M3M6: Methods of Mathematical Physics

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1 Lecture 7: Matrix norms and matrix functions

This lecture we start to introduce an application of Cauchy's integral formula and trapezium rule: computing matrix functions, e.g., the matrix exponential e^A . There are three possible definitions for matrix functions:

- 1. Taylor series
- 2. Diagonalisation/Jordan canonical form
- 3. Cauchy's integral formula

1.1 Matrix norms

Before discussing matrix functions we first review the notion of a matrix norm induced by a vector norm:

$$||A|| := \sup_{v:||v||=1} ||Av|| = \sup_{v} \frac{||Av||}{||v||}$$

some examples of matrix norms are the 1-norm

$$||A||_1 = \max_i ||A\mathbf{e}_i||_1$$

that is the maximum column sum, the ∞ -norm

$$||A||_{\infty} = \max_{k} ||A^{\top} \mathbf{e}_{k}||_{1}$$

that is the maximum row sum and the 2-norm

$$||A||_{2}$$

which equals the largest singular value, that is the square-root of the largest eigenvalue of $A^{\top}A$

Matrix norms have the usual norm properties, here α is constant and B has same dimensions as A:

1.

$$\|\alpha A\| = |\alpha| \|A\|$$

2.

$$||A + B|| \le ||A|| + ||B||$$

They have the extra feature that

$$||AB|| \le ||A|| ||B||$$

which implies that

$$||A^k|| \le ||A||^k.$$

1.1.1 Taylor series definition

One way to construct matrix exponentials is by Taylor series.

Def(Taylor series matrix function) Suppose

$$f(z) = \sum_{k=0}^{\infty} f_k z^k$$

converges in radius R. If ||A|| < R holds true for any matrix norm, then define

$$f(A) := \sum_{k=0}^{\infty} f_k A^k.$$

The well-posedness of this construction follows from the fact that the partial sums form a Cauchy sequence. In particular, let $\epsilon > 0$. Then for r = ||A|| < R we can choose N such that

$$\sum_{k=n}^{m} |f_k| r^k \le \epsilon$$

for all n, m > N. Therefore

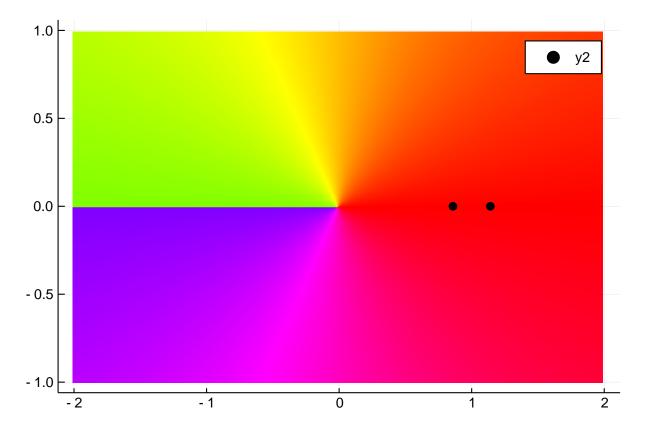
$$\|\sum_{k=n}^{m} f_k A^k\| \le \sum_{k=n}^{m} |f_k| \|A\|^k \le \epsilon.$$

The issue with Taylor series is that it requires analyticity to converge. We can see this clearly for the case \sqrt{A} with Taylor series around 1:

$$\sqrt{z+1} = 1 + z/2 - z^2/8 + z^3/16 - \dots = 1 + z/2 + \sum_{k=3}^{\infty} \frac{3 \cdots (2k-3)}{2^k k!} (-z)^k$$

Consider

using Plots, ComplexPhasePortrait, IntervalSets, LinearAlgebra $A = [1 \ 0.1; \ 0.2 \ 1]$ $\lambda = eigvals(A)$ phaseplot(-2..2, -1..1, z -> sqrt(z)) scatter!(real(λ),imag(λ); color=:black)



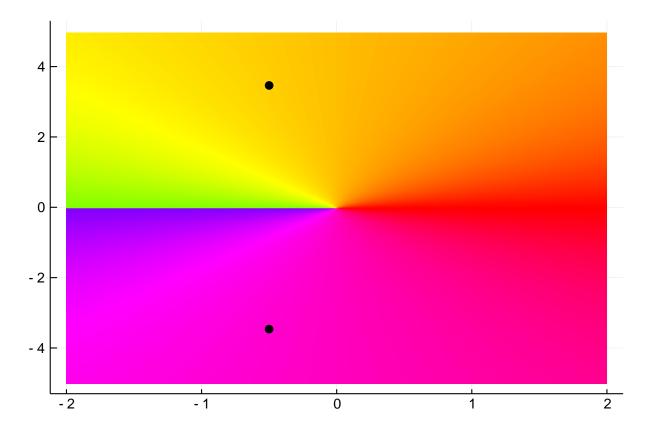
Then, using a slightly modified sqrt_n from Lecture 6 to compute the Taylor series and comparing with sqrt(A) which is Julia's implementation of matrix square root, we see convergence, as the spectrum of A lies inside the radius of convergence around 1:

```
function sqrt n(n,z,z_0)
    ret = sqrt(z_0) * one(A)
    c = 0.5*inv(ret)*(z-z_0*I)
    for k=1:n
        ret += c
        c *= -(2k-1)/(2*(k+1)*z_0)*(z-z_0*I)
    end
    ret
end
norm(sqrt(A) - sqrt_n(100,A,1))
```

7.738033469234878e-16

But if the eigenvalues become much larger this won't work. Here we see an example of a matrix whose eigenvalues are not in the radius of convergence:

```
using Plots, ComplexPhasePortrait, IntervalSets A = [-0.5 -4; 3 -0.5] \lambda = \text{eigvals(A)} phaseplot(-2..2, -5..5, z -> sqrt(z)) scatter!(real(\lambda),imag(\lambda); color=:black, legend=false)
```



Using the partial sum of the Taylor series completely fails, and catastrophically so: norm(sqrt(A) - sqrt_n(100,A,1))

2.1239250131186014e54

1.2 Diagonalisation/Jordan canonical form

Def (Diagonalisation matrix function) Suppose $A = V\Lambda V^{-1}$ where

$$\Lambda = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_d \end{pmatrix}$$

Then define

$$f(A) := V f(\Lambda) V^{-1} = V \begin{pmatrix} f(\lambda_1) & & \\ & \ddots & \\ & & f(\lambda_d) \end{pmatrix} V^{-1}$$

This works very well as a definition but is slow for large matrices and does not take advantage of sparsity.

We can extend it to Jordan canonical form:

Def (Jordan canonical form) Suppose

$$A = V \begin{pmatrix} J_1 & & \\ & \ddots & \\ & & J_{\tilde{d}} \end{pmatrix} V^{-1}$$

where J_k are Jordan blocks, that is,

$$J_k = \begin{pmatrix} \lambda_k & 1 & & \\ & \ddots & \ddots & \\ & & \lambda_k & 1 \\ & & & \lambda_k \end{pmatrix}$$

Then define

$$f(A) := V \begin{pmatrix} f(J_1) & & \\ & \ddots & \\ & & f(J_{\tilde{d}}) \end{pmatrix} V^{-1}$$

using

$$f\begin{pmatrix} \begin{pmatrix} \lambda & 1 & & \\ & \ddots & \ddots & \\ & & \lambda & 1 \\ & & & \lambda \end{pmatrix} = \begin{pmatrix} f(\lambda) & f'(\lambda) & \cdots & f^{(m-1)}(\lambda)/(m-1)! \\ & \ddots & \ddots & & \vdots \\ & & f(\lambda) & & f'(\lambda) \\ & & & f(\lambda) \end{pmatrix}.$$

This definition can be verified to be consistent with Taylor series when both are valid by direct inspection. For example, we have

$$\begin{pmatrix} \lambda & 1 & \lambda \end{pmatrix}^k = \begin{pmatrix} \lambda^k & k\lambda^{k-1} & \lambda^k \end{pmatrix}.$$

1.3 Caucy's integral formula

The last approach we detail in the next lecture is to use the Cauchy integral formula:

Def (Cauchy's integral matrix function) Suppose γ is a simple, closed contour that surrounds the spectrum of A. Then define

$$f(A) := \frac{1}{2\pi i} \oint_{\gamma} f(\zeta) (\zeta I - A)^{-1} d\zeta$$

Here the integrand is a matrix-valued function, hence consider the integral as defined entrywise.

Before we explain where this comes from, we can test on a simple example.

```
A = [-0.5 - 4; 3 - 0.5]

\lambda= eigvals(A)

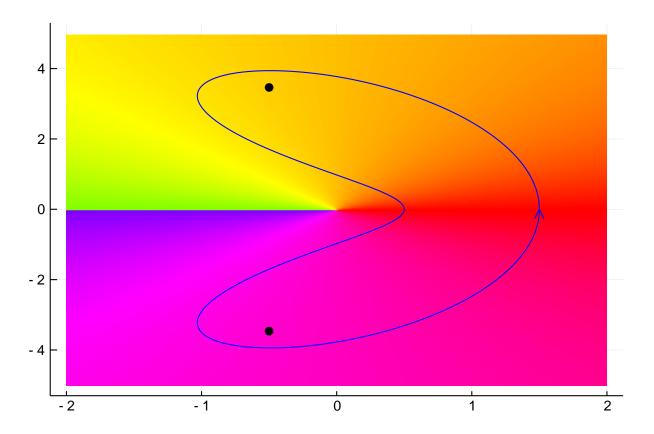
\theta = range(0,2\pi,length=1000)

\gamma = \theta -> (z = exp(im*\theta); 2z + z^2 - 1.5/z) # a curve containing \lambda

phaseplot(-2..2, -5..5, z -> sqrt(z))

scatter!(real(\lambda),imag(\lambda); color=:black, legend=false)

plot!(real(\gamma.(\theta)), imag(\gamma.(\theta)); color=:blue, arrow=true)
```



We use the periodic Trapezium rule to integrate over the contour, showing it is valid:

```
periodic_rule(N) = 2\pi/N*(0:(N-1)), 2\pi/N*ones(N)

\gamma p = \theta \rightarrow (z = exp(im*\theta); im*z*(2 + 2z + 1.5/z^2))

N = 1000

\theta,w = periodic_rule(N)

norm(sum(w .* \gamma p.(\theta).*sqrt.(\gamma.(\theta)) .* [inv(\gamma(\theta)*I-A) for \theta in \theta])/(2\pi*im) - sqrt(A))

1.6279683670392478e-15
```

We will discuss more next lecture.