Computing $A^\alpha$, log(A) and Related Matrix Functions by Contour Integrals

MIMS New Directions Workshop
Functions of Matrices
May 16th, 2008

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**A Definition**

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

- $f$ applied to a complex scalar value $z$
- positively orientated closed contour within region of analyticity of $f$, and surrounding the spectrum $\sigma(A)$
- square matrix
- analytic function
- resolvent

**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

\[ I(f) = \int f(z)\,dz = i \int_{0}^{2\pi} e^{i\theta} f(e^{i\theta})\,d\theta \]

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

**Theorem** (Poisson 1820, Davis 1950)

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

\[ |I(f) - I^T_N(f)| = O(R^{-N}) \]
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 \( 2\pi \) periodic and analytic in the strip \( |\text{Im}(z)| \leq \alpha \) then

\[ |I(f) - I_N^T(f)| = O(e^{-\alpha N}) \]
A Definition

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

analytic function

\( f \) applied to a complex scalar value \( z \)

square matrix

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

resolvent

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composite trapezium rule + analytic integrand geometric convergence
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square matrix

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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

\[ f(A) \approx \sum_{j=1}^{N} w_j f(z_j)(z_jI - A)^{-1} = f_N(A) \]
A Definition

An analytic function applied to a complex scalar value $z$ is given by:

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

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

An Idea

Approximate the integral above numerically via some quadrature scheme:

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

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

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

e.g. \[ \begin{array}{l}
\sqrt{A} \\
A^\alpha \\
\log(A) \\
\Gamma(A) \\
tanh A^{1/2}
\end{array} \] practical

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

suppose $f(z)$ is analytic in $\mathbb{C} \setminus (-\infty, 0]$ and $\sigma(A) \in [m, M] \subset (0, \infty)$
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let \( \Gamma \) be a circle about \([m, M]\)
passing through \((0, m)\)
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the rate of this convergence is determined by the width of the annulus
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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

\[ \subseteq \]
A Better Idea

use the whole region of analyticity

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

Elliptic function

\[ s \]

\[ t \]

\[ u \]

\[ z \]

\[ \log \]

\[ \text{Möbius} \]
A Conformal Map

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

\[ k = \sqrt{\frac{M}{m} - 1} \bigg/ \sqrt{\frac{M}{m} + 1} \]
A Method

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

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

\[ f_N(A) = \frac{2iK \sqrt{mM}}{N k \pi} \sum_{j=1}^{2N} f(z_j)(z_j I - A)^{-1} \frac{\text{cn}(t_j | k^2) \text{dn}(t_j | k^2)}{(k^{-1} - \text{sn}(t_j | k^2))^2} \]

complete elliptic integrals
A Method

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

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

\[ f_N(A)b = \frac{2iK \sqrt{mM}}{Nk\pi} \sum_{j=1}^{2N} f(z_j) \left[ (z_jI - A)b \right] \frac{\text{cn}(t_j|k^2)\text{dn}(t_j|k^2)}{(k^{-1} - \text{sn}(t_j|k^2))^2} \]
A Method

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\[
A \text{ Method}
\]

\[
A \text{ Theorem (HHT 2008)}
\]

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

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

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

Complete elliptic integrals

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

\[ f_N(A) = \frac{2iK\sqrt{mM}}{Nk\pi} \sum_{j=1}^{2N} f(z_j)(z_jI - A)^{-1} \frac{\text{cn}(t_j|k^2)\text{dn}(t_j|k^2)}{(k^{-1} - \text{sn}(t_j|k^2))^2} \]

**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 \( M/m \to \infty \)
A Method

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

complete elliptic integrals

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\[ f_N(A) = \frac{2iK\sqrt{mM}}{Nk\pi} \sum_{j=1}^{2N} f(z_j)(z_j I - A)^{-1} \frac{\text{cn}(t_j|k^2)\text{dn}(t_j|k^2)}{(k^{-1} - \text{sn}(t_j|k^2))^2} \]

A Theorem (HHT 2008)

\[ \| f(A) - f_N(A) \| = O\left(e^{-\pi^2 N/(\log(M/m)+3)}\right) \]
% method1.m - evaluate f(A) by contour integral. The functions
% ellipkdp 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] = ellipkdp(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, error)
end

An Example

>> 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

M/m ≈ 10^5
Complex Eigenvalues
A Complex Example

\begin{verbatim}
n = 32;
D = gallery('chebspec',n);
D = D(2:n,2:n);
I = eye(n-1);
A = I - (0.2/n)*D
\end{verbatim}

\[ \Gamma(A) \]

50\% of predicted rate
m = 0.25, M = 2
Extensions

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

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

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**

\[
A = \text{gallery('poisson',n)};
b = \text{ones}(n^2,1);
\]

\[
M = 2\pi^2 / (n+1)^2
\]

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

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

Large enough for 10 digits of relative accuracy!
An Example for Brian Davies

\[ A = \text{gallery('frank',12)}; \]

\[
\begin{array}{cccccccccccc}
12 & 11 & 10 & 9 & 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 \\
11 & 11 & 10 & 9 & 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 \\
10 & 10 & 9 & 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 \\
9 & 9 & 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 \\
8 & 8 & 7 & 6 & 5 & 4 & 3 & 2 & 1 \\
7 & 7 & 6 & 5 & 4 & 3 & 2 & 1 \\
6 & 6 & 5 & 4 & 3 & 2 & 1 \\
5 & 5 & 4 & 3 & 2 & 1 \\
4 & 4 & 3 & 2 & 1 \\
3 & 3 & 2 & 1 \\
2 & 2 & 1 & 1 \\
1 & 1 \\
\end{array}
\]

\[ m \approx 0.031 \]

\[ M \approx 32.2 \]
An Example for Brian Davies

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A = \text{gallery('frank',12)};
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\[
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?

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Parallelisation

trivial parallelisation using MATLAB's parallel toolbox