Ten things you should know about quadrature

Nick Trefethen, Vanderbilt, Wed. 28 May 2014 @ 8:35 PM
1. If the integrand is analytic, Gauss quadrature converges geometrically.

\( f \) is analytic and bounded by \( M \) in Bernstein \( \rho \)-ellipse with foci \( \pm 1 \), \( \rho = \) semimajor + semiminor axis lengths > 1.

\[
\begin{align*}
\rho &= \exp(a) \\
\sinh(a) &= 1 \\
\cosh(a) &= -1
\end{align*}
\]
Expand $f$ in a Chebyshev series. Bernstein (1912) showed

$$|a_k| \leq 2M \rho^{-k}$$

This implies a bound for the truncated series:

$$|f - f_n| \leq \frac{2M \rho^{-n}}{\rho - 1}$$

which implies for (n+1)-point Gauss quadrature

$$|I - I_n| \leq \frac{5M \rho^{-2n}}{\rho^2 - 1}$$

since Gauss q. is exact for polynomials of degree 2n+1. QED.
2. The equispaced trapezoidal rule also converges geometrically if the integrand is analytic and periodic (or on the real line).

André Weideman, U. Stellenbosch review article to appear in SIAM Review
Poisson, 1820s

Poisson's example: perimeter of ellipse with axes $1/\pi$ and $0.6/\pi$:

$$I = \frac{1}{2\pi} \int_{0}^{2\pi} (1 - 0.36\sin^2\theta)^{1/2} \, d\theta$$

Take advantage of 4-fold symmetry.

2 points: 0.9000000000
3 points: 0.9027692569
5 points: 0.9027798586
9 points: 0.9027799272

"La valeur approchée de I sera $I = 0,9927799272$."
Exponential convergence

Suppose $f$ is analytic, bounded, periodic in $S_\alpha = \{z: -\alpha < \text{Im } z < \alpha\}$.

Error in trapezoidal rule quadrature: $O(e^{-2\pi\alpha/h})$

Phil Davis 1959. He calls the result "folklore".
Three methods of proof

Proof method 1: Fourier series and aliasing
The trapezoidal rule returns the integral of a trigonometric interpolant. The error comes from Fourier components $e^{2\pi i x/h}$, $e^{4\pi i x/h}$, etc. that are indistinguishable from 1 on the grid.

Proof method 2: contour integral
The error can be written as a contour integral involving a function with a pole at each grid point. Moving the contour out into the complex plane gives the $O(e^{-2\pi \alpha/h})$ factor.

Proof method 3: trigonometric interpolation
The trapezoidal rule delivers the exact integral of a trigonometric interpolant. (This observation gets the geometric convergence, but underestimates its rate by a factor of 2 due to aliasing.)
3. This effect generalizes to nonequispaced points (quadrature via trigonometric interpolation).

The Fejér-Kalmár theorem (1926) in some sense says this works.

But it’s numerically unstable, not caring if points coalesce, although Lebesgue constants must explode.

I don’t know if anyone has a robust theory of such things.

Related to sampling theory.
4. The Euler-Maclaurin and Gregory formulas, too, come from integrating interpolants.

Euler-Maclaurin: trapezoidal rule + endpoint corrections based on derivatives.
Gregory: same, but with endpoint corrections based on finite differences (1670!)

Mohsin Javed and T., Numer. Math., submitted
GREGORY vs. SIMPSON (1638-1675, 1710-1761)

Simpson’s rule: \[ \frac{1}{3} \quad \frac{4}{3} \quad \frac{2}{3} \quad \frac{4}{3} \quad \frac{2}{3} \quad \frac{4}{3} \quad \frac{2}{3} \quad \ldots \]

degree 2 Gregory formula: \[ \frac{3}{8} \quad \frac{7}{6} \quad \frac{23}{24} \quad 1 \quad 1 \quad 1 \quad 1 \quad \ldots \]

\( O(h^4) \) convergence for \( f(x) = \exp(x) \):

![Graph showing convergence comparison between Gregory and Simpson's methods with a ratio of 4.75]
Euler-Maclaurin formula

For the trapezoidal rule applied to smooth nonperiodic \( f \) on \([a,b]\),

\[
I_h - I \sim h^2 [f'(b) - f'(a)] B_2 / 2! + h^4 [f'''(b) - f'''(a)] B_4 / 4! + \ldots
\]

where \( B_k \) is the \( k \)th Bernoulli number.

The trapezoidal rule gives the integral of a trig. interpolant. Do E-M formulas also give integrals of certain interpolants?

Yes. Euler-Maclaurin interpolant = trig. poly. + algebraic poly.

Similarly we get a Gregory interpolant of the same form.
5. Gauss nodes and weights can be computed in $O(n)$ time.
Carl Gauss, age 37


(No hits at Google Scholar)

Gene Golub, age 37


(907 hits at Google Scholar)
Nodes and weights in $O(n)$ time

all in SIAM J Sci Comp

$s, w = \text{legpts}(n)$
6. Clenshaw-Curtis quadrature usually converges as fast as Gauss (i.e., not just half as fast).

C-C quad is only exact through polynomial degree $n$, not $2n+1$. But the errors in integrating $T_{n+1}, T_{n+2}, \ldots$ are very small.
7. All such polynomial-based formulas are suboptimal by a factor of $\pi/2$.

... because ellipses are fatter in the middle than at the ends. The resolution power of polynomials is nonuniform: outstanding at the endpoints, paying a price in the middle.

Bakhvalov 1967    Hale + T. 2008

strip_vs_gauss
8. Bending around the negative real axis evaluates inverse Laplace transforms and special functions.
Laplace transform

\[ \hat{f}(z) = \int_0^\infty e^{-st} f(t) \, dt \]

Inverse Laplace transform

\[ f(t) = \frac{1}{2\pi i} \int_{\sigma-i\infty}^{\sigma+i\infty} e^{zt} \hat{f}(z) \, dz, \quad \sigma > \sigma_0 \]

**BROMWICH INTEGRAL**

Idea: bend the contour around \((-\infty,0]\) to exploit decay of \(\exp(zt)\).

**HANKEL CONTOUR**

- Green 1955
- Butcher 1955
- Talbot 1976, 1979
- Gavrilyuk, López-Fernández, Lubich, Palencia, Schädle,...
- Weideman 2005

- cotangent
- parabola
- cotangent
- hyperbola, parabola
- cotangent

\[ \int f(z) \, dz = \int f(g(s)) \, g'(s) \, ds \]
Optimal quadrature points for four types of contour

Assuming $|f(z)| \sim \exp(z)$ as $\text{Re}z \to -\infty$. $n$ chosen big enough for 16-digit precision.

(Weideman)
Example — gamma function  (T., "Ten digit algorithms", 2005)

Formula due to Hankel: \[ \frac{1}{\Gamma(t)} = \frac{1}{2\pi i} \int e^z z^{-t} dz \]

% gamma_talbot.m Compute complex gamma function via Talbot contour
% Hankel's integral formula is 1/Gamma(z) = (2*pi*i)^(-1) int_C e^t t^(-z) dt
% where the contour C passes from -infty-0i around 0 to -infty+0i. We evaluate
% the integral by the trapezoid rule transplanted to a cotangent contour due to
% Talbot (1979) with parameters optimized by Weideman (2005).

N = 40; % no. of quadrature pts
th = (-N/2+.5:N/2-.5)*pi/(N/2); % trapezoid pts in [-pi,pi]
a = -.2407; b = .2387; c = .7409; d = .1349i; % Weideman's parameters
z = N*(a + b*th.*cot(c*th) + d*th); % Talbot pts in z-plane
zp = b*cot(c*th) - b*c*th./sin(c*th).^2 + d; % N^(-1) times derivative
x = -3.5:.1:4; y = -2.5:.1:2.5; % N^(-1) times derivative
[xx,yy] = meshgrid(x,y); % plotting grid
gaminv = zeros(size(zz)); % no. of pts on contour
Npts = length(th); % Loop goes over contour
for k = 1:Npts % points, not grid pts
    t = z(k); % (which are vectorized)
gaminv = gaminv + exp(t)*t.^(-zz)*zp(k);
end
gam = 1i./gaminv; % Gamma(z) on the grid
mesh(xx,yy,abs(gam)); % plot |Gamma(z)|
disp(gam(26,46:10:76).'); % approxs. to Gamma(1:4)

This code uses 40 quadrature nodes to evaluate \( \Gamma(t) \) on a 50x75 grid
9. Taking the integrand to be a matrix or operator gives methods for computing $f(A)$. 
Example: \( \sqrt{A} \), \( \log(A) \)

For a matrix or operator \( A \), \( f(A) \) is defined by a resolvent integral

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

where \( C \) encloses \( \text{spec}(A) \).

Suppose \( f \) is analytic except on \((-\infty, 0]\), and \( A \) has spectrum in \([m, M] \), \( M \gg m > 0 \).

E.G. \( \sqrt{A} \), \( A^\alpha \), \( \log(A) \)

A bad idea: circular contour \( C \) surrounding the spectrum. Requires \( O(M/m) \) quad. points.
A better idea: first, conformal map from an annulus

As always we use a change of variables:

\[ \int f(z) (z-A)^{-1} \, dz = \int f(g(s)) (g(s)-A)^{-1} g'(s) \, ds \]

Requires just \( O(\log(M/m)) \) quadrature points.

Example: $\sqrt{A}$, $M/m \approx 10^5$

<table>
<thead>
<tr>
<th>n</th>
<th>error</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>5.983430140320</td>
</tr>
<tr>
<td>10</td>
<td>0.371941566087</td>
</tr>
<tr>
<td>15</td>
<td>0.017487132460</td>
</tr>
<tr>
<td>20</td>
<td>0.000741934280</td>
</tr>
<tr>
<td>25</td>
<td>0.000029716444</td>
</tr>
<tr>
<td>30</td>
<td>0.000001146690</td>
</tr>
<tr>
<td>35</td>
<td>0.000000043108</td>
</tr>
<tr>
<td>40</td>
<td>0.00000001590</td>
</tr>
<tr>
<td>45</td>
<td>0.000000000058</td>
</tr>
<tr>
<td>50</td>
<td>0.000000000002</td>
</tr>
</tbody>
</table>

Example: $\sqrt{A \cdot b}$

$A = 50\times50$ discrete Laplacian (dimension 2500), $b =$ random

Matlab $\texttt{sqrtm}$: 4 min. 48 secs. on a laptop

Contour integral & conformal map: 0.76 secs.
10. Every quadrature formula is a rational or meromorphic approximation.

We use the approximations to estimate accuracy of quadrature formulas for analytic integrands.

Conversely, we can use the quadrature formulas to generate approximations.
Jacobi 1825
(thesis, Berlin)

A rational function can be written as a sum of poles.

Cauchy 1826
(Exercices, Paris)

The strength of a pole (its residue) is given by a contour integral.

So every sum \( \sum_j w_j f(x_j) \) is equal to an integral \( \int_{\Gamma} r(z)f(z)\,dz \).

Nodes \( \leftrightarrow \) poles.  Weights \( \leftrightarrow \) residues.
Trapezoidal rule on unit circle

$|1-z^n|^{-1}, \ n=32$

Rational approximations of $\exp(z)$ on the negative real axis

Quadrature on a Hankel contour
(Talbot, Weideman,...)

Best approximation
(Cody-Meinardus-Varga, Gonchar-Rakhmanov, ...)

![Graph showing quadrature on a Hankel contour and best approximation on the negative real axis.](image-url)