Computing A^α, log(A) and Related Matrix Functions by Contour Integrals

MIMS New Directions Workshop

Functions of Matrices

May 16th, 2008

Nick Hale
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University of Oxford

with

Nick Higham

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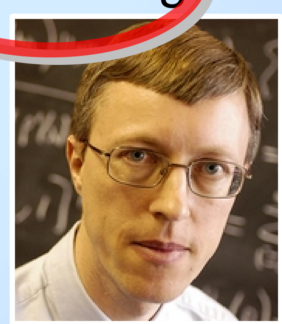


University of Manchester

University of Oxford

A Definition

f applied to a complex scalar value z

analytic function

$$f(A) := \frac{1}{2\pi i}\int_\Gamma f(z)(zI - A)^{-1}dz$$

square matrix

resolvent

positively orientated closed contour within region of analyticity of f, and surrounding the spectrum $\sigma(A)$

An Idea

approximate the integral above numerical via some quadrature scheme

composite trapezium rule + analytic integrand → geometric convergence

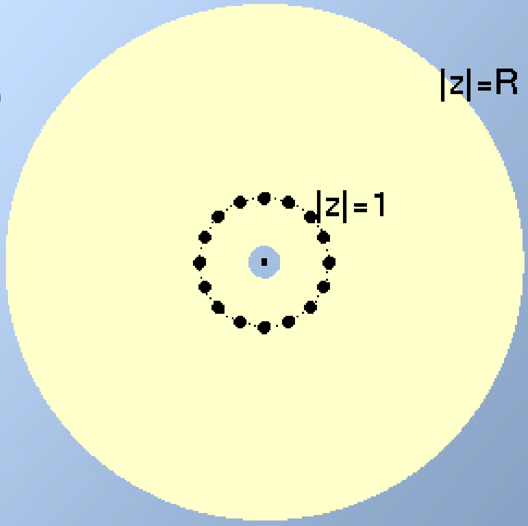
Whistle-stop Trapezium Rule Revision (part 1)

$$I(f) = \int_\Gamma f(z)dz \approx \sum_{j=1}^{N} w_k f(z_k) = I_N(f)$$

- trapezium rule over a circle in the complex plane

$$I(f) = \int_{|z|=1} f(z)dz = i\int_0^{2\pi} e^{i\theta} f(e^{i\theta})d\theta$$

$$\approx \frac{2\pi i}{N}\sum_{j=1}^{N} z_j f(z_j) = I_N^T(f)$$



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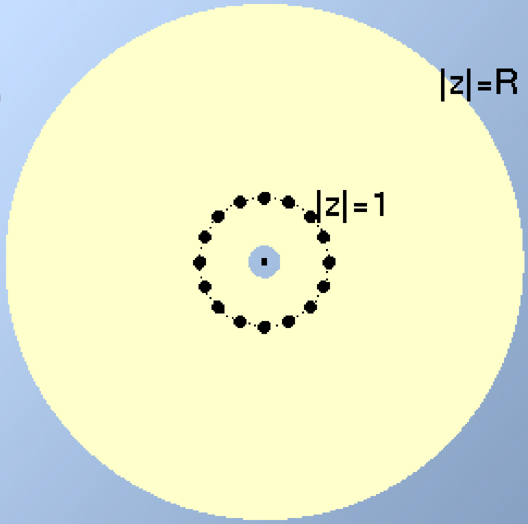


Theorem (Poisson 1820, Davis 1950)

if $f(z)$ is analytic in the annulus $1/R \leq |z| \leq R$ for some $R > 1$ then

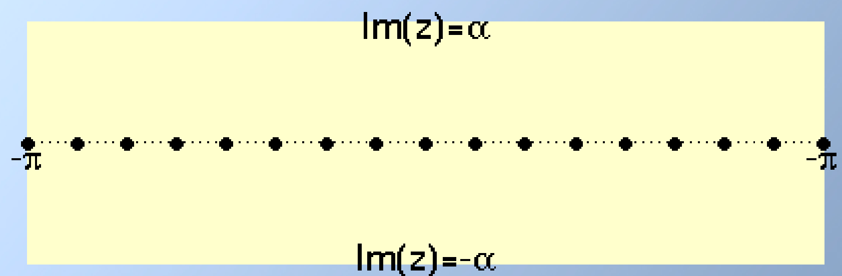
$$|I(f) - I_N^T(f)| = O(R^{-N})$$

Whistle-stop Trapezium Rule Revision (part 2)

$$I(f) = \int_\Gamma f(z)dz \approx \sum_{j=1}^{N} w_k f(z_k) = I_N(f)$$

- trapezium rule over a periodic interval

$$I(f) = \int_0^{2\pi} f(t)dt \approx \frac{2\pi}{N}\sum_{j=1}^{N} f(t_j) = I_N^T(f)$$



Corollary

if $f(z)$ is 2π periodic and analytic in the strip $|\mathrm{Im}(z)| \leq \alpha$
then

$$|I(f) - I_N^T(f)| = O(e^{-\alpha N})$$

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approximate the integral above numerical via some quadrature scheme

$$f(A) \approx \sum_{j=1}^{N} w_j f(z_j)(z_j I - A)^{-1} = f_N(A)$$

A Definition

f applied to a complex scalar value z

analytic function

$$f(A)b = \frac{1}{2\pi i}\int_\Gamma f(z)[(zI - A)\backslash b]dz$$

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solution to shifted linear system

positively orientated closed contour within region of analyticity of f, and surrounding the spectrum $\sigma(A)$

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approximate the integral above numerical via some quadrature scheme

$$f(A)b \approx \sum_{j=1}^{N} w_j f(z_j)[(z_j I - A)\backslash b] = f_N(A)b$$

An Example

suppose $f(z)$ is analytic in $\mathbb{C}\backslash(-\infty, 0]$ and $\sigma(A) \in [m, M] \subset (0, \infty)$

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e.g. $\sqrt{A}$, A^{α}, $\log(A)$ } practical

$\Gamma(A)$, $\tanh A^{1/2}$ } ?

e.g. positive definite
(this will be relaxed a little later on)

An Example

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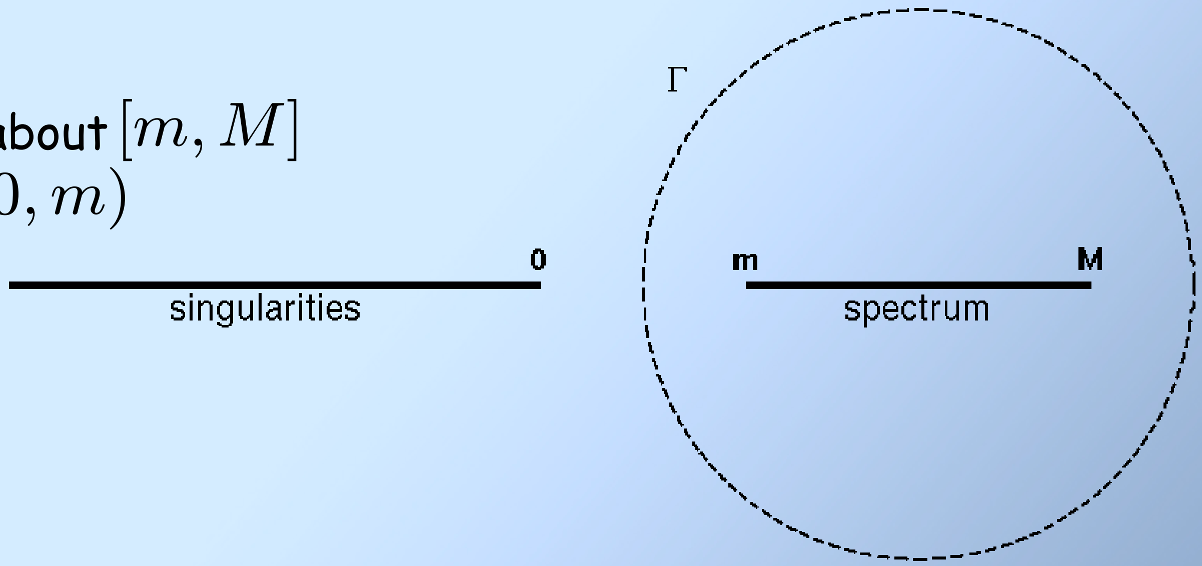
suppose $f(z)$ is analytic in $\mathbb{C} \backslash (-\infty, 0]$ and $\sigma(A) \in [m, M] \subset (0, \infty)$

let Γ be a circle about $[m, M]$
passing through $(0, m)$



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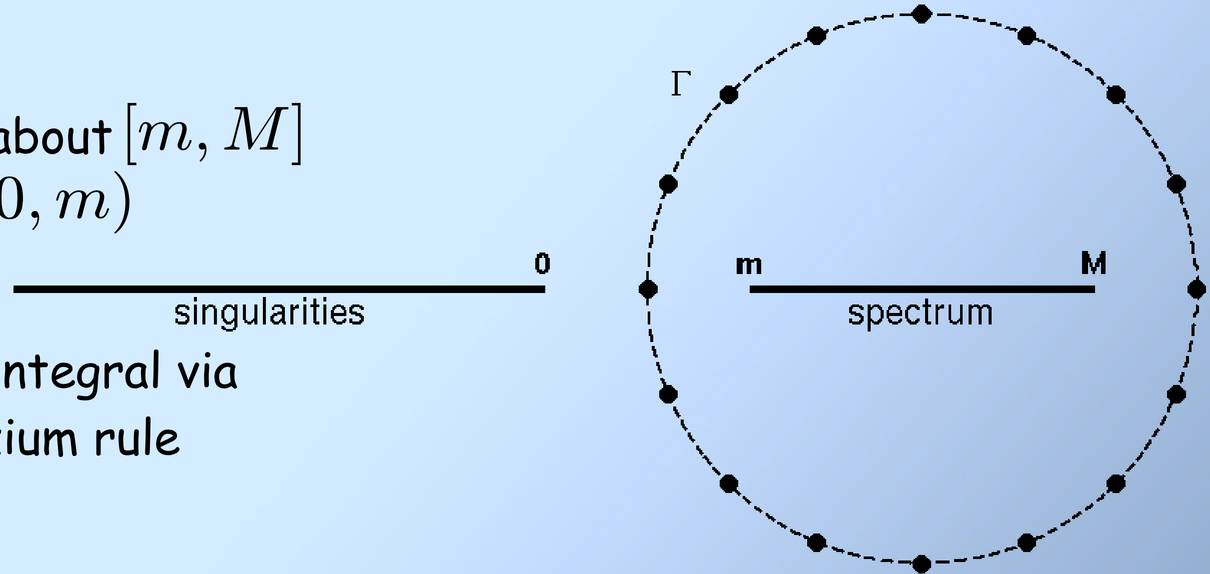

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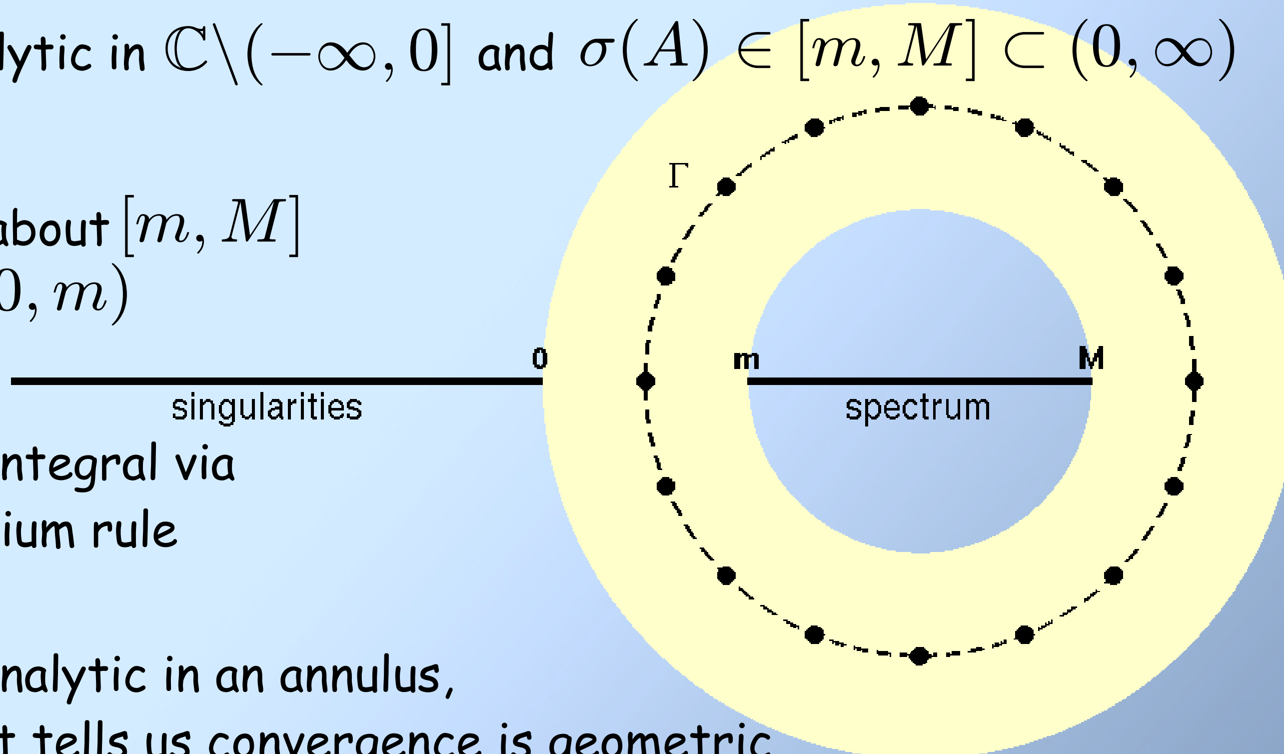

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the integrand is analytic in an annulus,
so Poisson's result tells us convergence is geometric

the rate of this convergence is determined by the width of the annulus

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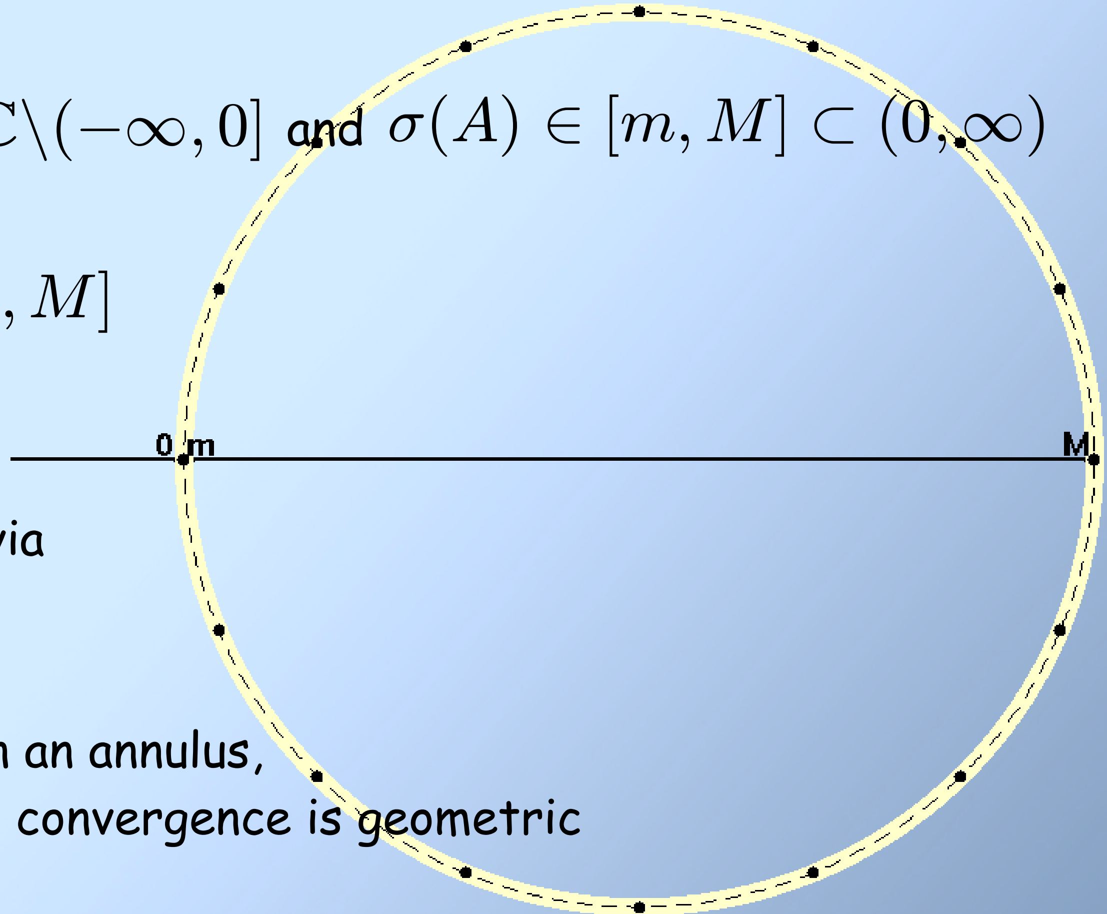

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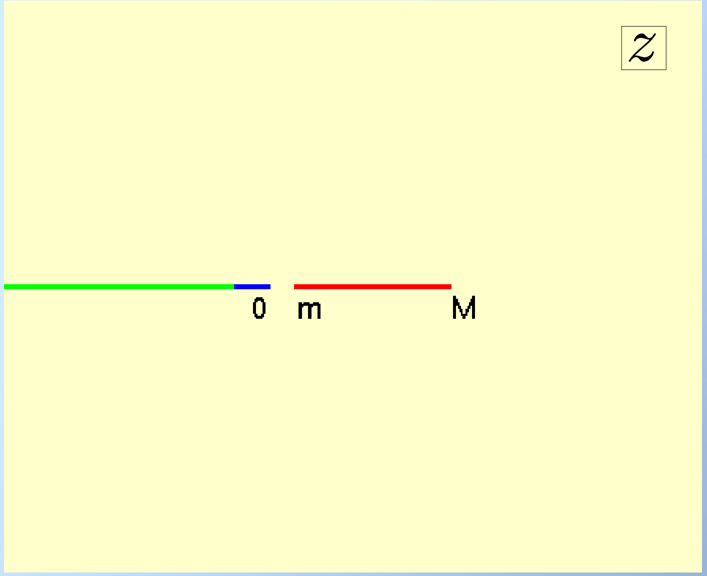
if A is ill-conditioned, i.e. $0<m\ll M$, this method will require at least $O(M/m)$ matrix inversions (or linear solves) to get any accuracy at all

A Better Idea

use the whole region of analyticity



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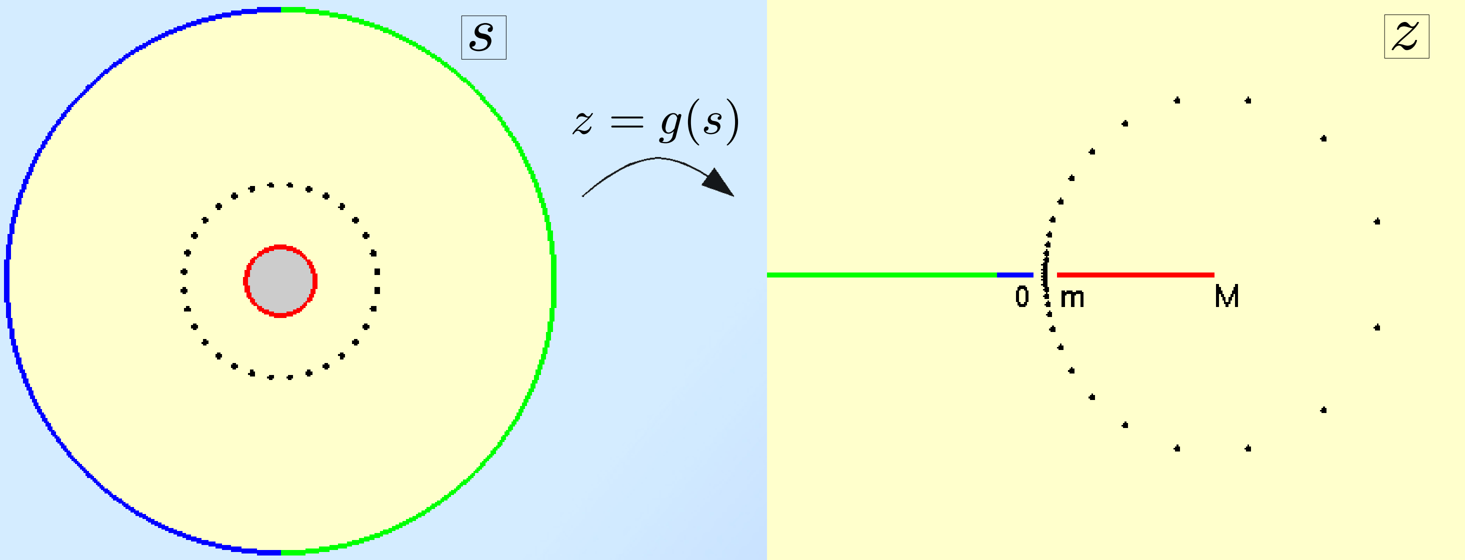
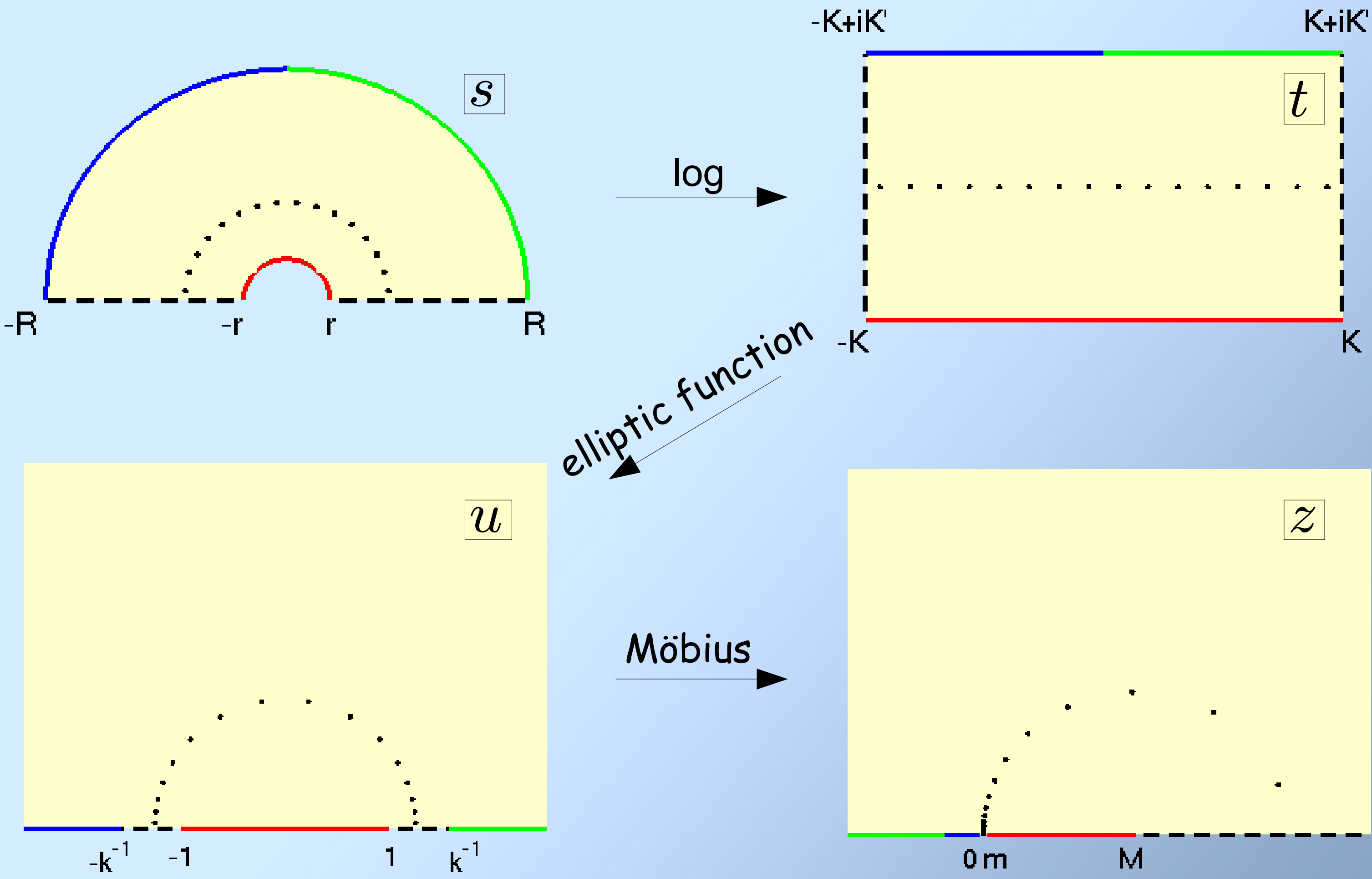


by finding a conformal map
from a much thicker annulus

i.e. introduce a change of variables in the integral

$$\int_\Gamma f(z)(zI - A)^{-1} dz = \int_\gamma f(g(s))(g(s)I - A)^{-1} g'(s) ds$$

A Conformal Map



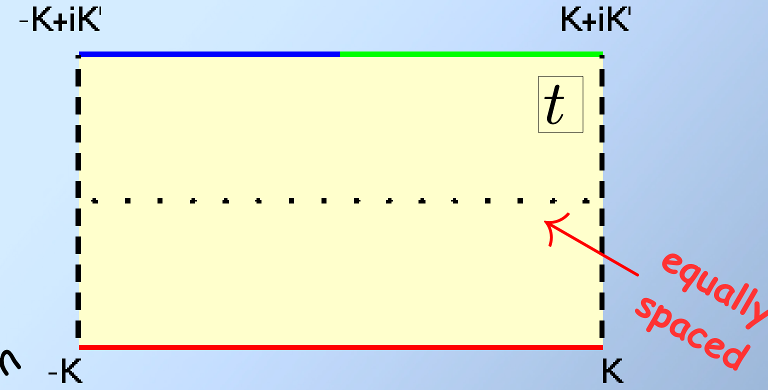
A Conformal Map

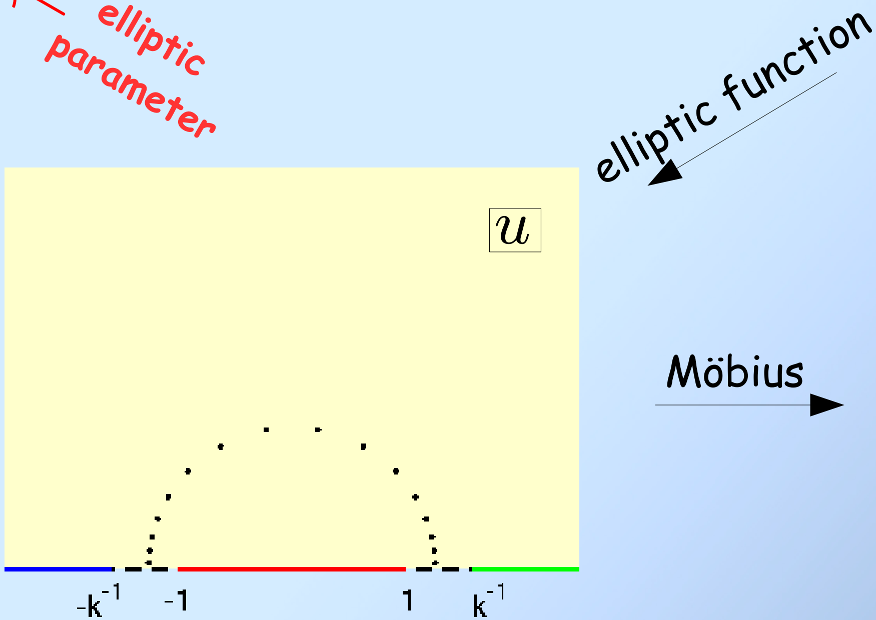
$$z(t) = \sqrt{mM}\left(\frac{k^{-1} + \operatorname{sn}(t|k^2)}{k^{-1} - \operatorname{sn}(t|k^2)}\right)$$

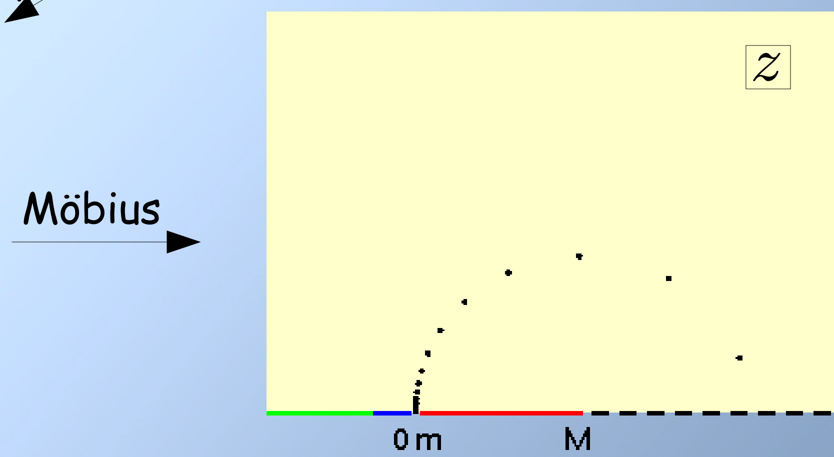
Jacobi elliptic sine function

$$k = \sqrt{M/m} - 1 \Big/ \sqrt{M/m} + 1$$

elliptic parameter



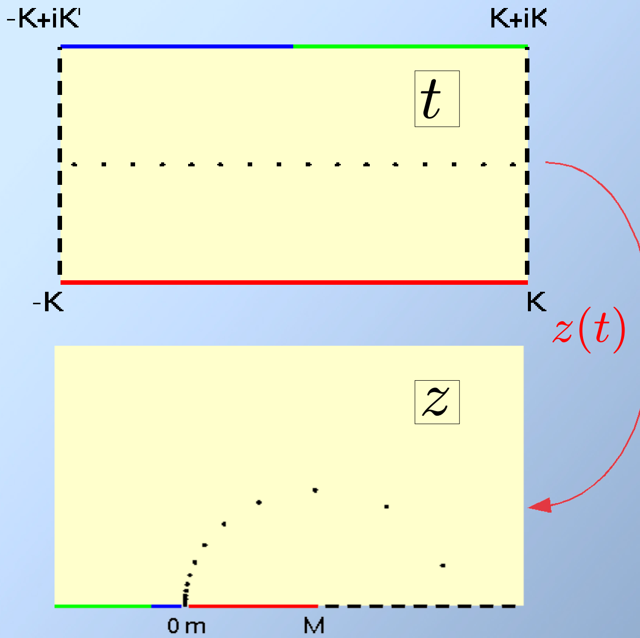




A Method

$$t_j = -K + \frac{iK'}{2} + 2\frac{(j-\frac{1}{2})K}{N}, \quad j = 1\ldots 2N$$

complete elliptic integrals



$$z_j = z(t_j) = \sqrt{mM}\left(\frac{k^{-1}+\mathrm{sn}(t_j|k^2)}{k^{-1}-\mathrm{sn}(t_j|k^2)}\right)$$

$$f_N(A) = \frac{2iK\sqrt{mM}}{Nk\pi}\sum_{j=1}^{2N} f(z_j)(z_jI-A)^{-1}\underbrace{\frac{\mathrm{cn}(t_j|k^2)\mathrm{dn}(t_j|k^2)}{(k^{-1}-\mathrm{sn}(t_j|k^2))^2}}_{dz/dt}$$

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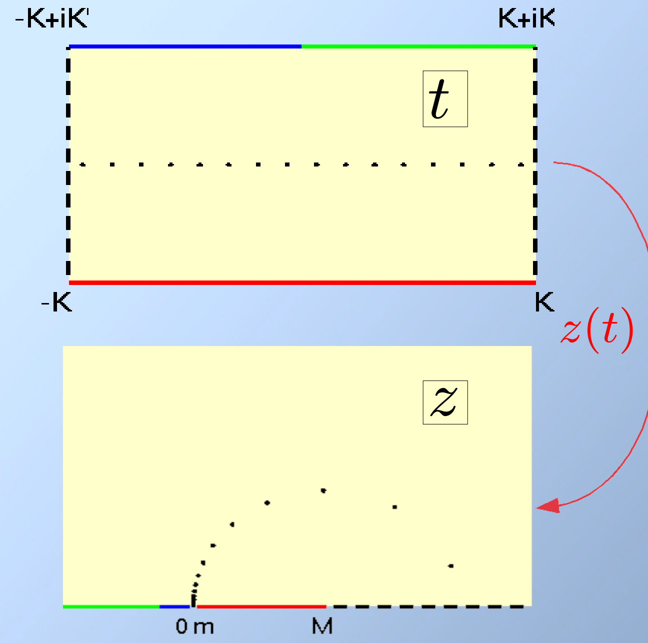

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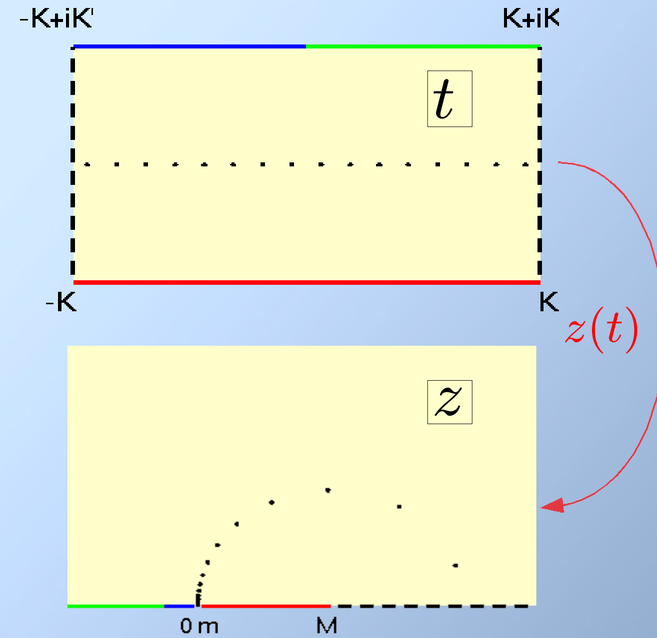

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A Theorem (HHT 2008)

$$\|f(A) - f_N(A)\| = O(e^{\varepsilon - \pi K' N/(2K)})$$

where $\pi K'/(2K) \sim \pi^2/\log(M/m)$ as $M/m \to \infty$

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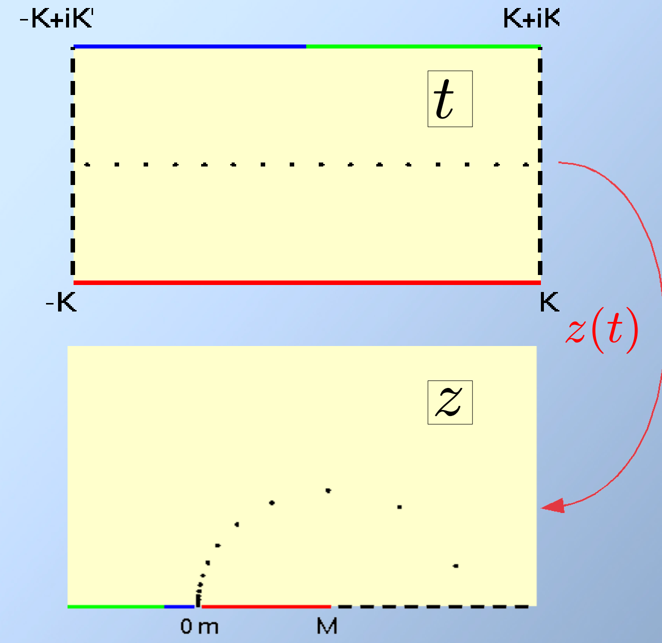

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$\leftarrow$ log!!

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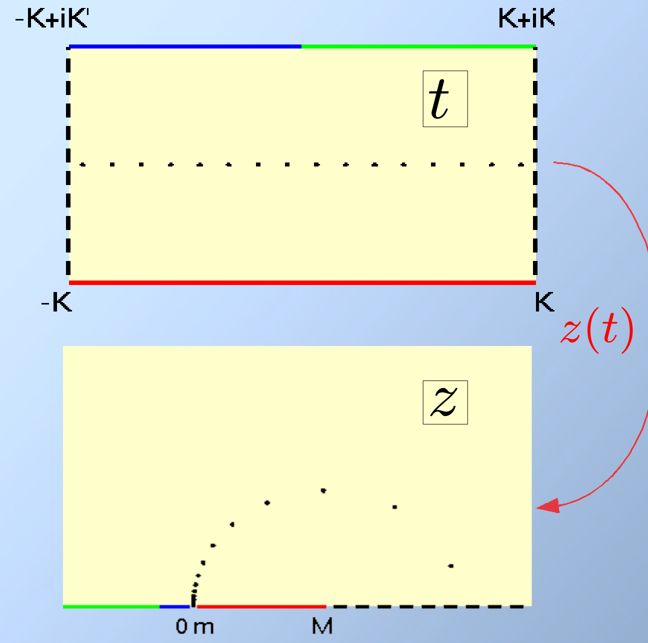

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$$\|f(A) - f_N(A)\| = O(e^{-\pi^2 N/(\log(M/m)+3)})$$

An Example

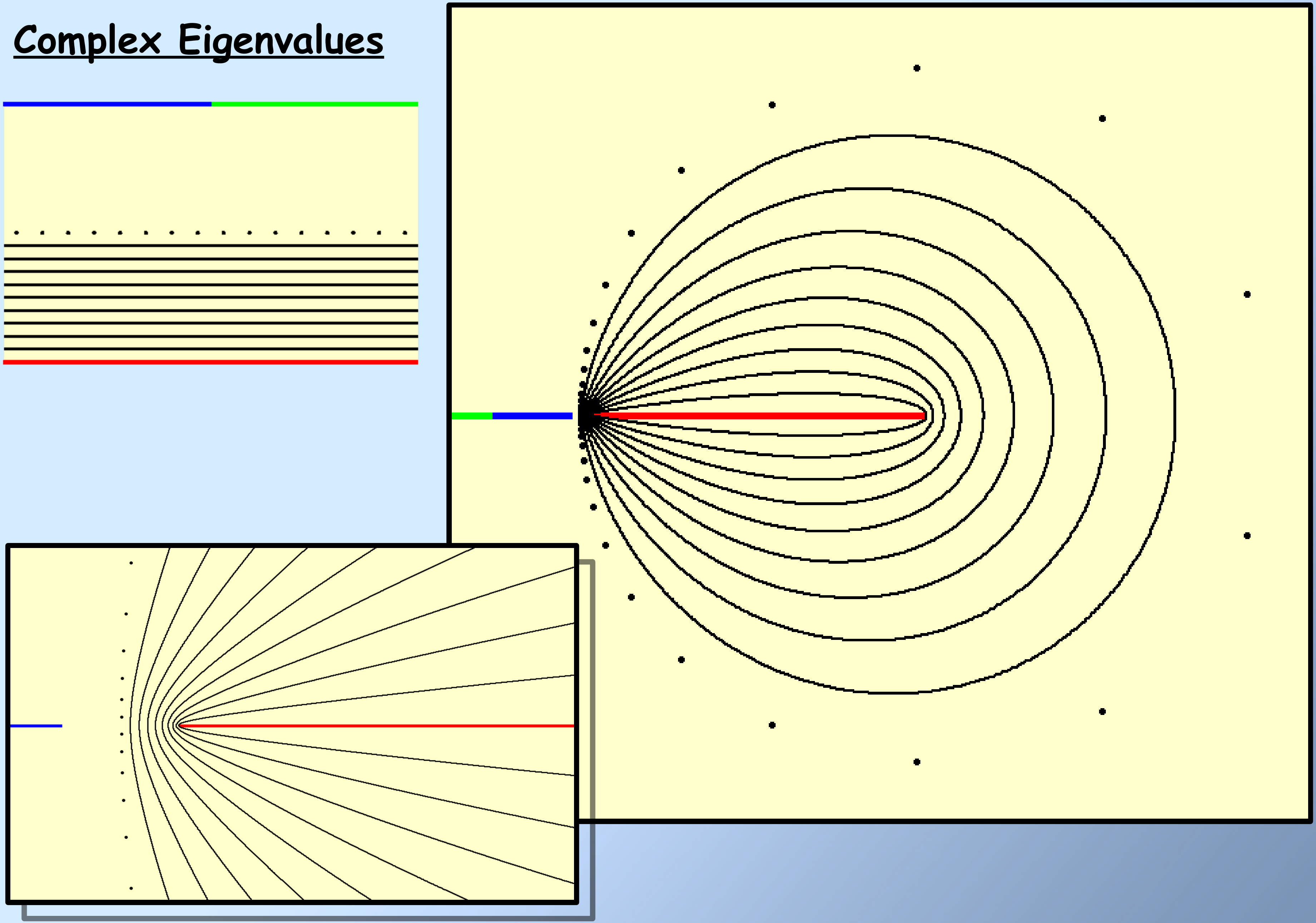
```
% method1.m - evaluate f(A) by contour integral. The functions
%             ellipkkp and ellipjc are from Driscoll's SC Toolbox.

f = @sqrt;                         % change this for another function f
A = pascal(6);                     % change this for another matrix A
fA = sqrtm(A);                     % change this if f is not sqrt
I = eye(size(A));
e = eig(A); m = min(e); M = max(e); % in practice these would be estimated
k = (sqrt(M/m)-1)/(sqrt(M/m)+1);
L = -log(k)/pi;
[K,Kp] = ellipkkp(L);
for N = 5:5:45
  t = .5i*Kp - K + (.5:N)*2*K/N;
  [sn,cn,dn] = ellipjc(t,L);
  z = sqrt(m*M)*((1/k+sn)./(1/k-sn));
  dzdt = sqrt(m*M)/k*cn.*dn./(1/k-sn).^2;
  fNA = zeros(size(A));
  for j = 1:N
    fNA = fNA + f(z(j))*inv(z(j)*I-A)*dzdt(j);
  end
  fNA = -4*K*imag(fNA)/(pi*N);
  error = norm(fNA-fA)/norm(fA);
  fprintf('%4d   %16.12f\n', N, error)
end
```

$\leftarrow M/m \approx 10^5$

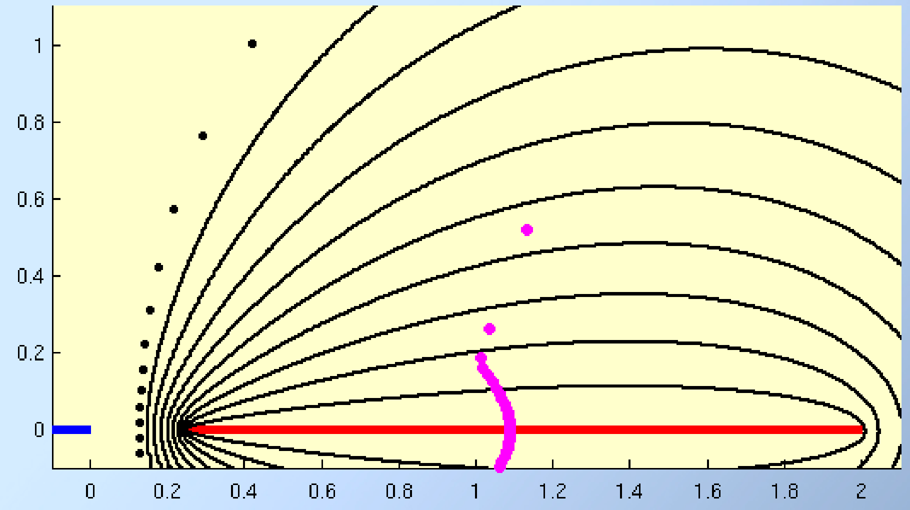
```
>> method1
   5       0.327965641207
  10       0.020386977261
  15       0.000958510165
  20       0.000040667133
  25       0.000001628827
  30       0.000000062853
  35       0.000000002363
  40       0.000000000087
  45       0.000000000003
```

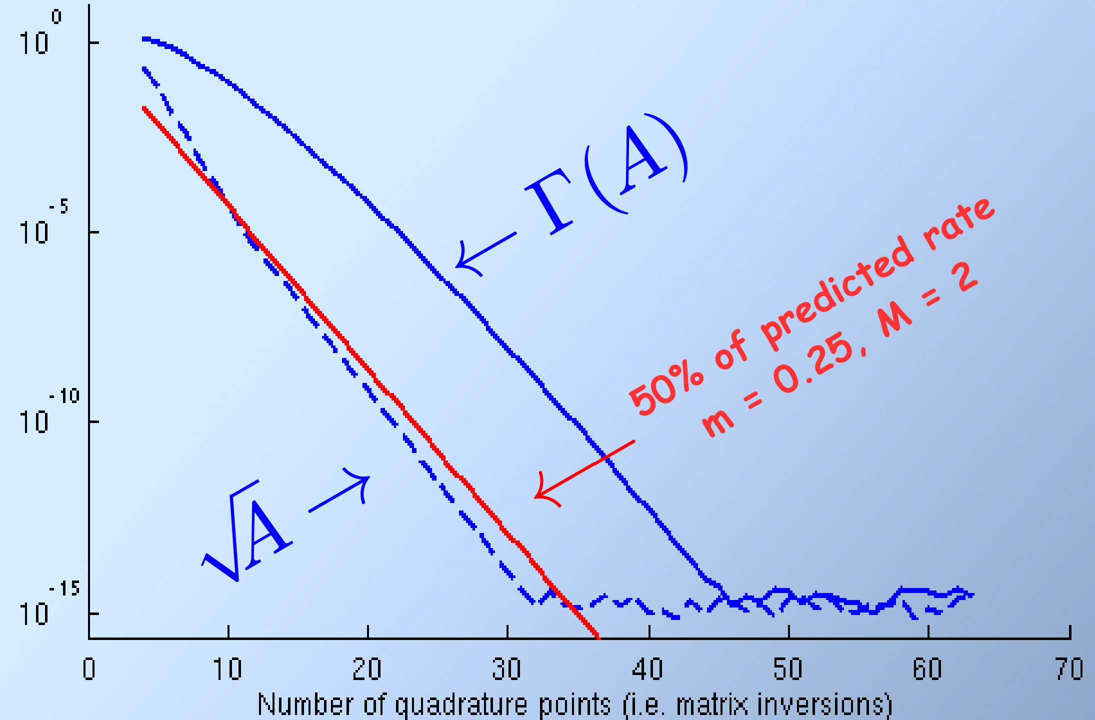
Complex Eigenvalues



A Complex Example

```
n = 32;
D = gallery('chebspec',n);
D = D(2:n,2:n);
I = eye(n-1);
A = I - (0.2/n)*D
```





Extensions

method2: when $(-\infty, 0)$ is just a branch cut, e.g. $\log z, z^{\alpha}$

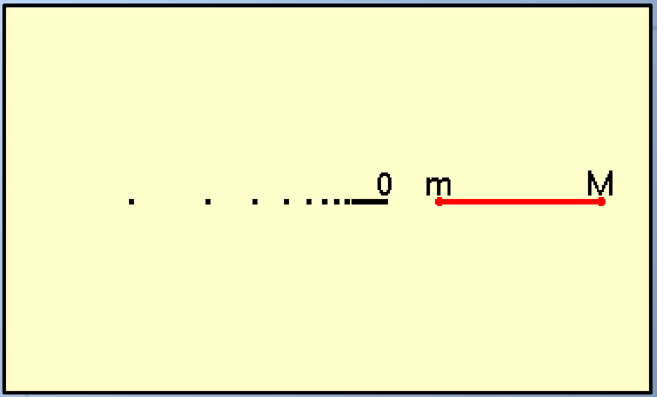
$$\|f(A) - f_N(A)\| = O(e^{-2\pi^2 N/(\log(M/m)+6)})$$

further factor of two speed-up

method3: when $f(z) = \sqrt{z}$

$$\|f(A) - f_N(A)\| = O(e^{-2\pi^2 N/(\log(M/m)+3)})$$

- no complex arithmetic
- save factor of two in symmetry, regardless of whether A is real
- connections to best rational approximation (Zolotarev)



A Practical Example

```
A = gallery('poisson',n);
b = ones(n^2,1);
```

$m = 2\pi^2 / (n+1)^2$

$M = 8$

Compute $A^{1/2}b$ using both **method3** and **sqrtm(full(A))*b**

large enough for 10 digits of relative accuracy →

n^2	M/m	N	time	time (sqrtm)
16	10.1	8	0.01	0.0006
64	32.8	9	0.02	0.005
256	117.	10	0.04	0.2
1024	441.	12	0.2	21.
4096	1712.	14	1.0	26 minutes
16384	6744.	15	6.0	<1 day?

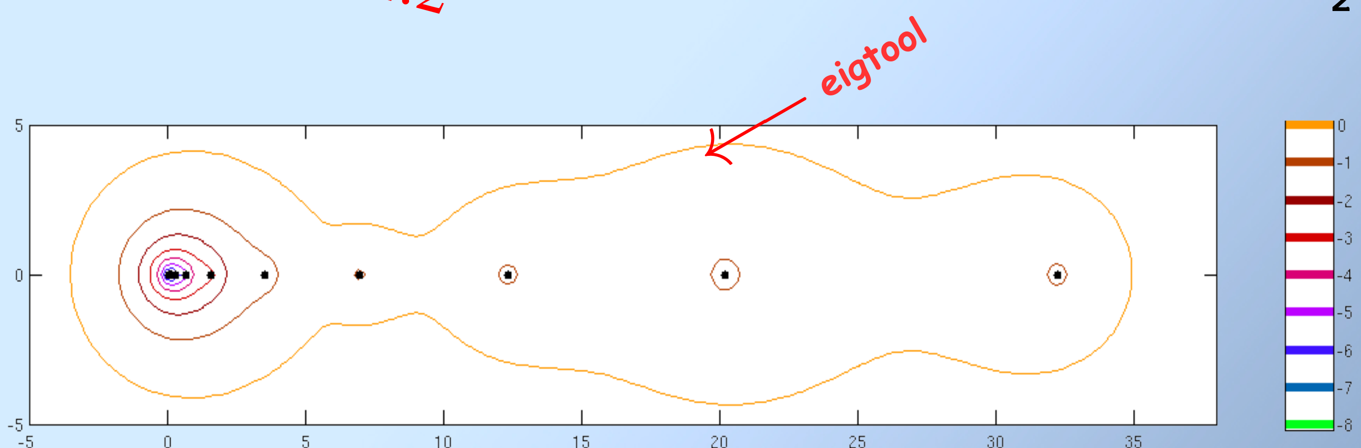
An Example for Brian Davies

```
A = gallery('frank',12);
```

12	11	10	9	8	7	6	5	4	3	2	1
11	11	10	9	8	7	6	5	4	3	2	1
	10	10	9	8	7	6	5	4	3	2	1
		9	9	8	7	6	5	4	3	2	1
			8	8	7	6	5	4	3	2	1
				7	7	6	5	4	3	2	1
					6	6	5	4	3	2	1
						5	5	4	3	2	1
							4	4	3	2	1
								3	3	2	1
									2	2	1
										1	1

$m \approx 0.031$

$M \approx 32.2$



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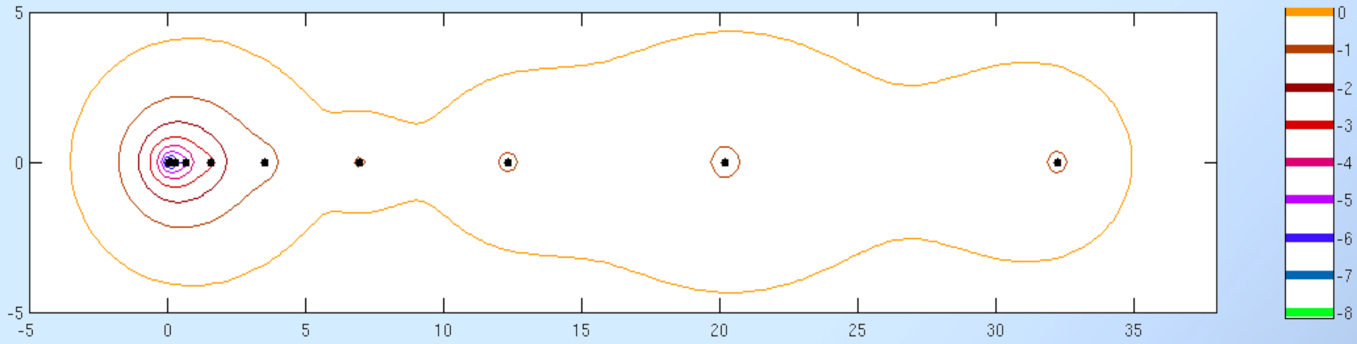

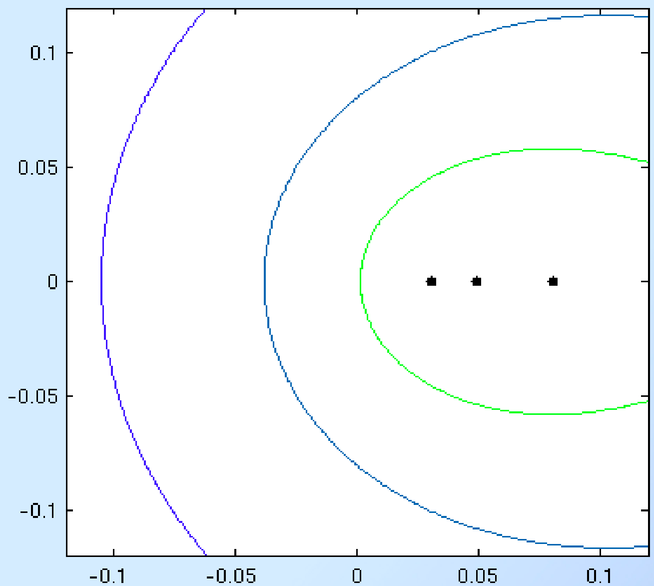

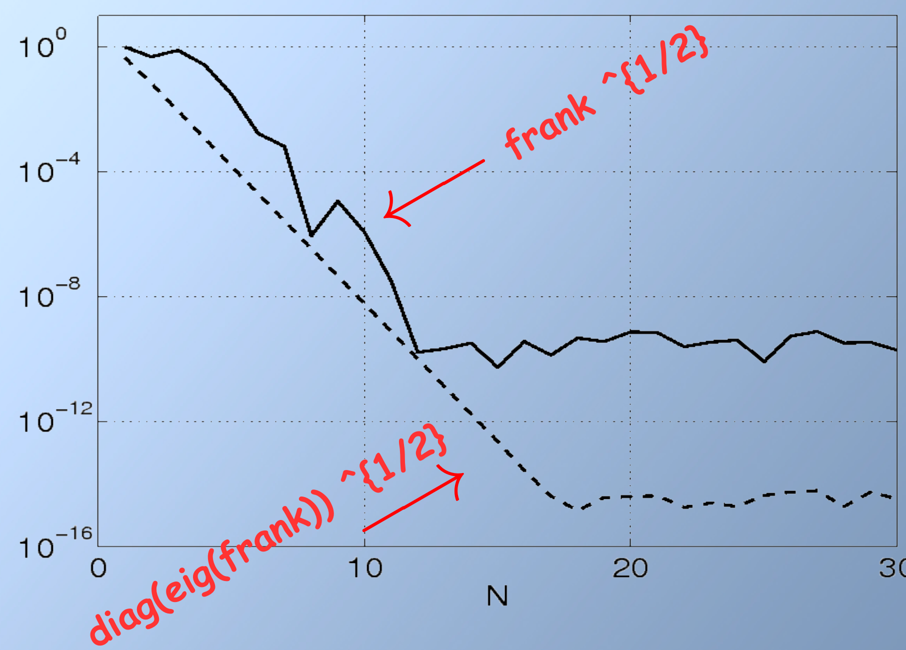

Comments

- most suitable for (but not limited to) f(A)b problems
- fully parallelisable – one matrix inversion / system solve per processor
- a slick way of solving shifted systems? Hessenberg form
- need some heuristic for choosing m & M when eigenvalues are complex
- more general analyticity / eigenvalue assumptions?

References

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  dzdt = sqrt(m*M)/k*cn.*dn./(1/k-sn).^2;
  fNA = zeros(size(A));
  parfor j = 1:N
    fNA = fNA + f(z(j))*inv(z(j)*I-A)*dzdt(j);
  end
  fNA = -4*K*imag(fNA)/(pi*N);
  error = norm(fNA-fA)/norm(fA);
  fprintf('%4d   %16.12f\n', N, error)
end
```

trivial parallelisation using MATLAB's parallel toolbox