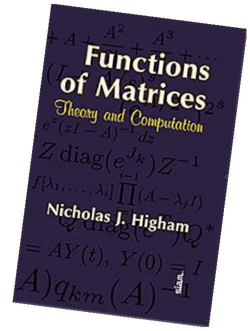
Nick Trefethen, 15 Sept. 2021

Computing $f(A)$ and in particular e^A

1. Why do we want $f(A)$?



For all sorts of reasons. That said, it's rare to need exotic functions like $\Gamma(A)$ or $\zeta(A)$ or $Ai(A)$. More often we want e^A, $\log(A)$, $A^{1/2}$. Also $\mathrm{sign}(A)$ and other projectors.

One reason f tends to be simple is that it often comes from differential equations or operators.

- Most fundamental example: $\frac{\mathrm{d}u}{\mathrm{d}t} = Au$ has solution $u(t) = \mathrm{e}^{tA}u(0)$.
- Exponential integrators: high-order solns via "phi functions," e.g. $\varphi_2(A) = A^{-2}(\mathrm{e}^A - I - A)$.
- Anomalous diffusion example: $\partial_t u = \Delta^{1/2} u$ can be approximated via $A^{1/2}$ with $A \approx \Delta$.
- More anomalous diffusion: $(\partial_t)^{1/2} u = \Delta u$ leads to the Mittag-Leffler function of a matrix A.

2. How do we define $f(A)$?

I. Diagonalization / Jordan decomposition

If A is diagonal, $f(A)$ has the obvious elementwise definition.
If A is diagonalizable with $A = SDS^{-1}$, we define $f(A) = Sf(D)S^{-1}$.
If A is nondiagonalizable with $k \times k$ Jordan block at eigenvalue λ, this definition generalizes using $f(\lambda), f'(\lambda), \dots, f^{(k-1)}(\lambda)$.

II. Polynomial interpolation

If A is diagonalizable, $f(A) = p(A)$, where p interpolates f at the eigenvalues.
If A is nondiagonalizable, p becomes Hermite interpolant involving $f(\lambda), f'(\lambda), \dots, f^{(k-1)}(\lambda)$.

III. Contour integral

The Cauchy integral for scalar analytic functions is $f(a) = \frac{1}{2\pi \mathrm{i}} \int_\Gamma \frac{f(z)}{z-a} \mathrm{d}z$. For matrices, $f(A) = \frac{1}{2\pi \mathrm{i}} \int_\Gamma (zI - A)^{-1} f(z) \mathrm{d}z$.

Γ must lie in the region of analyticity of f and enclose the spectrum of A.
For projectors such as $(\mathrm{sign}(A) + I)/2$, Γ may enclose just certain parts of the spectrum.

3. How do we compute $f(A)$?

I. Schur-Parlett algorithm

Compute Schur form, $A = U\,T\,U^*$ with U unitary and T triangular.
With considerable clever engineering, one can then compute
$f(A) = Uf(T)U^*$. Worst case $O(n^4)$ work. → MATLAB funm(A).

Davies & Higham, SIMAX 2003

II. Polynomial and rational approximation

Approximate $f(z)$ by $p(z)$ or $r(z) = p(z)/q(z)$ for z in nbhd of spectrum of A.
Often r is a composite of simpler rational functions. Then use $f(A) \approx p(A)$ or $r(A)$.
→ MATLAB expm(A), based on type (13,13) Padé approx $\mathrm{e}^z \approx r(z)$.

Higham, SIREV 2009

III. Discretized contour integrals

Discretize $f(A) = \frac{1}{2\pi \mathrm{i}} \int_\Gamma (zI - A)^{-1} f(z) \mathrm{d}z$ by e.g. m-point trapezoidal rule over a circle.
Geometric convergence as $m \to \infty$, independent of dimension of A.
This reduces $f(A)b$ to m linear systems $(z_j I - A)w_j = b$.
Transformation by a conformal map may speed this up dramatically.

Hale-Higham-T., SINUM 2008

4. What's special for e^A?

One can use ODE methods to compute e^{tA}. But more often it's the other way around.

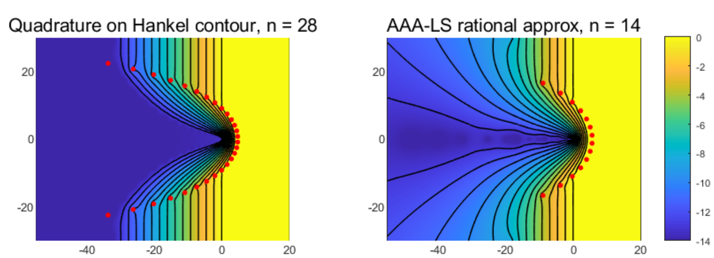
Moler & Van Loan, SIREV 2003

expm(A) uses "scaling-and-squaring": $\mathrm{e}^A = \left(\mathrm{e}^{A/2^s}\right)^{2^s}$. So it's a composite of Padé approximations.

Contour integrals: $\mathrm{e}^A = \frac{1}{2\pi \mathrm{i}} \int_\Gamma (zI - A)^{-1} \mathrm{e}^z \mathrm{d}z$ is the inverse Laplace transform.

Expert: J. A. C. Weideman

Quadrature formulas all implicitly involve rational approximations.
So contour integral and rational approximation methods for $f(A)$ are very close.
For $f(A) = \mathrm{e}^A$ this is particularly well studied.



← 14-digit eval. of e^A: 7 backslashes

T.-Weideman-Schmelzer, BIT 2006
Costa & T., 8ECM 2021