Numerical Integration

Gauss or Gauss-Legendre Quadrature

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References

- S. Chapra and R. Canale, Numerical Methods for Engineers
- Carnahan and Wilkes, Applied Numerical Methods, University of Michigan, Class Notes, 1996.
- Pal, Numerical Analysis for Scientists and Engineers, 2007.
- Holistic Numerical Methods Institute webpage
- Samir Al-Amer, Class Notes
- wikipedia.org

Motivation

Multistep trapezoidal with equally spaced points

$$\int_a^b f(x)dx \approx h\left[\frac{f(x_0)+f(x_n)}{2}+\sum_{i=1}^{n-1} f(x_i)\right]$$

Think of this as:

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} w_i f(x_i)$$

with

$$w_i = \begin{cases} h & \text{for } i = 1, 2, ...n-1 \\ h/2 & \text{for } i = 0 \text{ and } n \end{cases}$$

Motivation

- Can I relax the requirement "interval size is constant"?
- Can I get a higher order polynomial approximation for a given n in return?
- I want to "select" both w_i and x_i to generate a formula of the type
$$\int_a^b f(x)dx \approx \sum_{i=0}^{n} w_i f(x_i)$$
which allows me to compute integrals of polynomials of order $2n+1$ perfectly (Gauss-Legendre)
- Note that there are $n+1$, w_i and x_is in the equation above.

Quick Review

- For Newton-Cotes, Simpson's 1/3 for example

$$e = \frac{(b-a)^5}{2880n^4} \underbrace{\max_{x \in [a,b]} f^{(4)}(x)}_{\text{zero for up to } p_3(x)}$$

- Changing n in a multi-step method, increases the numerical accuracy but does not affect (is independent of) the polynomial order accuracy
- In Gaussian Quadrature n simultaneously relates to both accuracies
- Error bounds, however, are not as easy to estimate as in Newton-Cotes

Simple Example

- Select nodes and weights so that $(n+1) = 2$ nodes allow us to write a formula that is exact for polynomials of degree $(2n+1) = 3$.

$$\int_{-1}^{1} f(x)dx = w_0 f(x_0) + w_1 f(x_1)$$

- Do not worry about the limits right now, we will learn how to generalize later.
- Here we are going to use brute force to set up equations for all polynomials degree 0 to $2n+1 = 3$

Equations

Yields the system of equations:

$$
\begin{aligned}
f(x) = 1; &\quad w_0 + w_1 = \int_{-1}^{1} 1 \; dx = 2 \\
f(x) = x; &\quad w_0 x_0 + w_1 x_1 = \int_{-1}^{1} x \; dx = 0 \\
f(x) = x^2; &\quad w_0 x_0^2 + w_1 x_1^2 = \int_{-1}^{1} x^2 \; dx = 2/3 \\
f(x) = x^3; &\quad w_0 x_0^3 + w_1 x_1^3 = \int_{-1}^{1} x^3 \; dx = 2
\end{aligned}
$$

which has the solution:

$$w_0 = w_1 = 1$$

$$x_0 = -\frac{1}{\sqrt{3}}, \quad x_1 = \frac{1}{\sqrt{3}}$$

Generalize

- To generalize this method, and compute the w_i and x_i efficiently, we need to learn about orthogonal polynomials
- I won't get into that in this class, but will point out that the x_is correspond to the zeros of well-studied class of orthogonal polynomials called Legendre Polynomials.*

$n+1$	x_i	w_i
1	0	2
2	$\pm 1/\sqrt{3}$	1
3	0 $\pm\sqrt{3/5}$	8/9 5/9
4	$\pm\sqrt{\left(3-2\sqrt{6/5}\right)/7}$ $\pm\sqrt{\left(3+2\sqrt{6/5}\right)/7}$	$\frac{18+\sqrt{30}}{36}$ $\frac{18-\sqrt{30}}{36}$
5	0 $\pm\frac{1}{3}\sqrt{5-2\sqrt{10/7}}$ $\pm\frac{1}{3}\sqrt{5+2\sqrt{10/7}}$	128/225 $\frac{322+13\sqrt{70}}{900}$ $\frac{322-13\sqrt{70}}{900}$

*wikipedia.org

Gauss-Legendre Quadrature

- Discovered by Gauss in his mid-thirties (early 1800s)
- Computation of nodes and weights for larger n is tedious (irrational numbers)
- In 1969, Golub and Welsch published an algorithm which made it practical to compute nodes and weights using computers[†]
- Matlab Implementation on next slide
- Eig() does not exploit the fact that the matrix is tridiagonal
- Factorization of a symmetric tridiagonal matrix can be accomplished $O(n^2)$ compared to $O(n^3)$ for general matrices

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[†] Golub and Welsch, Calculation of Gauss quadrature rules, Math. Comp. 23 (1969), 221-230.

Matlab Code[‡]

```
% (n+1)-pt Gauss quadrature of f
function I = gauss(f,n)

  % 3-term recurrence coeffs
  beta = .5./sqrt(1-(2*(1:n)).^(-2));

  % Jacobi matrix
  T = diag(beta,1) + diag(beta,-1);

  [V,D] = eig(T);    % eigenvalue decomposition
  x     = diag(D);
  [x,i] = sort(x);   % nodes (= Legendre points)

  w = 2*V(1,i).^2;   % weights
  I = w*feval(f,x);  % the integral
```

[‡]Algorithm from Trefethen, "Is Gauss Quadrature better than Clenshaw-Curtis?"

What about arbitrary limits?

- When the limits of integration are not -1 and 1, we need to apply a suitable transformation.

$$\int_a^b f(x)dx = \frac{b-a}{2} \sum_{i=0}^{n} w_i f\left(\frac{b-a}{2} x_i + \frac{b+a}{2}\right)$$

  where the weights and the abscissa are still the same
- This formula applies to Gauss-Legendre quadrature
- Next, we'll see how this is derived

What about arbitrary limits?

- We want to transform a problem that we don't know how to solve, to a problem we can deal with

$$\int_a^b g(t)dt = \int_{-1}^1 f(x)dx$$

- We need to transform x in $[-1, 1]$ to t in $[a, b]$
- Consider a linear transformation since it preserves the degree of the quadrature rule

$$t = \frac{(b-a)x + a + b}{2}.$$

When $x = -1, t = a$, and $x = 1, t = b$.

What about arbitrary limits?

- Using this substitution,

$$\int_a^b g(t)\ dt = \int_{-1}^1 g\left(\frac{(b-a)x+a+b}{2}\right)\frac{dt}{dx}dx$$

- Thus,

$$\begin{aligned}\int_a^b g(t)dt &= \frac{b-a}{2}\int_{-1}^1 g\left(\frac{(b-a)x+a+b}{2}\right)dx \\ \int_a^b g(t)dt &= \frac{b-a}{2}\sum_{i=0}^n w_i g\left(\frac{b-a}{2}x_i+\frac{b+a}{2}\right)\end{aligned}$$

Example

Problem: Integrate using Gauss-Legendre, with $n = 2$, 4 and 6

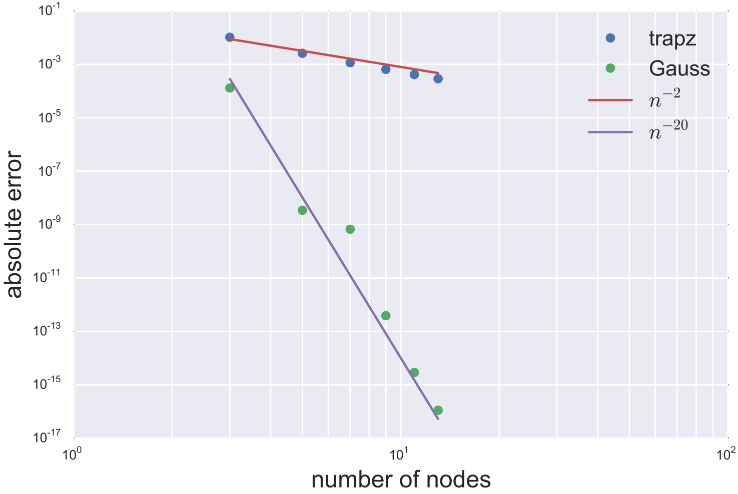
$$\int_a^b f(x)dx = \int_0^1 \frac{1}{1+x^2}dx = \frac{\pi}{4}$$

Solution: For $n = 2, a = 0, b = 1$

$$\begin{aligned} I &= \frac{1}{2}\left[w_0 f\left(\frac{x_0}{2} + \frac{1}{2}\right) + w_1 f\left(\frac{x_1}{2} + \frac{1}{2}\right)\right] \\ &= 0.78688524 \end{aligned}$$

- with $n = 4$, $I = 0.78540297$
- with $n = 6$, $I = 0.78539814$

Gauss Quadrature versus Trapezoidal Rule



Newton-Cotes v/s Gauss Quadrature

- Gauss Quadrature going from n to higher n, recompute all the points
- Error bounds are not readily available
- Newton-Cotes (Romberg) can reuse abscissa
- For smooth functions Gauss Quadrature is preferable but needs more work (find coefficients, etc.)

Beyond Newton-Cotes and Gauss

- If integrand is very noisy, very high-dimensional, or has complicated boundaries one can use Monte Carlo integration where the abscissa are drawn randomly
- There are other Gauss-quadrature methods (Gauss-Laguerre, Gauss-Hermite) than can integrate bounded integrals with infinity as one of the limits
- Gauss-Kronrod methods are nested quadrature rules that seek to solve the problem of having to recompute all the points. They can be used to arrive at error estimates as well.
- In Clenshaw-Curtis quadrature, we use Chebyshev points as the abscissa. Although the method is of lower order than Gauss quadrature, in practice, it seems to have comparable performance. In addition, finding the nodes and weights is simple and cheap.

Integrable Singularities

- The integral

$$\int_0^1 \log x \; dx = (x \log x - x)\Big|_0^1 = -1$$

  even though $\log(0) \to -\infty$. This is an example of an integrable singularity.
- More precisely, the singularity can be isolated to an arbitrary interval which can be shrunk to zero.

$$\int_0^1 \log x \; dx = \lim_{\epsilon \to 0} \int_\epsilon^1 \log x \; dx = -1$$

- Integrating such functions numerically poses problems
- There are two common strategies to handle integrable singularities: (i) change of variables, and (ii) dividing or subtracting an analytically tractable function with the same kind of singularity.

Change of Variables

- Consider the integral

$$\int_0^{\pi/2} \frac{\cos x}{\sqrt{x}}\ dx$$

  which has a singularity at $x = 0$, since $\cos(0)/\sqrt{0} \to \infty$.

- Consider the transformation $x = t^2$

$$\int_0^{\pi/2} \frac{\cos x}{\sqrt{x}}\ dx = \int_0^{\sqrt{\pi/2}} \frac{\cos t^2}{t} 2t\ dt = 2\int_0^{\sqrt{\pi/2}} \cos t^2 dt$$

  which can be integrated easily since the singularity there is no singularity at $t = 0$.

Subtracting/Dividing Singularities

- Consider the integral

$$\int_0^{\pi/2} \frac{1}{\sqrt{\sin x}} \, dx$$

  which again has a singularity at $x = 0$.
- Consider rewriting the integral as:

$$\int_0^{\pi/2} \left(\frac{1}{\sqrt{\sin x}} - \frac{1}{\sqrt{x}} \right) \, dx + \int_0^{\pi/2} \frac{1}{\sqrt{x}} \, dx$$

  Note here I used my knowledge of Taylor series expansions: $\sin x \sim x$ for x near 0.

Subtracting/Dividing Singularities

- The first integrand is well-behaved near $x = 0$ (it can be replaced with 0)
- The second integrand is analytically integrable ($2\sqrt{2\pi}$)