How and How Not to Compute the Exponential of a Matrix

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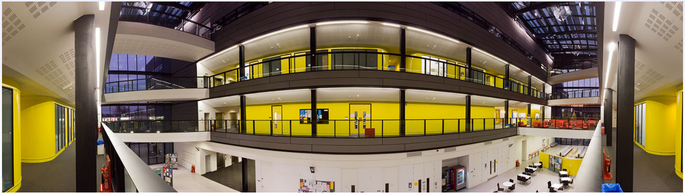
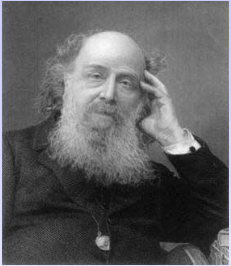


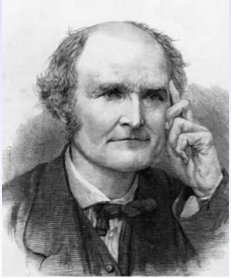
Outline

Cayley and Sylvester

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



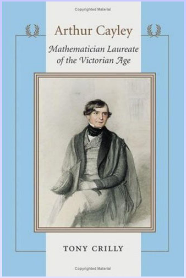
- **Matrix algebra** developed by Arthur Cayley, FRS (1821–1895).
  Memoir on the Theory of Matrices (1858).



Cayley and Sylvester on Matrix Functions

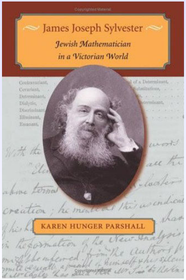
- Cayley considered matrix square roots in his 1858 memoir.

  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):

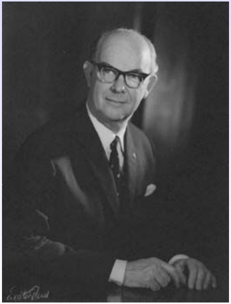
$$\mathbf{x} = \left[1 + \mathbf{R}t + \frac{1}{2!}(\mathbf{R}t)^2 + \cdots\right]\mathbf{a},$$

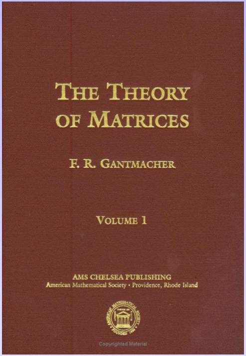
ou, en posant $e^{\mathbf{R}} = 1 + \mathbf{R} + \frac{1}{2!}\mathbf{R}^2 + \cdots,$

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

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"*.

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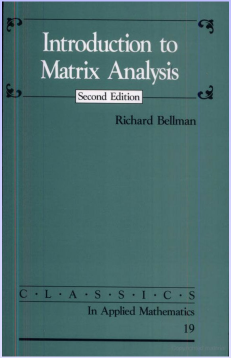
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In Applied Mathematics
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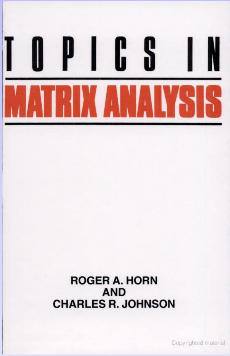
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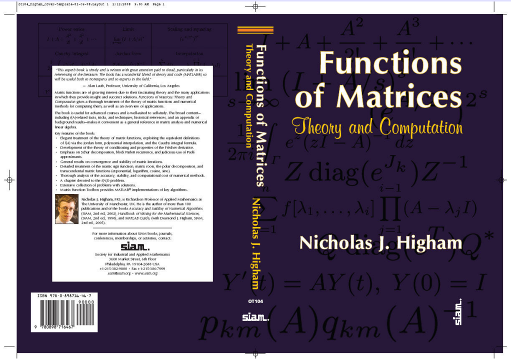
Functions of Matrices
Theory and Computation
Nicholas J. Higham
OT104
siam.

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** $p_{km}(A)q_{km}(A)^{-1}$

Exponential of Sum

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 $AB = BA$.

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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 $A \oplus B = A \otimes I_m + I_n \otimes B$.

Taylor Series

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

1. History & Properties
2. Applications
3. Methods

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`.

Phi Functions: Definition

$$\varphi_0(z) = e^z, \quad \varphi_1(z) = \frac{e^z - 1}{z}, \quad \varphi_2(z) = \frac{e^z - 1 - z}{z^2}, \ldots$$

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

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

Phi Functions: Solving DEs

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

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

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$$\frac{dy}{dt} = Ay + b, \quad y(0) = 0 \quad \Rightarrow \quad y(t) = t\,\varphi_1(tA)b.$$

$$\frac{dy}{dt} = Ay + ct, \quad y(0) = 0 \quad \Rightarrow \quad y(t) = t^2\,\varphi_2(tA)c.$$

$$\vdots$$

Exponential Integrators

Consider

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

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

$$y(t) \approx e^{tL} y_0 + t\varphi_1(tL)N(y(0)).$$

Exponential Euler method:

$$\boxed{y_{n+1} = e^{hL} y_n + h\varphi_1(hL)N(y_n).}$$

Lawson (1967); recent resurgence.

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 $\exp(m^{-1}\sum_{i=1}^{m}\log(T_i))$.

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).

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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)

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

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 $q_m(x) = p_m(-x)$.

Henri Padé
1863–1953

Error satisfies

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

Truncation Analysis

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

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

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

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

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$A_2 = A^2$, $A_4 = A_2^2$, $A_6 = A_2 A_4$

$$U = A\big[A_6(b_{13}A_6 + b_{11}A_4 + b_9A_2) + b_7A_6 + b_5A_4 + b_3A_2 + b_1 I\big]$$

$$V = A_6(b_{12}A_6 + b_{10}A_4 + b_8A_2) + b_6A_6 + b_4A_4 + b_2A_2 + b_0 I$$

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	`expm`(A)	s	`funm`(A)
10^3	1.7e-15	8	1.9e-16
10^4	1.8e-13	11	3.8e-20
10^5	7.5e-13	15	1.2e-16
10^6	1.3e-11	18	2.0e-16
10^7	7.2e-11	21	1.6e-16
10^8	3.0e-12	25	1.3e-16

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.

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x	$e^x - (1+x)$	$e^x - (1+x/2)^2$
9.9e-9	2.2e-16	6.7e-16
8.9e-9	0	6.7e-16

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

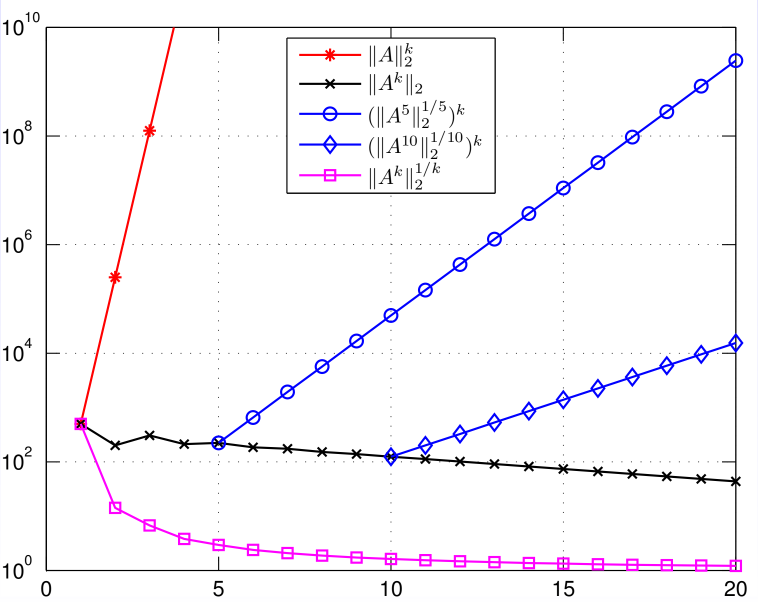
Insight

- 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.

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



New Alg (Al-Mohy & H, 2009)

- Truncation bounds use $\|A^k\|^{1/k}$ rather than $\|A\|$, leading to major benefits in speed and accuracy.

- Special treatment of triangular matrices leads to more stable squaring phase.

Example

$$A = \begin{bmatrix} 1 & b \\ 0 & -1 \end{bmatrix}, \quad A^{2k} \equiv I, \quad A^{2k+1} \equiv A.$$

New alg selects $s = 0$, $m = 9$ for all b.

b	expm	expm_new	cost: $\frac{\texttt{expm}}{\texttt{expm\_new}}$
10^3	1.7e-15	0	2.8
10^4	1.8e-13	0	3.4
10^5	7.5e-13	0	4.2
10^6	1.3e-11	2.0e-16	4.8
10^7	7.2e-11	0	5.4
10^8	3.0e-12	1.3e-16	6.2
10^{17}	1.5e-1	1.4e-16	12.2

Summary of New Algorithm

- Overscaling problem alleviated.
- New algorithm is no slower than **`expm`**, potentially faster, potentially more accurate.

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- Overscaling problem alleviated.
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Stability of squaring phase for full matrices remains an **open problem**.

The $e^A B$ Problem

Exploit, for integer s,

$$e^A B = (e^{s^{-1}A})^s B = \underbrace{e^{s^{-1}A} e^{s^{-1}A} \cdots e^{s^{-1}A}}_{s \text{ times}} B.$$

Choose s so $T_m(s^{-1}A) = \sum_{j=0}^{m} \dfrac{(s^{-1}A)^j}{j!} \approx e^{s^{-1}A}$. Then

$$B_{i+1} = T_m(s^{-1}A)B_i, \quad i = 0\colon s-1, \qquad B_0 = B$$

yields $B_s \approx e^A B$.

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Choose s and m using $\|A^k\|^{1/k}$ approach.

Algorithm for $F = e^{tA}B$ (Al-Mohy & H, 2010)

$\mu = \mathrm{trace}(A)/n$

$A = A - \mu I$

$[m, s] = \mathrm{parameters}(tA)$

$F = B,\ \eta = e^{t\mu/s}$

for $i = 1\colon s$

  $c_1 = \|B\|_\infty$

  for $j = 1\colon m$

    $B = tAB/(sj),\ c_2 = \|B\|_\infty$

    $F = F + B$

    if $c_1 + c_2 \le \mathrm{tol}\|F\|_\infty$, quit, end

    $c_1 = c_2$

  end

  $F = \eta F,\ B = F$

end

The Sixth Dubious Way

Moler & Van Loan (1978, 2003)

METHOD 6. SINGLE STEP O.D.E. METHODS. Two of the classical techniques for the solution of differential equations are the fourth order Taylor and Runge–Kutta methods with fixed step size. For our particular equation they become

$$x_{j+1} = \left(I + hA + \cdots + \frac{h^4}{4!}A^4\right)x_j = T_4(hA)x_j$$

and

$$x_{j+1} = x_j + \tfrac{1}{6}k_1 + \tfrac{1}{3}k_2 + \tfrac{1}{3}k_3 + \tfrac{1}{6}k_4,$$

where $k_1 = hAx_j$, $k_2 = hA(x_j + \frac{1}{2}k_1)$, $k_3 = hA(x_j + \frac{1}{2}k_2)$, and $k_4 = hA(x_j + k_3)$. A little manipulation reveals that in this case, the two methods would produce identical results were it not for roundoff error. As long as the step size is fixed, the matrix $T_4(hA)$ need be computed just once and then x_{j+1} can be obtained from x_j with just one matrix-vector multiplication. The standard Runge–Kutta method would require 4 such multiplications per step.

Let us consider $x(t)$ for one particular value of t, say $t = 1$. If $h = 1/m$, then

$$x(1) = x(mh) \simeq x_m = [T_4(hA)]^m x_0.$$

Advantages of New Algorithm

Versus **one-step ODE integrators**:

- Fully exploits the **linearity** of the ODE.
- **Variable order**, up to $m = 55$.
- **Backward error** based; ODE integrator controls local (forward) errors.
- **Overscaling** avoided.

Versus **Krylov methods**:

- Very competitive in cost and storage.
- Cost dominated by matrix–vector multiplications.
- Black box: no need to choose/tune parameters.

Frechét Derivative

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

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

- 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

- Growing number of applications of $f(A)$.
- $f(A)$ algorithms ready for library deployment.
- Need better understanding of conditioning of $f(A)$.
- How to exploit structure?
- More work needed on $f(A)b$ problem.

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