C++ templates for universal Clifford algebras: exp, log, square root, trig functions.
  `http://glucat.sourceforge.net`.
- Group exponential of a diffeomorphism in computational anatomy to study variability among medical images (Bossa et al., 2008).

Outline

Sengupta (Adv. Appl. Prob., 1989)

Note that e^T is a power series in T. This means that a wide variety of methods in linear algebra can also be used to evaluate e^T. ... brute force evaluation of the power series, ... matrix decomposition methods or polynomial methods based on the Cayley-Hamilton theorem ...

Sengupta (Adv. Appl. Prob., 1989)

Note that e^T is a power series in T. This means that a wide variety of methods in linear algebra can also be used to evaluate e^T. ... brute force evaluation of the power series, ... matrix decomposition methods or polynomial methods based on the Cayley-Hamilton theorem ...

Since evaluation of functions of matrices may be fraught with difficulties (such as roundoff and truncation errors, ill conditioning, near confluence of eigenvalues, etc.), there is a distinct advantage in having a rich class of solution techniques available for finding e^T. If one method fails to find an accurate answer, one can always fall back on a different method.

Cayley–Hamilton Theorem

Theorem (Cayley, 1857)

If $A, B \in \mathbb{C}^{n\times n}$, $AB = BA$, and $f(x, y) = \det(xA - yB)$ then $f(B, A) = 0$.

- $p(t) = \det(tI - A)$ implies $p(A) = 0$.
- $A^n = \sum_{k=0}^{n-1} c_n A^k$.
- $e^A = \sum_{k=0}^{n-1} d_n A^k$.

Walz's Method

Walz (1988) proposed computing

$$C_k = (I + 2^{-k}A)^{2^k}$$

with Richardson extrapolation to accelerate cgce of the C_k.

Numerically unstable in practice (Parks, 1994).

Diagonalization (1)

$A = Z\text{diag}(\lambda_i)Z^{-1}$ implies $f(A) = Z\text{diag}(f(\lambda_i))Z^{-1}$.

But

- Z may be ill conditioned ($\kappa(Z) = \|Z\|\|Z^{-1}\| \gg 1$).
- A may not be diagonalizable.

Diagonalization (2)

```
>> A = [3 -1; 1 1]; X = funm_ev(A,@exp)
X =
   14.7781   -7.3891
    7.3891         0
>> norm(X - expm(A))/norm(expm(A))
ans =  1.3431e-009
>>  expm_cond(A)
ans =  3.4676

>> [Z,D]=eig(A)
Z =                        D =
    0.7071     0.7071          2.0000          0
    0.7071     0.7071               0     2.0000
```

Scaling and Squaring Method

- $B \leftarrow A/2^s$ so $\|B\|_\infty \approx 1$
- $r_m(B) = [m/m]$ Padé approximant to e^B
- $X = r_m(B)^{2^s} \approx e^A$

- Originates with **Lawson (1967)**.
- **Ward (1977)**: algorithm, with rounding error analysis and a posteriori error bound.
- **Moler & Van Loan (1978)**: give backward error analysis allowing choice of s and m.
- **H (2005)**: sharper analysis giving optimal s and m. MATLAB's **`expm`**, Mathematica, NAG Library Mark 22.

Padé Approximants r_m to e^x

$r_m(x) = p_m(x)/q_m(x)$ known explicitly:

$$p_m(x) = \sum_{j=0}^{m} \frac{(2m-j)!\, m!}{(2m)!\,(m-j)!} \frac{x^j}{j!}$$

and $q_m(x) = p_m(-x)$. Error satisfies

$$e^x - r_m(x) = (-1)^m \frac{(m!)^2}{(2m)!(2m+1)!} x^{2m+1} + O(x^{2m+2}).$$

Scaling and Squaring Method

$$h_{2m+1}(X) := \log(e^{-X} r_m(X)) = \sum_{k=2m+1}^{\infty} c_k X^k.$$

Then $r_m(X) = e^{X + h_{2m+1}(X)}$. Hence

$$r_m(2^{-s}A)^{2^s} = e^{A + 2^s h_{2m+1}(2^{-s}A)} =: e^{A + \Delta A}.$$

Want $\|\Delta A\| / \|A\| \le u$.

- Moler & Van Loan (1978): a priori bound for h_{2m+1}; $m = 6$, $\|2^{-s}A\| \le 1/2$ in MATLAB.
- H (2005): sharp normwise bound using symbolic arithmetic and high precision. Choose (s, m) to minimize computational cost.

Scaling & Squaring Algorithm (H, 2005)

m	3	5	7	9	13
θ_m	0.015	0.25	0.95	2.1	5.4

for $m = [3\ 5\ 7\ 9\ 13]$
    if $\|A\|_1 \le \theta_m$, $X = r_m(A)$, quit, end
end

Scaling & Squaring Algorithm (H, 2005)

m	3	5	7	9	13
θ_m	0.015	0.25	0.95	2.1	5.4

for $m = [3\ 5\ 7\ 9\ 13]$
    if $\|A\|_1 \le \theta_m$, $X = r_m(A)$, quit, end
end

$A \leftarrow A/2^s$ with $s \ge 0$ minimal s.t. $\|A/2^s\|_1 \le \theta_{13} = 5.4$

Scaling & Squaring Algorithm (H, 2005)

m	3	5	7	9	13
θ_m	0.015	0.25	0.95	2.1	5.4

for $m = [3\ 5\ 7\ 9\ 13]$
    if $\|A\|_1 \le \theta_m$, $X = r_m(A)$, quit, end
end

$A \leftarrow A/2^s$ with $s \ge 0$ minimal s.t. $\|A/2^s\|_1 \le \theta_{13} = 5.4$
$A_2 = A^2$, $A_4 = A_2^2$, $A_6 = A_2 A_4$
$U = A\big[A_6(b_{13}A_6 + b_{11}A_4 + b_9A_2) + b_7A_6 + b_5A_4 + b_3A_2 + b_1 I\big]$
$V = A_6(b_{12}A_6 + b_{10}A_4 + b_8A_2) + b_6A_6 + b_4A_4 + b_2A_2 + b_0 I$
Solve $(-U + V)r_{13} = U + V$ for r_{13}.
$X = {r_{13}}^{2^s}$ by repeated squaring.

Example

$$A = \begin{bmatrix} 1 & b \\ 0 & -1 \end{bmatrix}, \qquad e^A = \begin{bmatrix} e & \frac{b}{2}(e - e^{-1}) \\ 0 & e^{-1} \end{bmatrix}.$$

b	$\texttt{expm}(A)$	s	$\texttt{expm}(A)^\dagger$	s	$\texttt{funm}(A)$
10^3	1.7e-15	8	1.9e-16	0	1.9e-16
10^4	1.8e-13	11	7.6e-20	0	3.8e-20
10^5	7.5e-13	15	1.2e-16	0	1.2e-16
10^6	1.3e-11	18	2.0e-16	0	2.0e-16
10^7	7.2e-11	21	1.6e-16	0	1.6e-16
10^8	3.0e-12	25	1.3e-16	0	1.3e-16

For $b = 10^8$, $r_m(x)^{2^{25}} \approx \left((1 + \frac{1}{2}x)/(1 - \frac{1}{2}x)\right)^{2^{25}}$ with $x = \pm 2^{-25} \approx \pm 10^{-8}$.

Overscaling

Kenney & Laub (1998); Dieci & Papini (2000).

A large $\|A\|$ causes a larger than necessary s to be chosen, with a harmful effect on accuracy.

$$\exp\left(\begin{bmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{bmatrix}\right) = \begin{bmatrix} e^{A_{11}} & \int_0^1 e^{A_{11}(1-s)} A_{12} e^{A_{22}s}\, ds \\ 0 & e^{A_{22}} \end{bmatrix}.$$

Insight

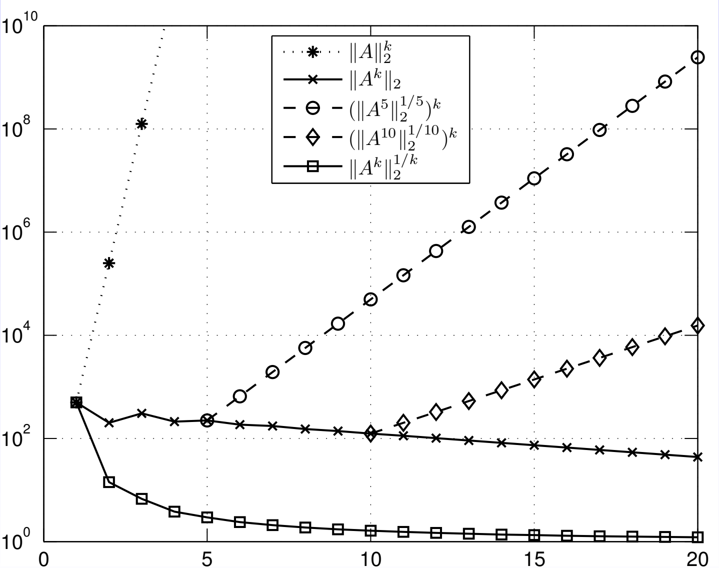
Al-Mohy & H (2009):

Existing method based on analysis in terms of $\|A\|$.
Why not instead use $\|A^k\|^{1/k}$?

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

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

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



Key Bounds (1)

Theorem

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

$$\Big\| \sum_{k=\ell}^{\infty} c_k A^k \Big\| \le \sum_{k=\ell}^{\infty} |c_k| \left(\|A^t\|^{1/t} \right)^k$$

where $\|A^t\|^{1/t} = \max\{ \|A^k\|^{1/k} : k \ge \ell,\ c_k \ne 0 \}$.

Proof. Use $\|A^k\| = \left(\|A^k\|^{1/k}\right)^k \le \left(\|A^t\|^{1/t}\right)^k$. $\square$

Key Bounds (2)

Lemma

If $k = pm_1 + qm_2$ *with* $p, q \in \mathbb{N}$ *and* $m_1, m_2 \in \mathbb{N} \cup \{0\}$,

$$\|A^k\|^{1/k} \le \max\left(\|A^p\|^{1/p}, \|A^q\|^{1/q}\right).$$

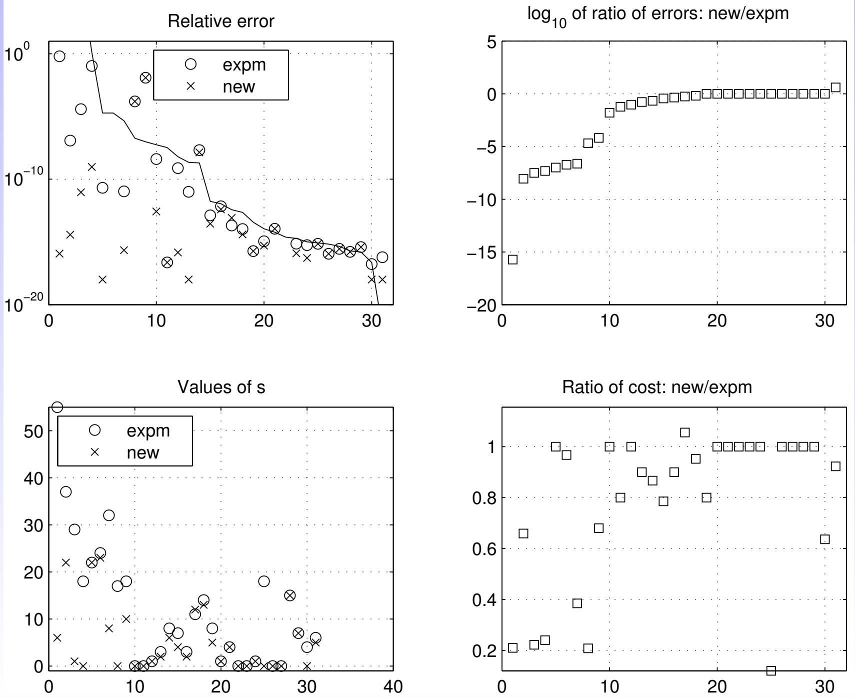
Proof. Let $\delta = \max(\|A^p\|^{1/p}, \|A^q\|^{1/q})$. Then

$$\begin{aligned} \|A^k\| &\le \|A^{pm_1}\| \, \|A^{qm_2}\| \\ &\le \left(\|A^p\|^{1/p}\right)^{pm_1} \left(\|A^q\|^{1/q}\right)^{qm_2} \\ &\le \delta^{pm_1}\delta^{qm_2} = \delta^k. \qquad \square \end{aligned}$$

- Take $\{p, q\} = \{r, r+1\}$ for $k \ge r(r-1)$.

New Scaling and Squaring Algorithm

- Truncation bounds use $\|A^k\|^{1/k}$ instead of $\|A\|$.
- Roundoff considerations: correction to chosen m.
- Use *estimates* of $\|A^k\|$ where necessary (alg of H & Tisseur (2000)).
- Special treatment of triangular matrices to ensure accurate diagonal.
- New alg no slower than `expm`, potentially faster, potentially more accurate.



Relative error
expm
new
10^0
10^{-10}
10^{-20}
0
10
20
30
$\log_{10}$ of ratio of errors: new/expm
5
0
−5
−10
−15
−20
Values of s
50
40
30
20
10
Ratio of cost: new/expm
1
0.8
0.6
0.4
0.2

Summary of New Alg

- Major benefits in speed and accuracy through using $\|A^k\|^{1/k}$ in place of $\|A\|^k$.
- Overscaling problem “solved”.
- Stability of squaring phase remains an open question.

Frechét Derivative

$$\boxed{f(A+E) - f(A) - L(A,E) = o(\|E\|).}$$

$$L(A,E) = \int_0^1 e^{A(1-s)} E e^{As} \, ds.$$

- Method based on

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

- Kenney & Laub (1998): Kronecker–Sylvester alg, Padé of $\tanh(x)/x$: $538n^3$ (complex) flops.
- **Al-Mohy & H (2009)**: e^A and $L(A,E)$ in only $48n^3$ flops.

In Conclusion

- Many applications of $f(A)$, e.g. control theory, Markov chains, theoretical physics.
- Need better understanding of conditioning of $f(A)$.
- How to exploit structure?
- Need “factorization-free” methods for large, sparse A.
- Specialize to $f(A)b$ problem.

References I

A. H. Al-Mohy and N. J. Higham.
Computing the Fréchet derivative of the matrix exponential, with an application to condition number estimation.
SIAM J. Matrix Anal. Appl., 30(4):1639–1657, 2009.

A. H. Al-Mohy and N. J. Higham.
A new scaling and squaring algorithm for the matrix exponential.
SIAM J. Matrix Anal. Appl., 31(3):970–989, 2009.

References II

R. Bellman.
Introduction to Matrix Analysis.
McGraw-Hill, New York, second edition, 1970. xxiii+403 pp.
Reprinted by Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 1997. ISBN 0-89871-399-4.

M. Bossa, E. Zacur, and S. Olmos.
Algorithms for computing the group exponential of diffeomorphisms: Performance evaluation.
In *Computer Vision and Pattern Recognition Workshops, 2008 (CVPRW '08)*, pages 1–8. IEEE Computer Society, 2008.

References III

T. Crilly.
Cayley's anticipation of a generalised Cayley–Hamilton theorem.
Historia Mathematica, 5:211–219, 1978.

T. Crilly.
Arthur Cayley: Mathematician Laureate of the Victorian Age.
Johns Hopkins University Press, Baltimore, MD, USA, 2006.
ISBN 0-8018-8011-4.
xxi+610 pp.

References IV

L. Dieci and A. Papini.
Padé approximation for the exponential of a block triangular matrix.
Linear Algebra Appl., 308:183–202, 2000.

R. A. Frazer, W. J. Duncan, and A. R. Collar.
Elementary Matrices and Some Applications to Dynamics and Differential Equations.
Cambridge University Press, Cambridge, UK, 1938.
xviii+416 pp.
1963 printing.

References V

- Glucat: Generic library of universal Clifford algebra templates.
  |http://glucat.sourceforge.net/|.

- N. J. Higham.
  The Matrix Function Toolbox.
  http://www.ma.man.ac.uk/~higham/mftoolbox.

References VI

N. J. Higham.
Functions of Matrices: Theory and Computation.
Society for Industrial and Applied Mathematics, Philadelphia, PA, USA, 2008.
ISBN 978-0-898716-46-7.
xx+425 pp.

R. A. Horn and C. R. Johnson.
Topics in Matrix Analysis.
Cambridge University Press, Cambridge, UK, 1991.
ISBN 0-521-30587-X.
viii+607 pp.

References VII

C. S. Kenney and A. J. Laub.
A Schur–Fréchet algorithm for computing the logarithm and exponential of a matrix.
SIAM J. Matrix Anal. Appl., 19(3):640–663, 1998.

M. J. Parks.
A Study of Algorithms to Compute the Matrix Exponential.
PhD thesis, Mathematics Department, University of California, Berkeley, CA, USA, 1994.

References VIII

K. H. Parshall.
James Joseph Sylvester. Jewish Mathematician in a Victorian World.
Johns Hopkins University Press, Baltimore, MD, USA, 2006.
ISBN 0-8018-8291-5.
xiii+461 pp.

B. Sengupta.
Markov processes whose steady state distribution is matrix-exponential with an application to the $GI/PH/1$ queue.
Adv. Applied Prob., 21(1):159–180, 1989.

References IX

G. Walz.
Computing the matrix exponential and other matrix functions.
J. Comput. Appl. Math., 21:119–123, 1988.