Topic and contents

UNSW, School of Mathematics and Statistics

MATH2089 – Numerical Methods

Week 06 – Numerical Integration

- MATLAB M-files
  - `numint.m`
  - `gauleg.m`
  - `spike.m`

Integration

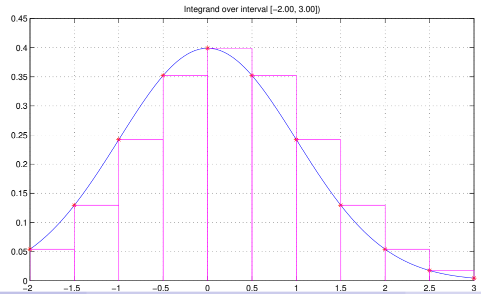
- One-dimensional integral of $f \in C([a,b])$

$$I(f) = \int_a^b f(x)\,dx$$

- Multi-dimensional integrals not in this course

Example (Standard normal probabilities)

$$X \sim N(0,1), \quad \mathbb{P}\left[a \le X \le b\right] = \int_a^b \frac{1}{\sqrt{2\pi}} e^{-u^2/2} du$$



Quadrature Rules

- Integral

$$I(f) = \int_a^b f(x)\,dx$$

Definition (Quadrature Rule)

A quadrature rule $Q_N(f)$ to approximate the integral $I(f)$ using the nodes $x_j \in [a,b]$ for $j = 1, \ldots, N$ and weights w_j, $j = 1, \ldots, N$ is

$$Q_N(f) = \sum_{j=1}^{N} w_j f(x_j)$$

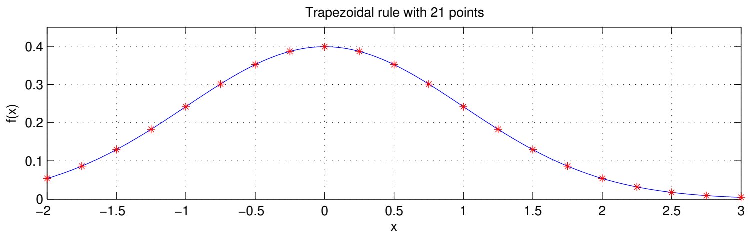
- Quadrature Error

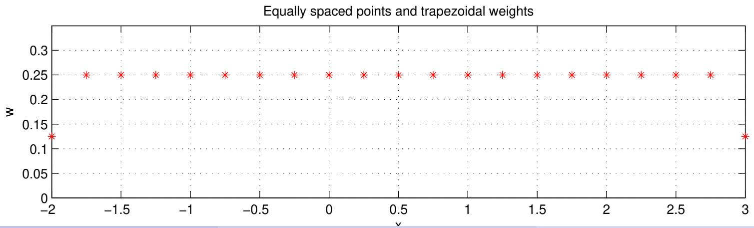
$$E_N(f) = I(f) - Q_N(f)$$

  - Want as $N \to \infty$: $\quad Q_N(f) \to I(f) \iff |E_N(f)| \to 0$
  - $E_N(f) > 0 \iff I(f) > Q_N(f), \quad E_N(f) < 0 \iff I(f) < Q_N(f)$

Quadrature rule

- Quadrature rule: $Q_N(f) = \sum_{j=1}^{N} w_j f(x_j)$, $\quad$ nodes x_j, weights w_j





Trapezoidal Rule

- Divide $[a, b]$ into N equal width intervals ($N+1$ points)

$$x_j = a + hj, \quad j = 0, \ldots, N, \quad \text{where} \quad h = \frac{b-a}{N}$$

- Function values $f_j \equiv f(x_j)$
- Approximate $f(x)$ on $[x_j, x_{j+1}]$ by a straight line joining f_j and f_{j+1}
- Trapezoidal rule

$$Q_N(f) = h\left(\tfrac{1}{2}f_0 + \sum_{j=1}^{N-1} f_j + \tfrac{1}{2}f_N\right)$$

- Weights $\quad w_0 = w_N = \frac{h}{2}, \quad w_j = h,\ j = 1, \ldots, N-1$
- Error for $f \in C^2([a, b])$

$$E_N(f) = -\frac{(b-a)h^2}{12} f''(\eta) \quad \text{some } \eta \in [a, b].$$

- $E_N(f) = O(h^2) = O\left(N^{-2}\right)$

Simpson's Rule

- N intervals, equal width h, N even
- Approximate f by a quadratic function over $[x_{j-1}, x_{j+1}]$
- Simpson's rule

$$Q_N(f) = \frac{h}{3}\left(f_0 + 4f_1 + 2f_2 + 4f_3 + 2f_4 + \cdots 2f_{N-2} + 4f_{N-1} + f_N\right)$$

- Weights

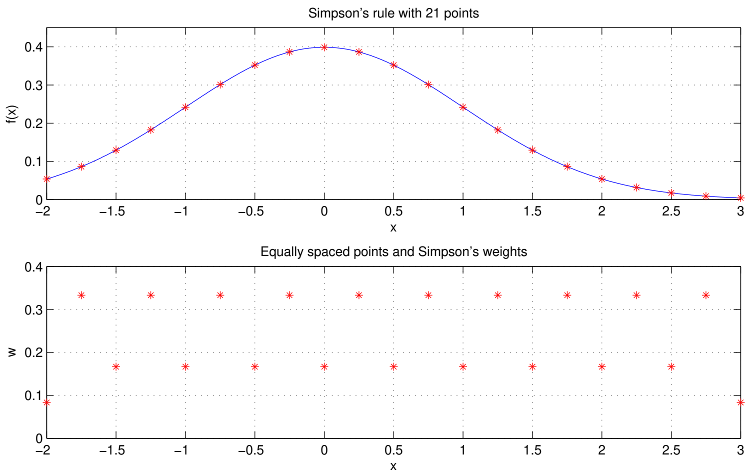
$$w_0 = w_N = \frac{h}{3},\ w_{2j-1} = \frac{4h}{3},\ w_{2j} = \frac{2h}{3},\ j = 1, \ldots, \frac{N}{2} - 1;\ w_{N-1} = \frac{4h}{3}.$$

- Error for $f \in C^4([a, b])$

$$E_N(f) = -\frac{(b-a)h^4}{180} f^{(4)}(\eta) \quad \text{some } \eta \in [a, b].$$

- $E_N(f) = O(h^4) \quad$ or $\quad E_N(f) = O\left(N^{-4}\right)$

Simpson's rule – example



Example - Standard normal probability

Example (Standard normal probability)

Estimate $I(\phi) = \int_{-2}^{3} \phi(x)dx$ using the Trapezoidal rule and Simpson's rule with $N = 2, 4, 8, 16, 32, 64, 128$. Tabulate the errors $E_N(\phi)$ and the ratios $E_{N/2}(\phi)/E_N(\phi)$ of the errors.

Solution (MATLAB script `numint.m`)

	Trapezoidal rule			Simpson's rule		
N	$Q_N(f)$	$E_N(f)$	Ratio	$Q_N(f)$	$E_N(f)$	Ratio
2	0.9531918356	2.27e-02		1.2222367683	-2.46e-01	
4	0.9608643565	1.50e-02	1.51	0.9634218635	1.25e-02	-19.7
8	0.9719937401	3.91e-03	3.85	0.9757035347	1.96e-04	63.5
16	0.9749155260	9.84e-04	3.97	0.9758894546	1.05e-05	18.7
32	0.9756533862	2.47e-04	3.99	0.9758993396	6.30e-07	16.7
64	0.9758382948	6.17e-05	4.00	0.9758999310	3.90e-08	16.2
128	0.9758845494	1.54e-05	4.00	0.9758999676	2.43e-09	16.0

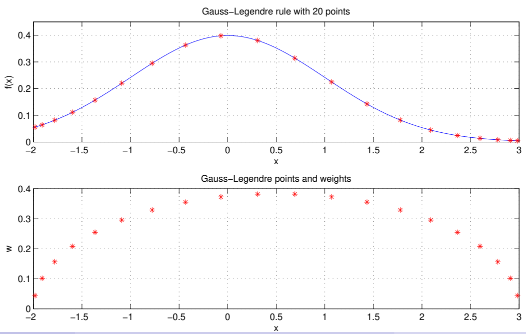
Table: Trapezoidal rule and Simpson's rule for $\int_{-2}^{3} \phi(x)dx$

Gauss-Legendre Rule

- Integral on $[-1, 1]$
$$I(f) = \int_{-1}^{1} f(x)dx \approx Q_N(f) = \sum_{j=1}^{N} w_j f(z_j)$$
- "Optimal" choice of both nodes z_j and weights w_j
- Nodes z_j: zeros of $P_N(x)$, degree N Legendre polynomial on $[-1, 1]$
  - Legendre polynomials, three-term recurrence
$$P_0(x) = 1,\ P_1(x) = x,\ (n+1)P_{n+1}(x) = (2n+1)xP_n(x) - nP_{n-1}(x)$$
- Weights w_j: $w_j = \dfrac{2}{(1 - z_j^2)[P_N'(z_j)]^2} \geq 0 \quad j = 1, \dots, N$
- MATLAB function `gauleg.m`
- Error for $f \in C^{2N}([-1, 1])$
$$E_N(f) = \frac{2^{2N+1}(N!)^4}{(2N+1)[(2N)!]^3} f^{(2N)}(\eta) \quad \text{some } \eta \in (-1, 1),$$

Gauss-Legendre Quadrature

- Given Gauss-Legendre nodes z_j and weights w_j for $[-1, 1]$
- Map $z \in [-1, 1]$ to $x \in [-2, 3]$ by $x = \frac{5}{2}z + \frac{1}{2}$, $\implies dx = \frac{5}{2}dz$
- Approximate integral
$$\int_{-2}^{3} f(x)dx = \int_{-1}^{1} f\left(\tfrac{5}{2}z + \tfrac{1}{2}\right)\tfrac{5}{2}dz \approx \sum_{j=1}^{N} \frac{5w_j}{2} f\left(\tfrac{5}{2}z_j + \tfrac{1}{2}\right)$$
- On interval $[-2, 3]$



Gauss-Legendre rule Example

Example (Standard normal probability – Gauss-Legendre rule)

N	$Q_N(f)$	$I(f) - Q_N(f)$
2	0.7900637402	1.86e-01
3	1.0083098187	-3.24e-02
4	0.9720865669	3.81e-03
5	0.9761640669	-2.64e-04
6	0.9759029512	-2.98e-06
7	0.9758959874	3.98e-06
8	0.9759006722	-7.02e-07
9	0.9758998852	8.48e-08
10	0.9758999783	-8.26e-09
15	0.9758999700	1.11e-14
20	0.9758999700	-5.55e-16

Table: Gauss-Legendre rule on $\int_{-2}^{3} \phi(x)dx$

Degree of precision

- Degree of precision is highest degree m such that

  $$E_N(1) = E_N(x) = E_N(x^2) = \ldots = E_N(x^m) = 0 \text{ but } E_N(x^{m+1}) \neq 0.$$

  - Degree of precision of trapezoidal rule is 1.
  - Degree of precision of Simpson's rule is 3.
  - Degree of precision of a Gauss-Legendre rule with N points is $2N - 1$.

Change of variables – Linear

- Map interval $[0, 1]$ to $[a, b]$
  - Change of variables

    $$y = a + (b - a)x, \qquad dy = (b - a)dx,$$

  - $$\int_a^b f(y)dy = (b - a)\int_0^1 f(a + (b - a)x)dx.$$

- Map interval $[-1, 1]$ to $[a, b]$
  - Change of variables

    $$y = \frac{a + b}{2} + \frac{b - a}{2}x, \qquad dy = \frac{b - a}{2}dx,$$

  - $$\int_a^b f(y)dy = \frac{(b - a)}{2}\int_{-1}^1 f\left(\frac{a + b}{2} + \frac{(b - a)}{2}x\right)dx.$$

Change of variables – Nonlinear

- Map $\mathbb{R}$ to $[0,1]$
  - Expected value of $f(X)$, random variable $X \sim N(0,1)$

$$\mathbb{E}[f] = \int_{\mathbb{R}} f(x)\phi(x)dx$$

  - ϕ standard normal pdf, Φ standard normal cdf

$$\phi(x) = \frac{1}{\sqrt{2\pi}} e^{\frac{-x^2}{2}}, \qquad \Phi(x) = \int_{-\infty}^{x} \phi(u)du$$

  - Change of variables $y = \Phi(x)$, $\quad x = \Phi^{-1}(y)$, MATLAB `norminv`
  - Derivative

$$\frac{dy}{dx} = \frac{d}{dx}\int_{-\infty}^{x} \phi(u)du = \phi(x)$$

  - Bounds of integration $x = -\infty \iff y = 0, \quad x = +\infty \iff y = 1$
  -

$$\int_{\mathbb{R}} f(x)\phi(x)dx = \int_0^1 f(\Phi^{-1}(y))dy.$$

Difficult integrals

Example

Approximate the integral

$$I = \int_0^1 \sqrt{x}\, dx = \frac{2}{3}$$

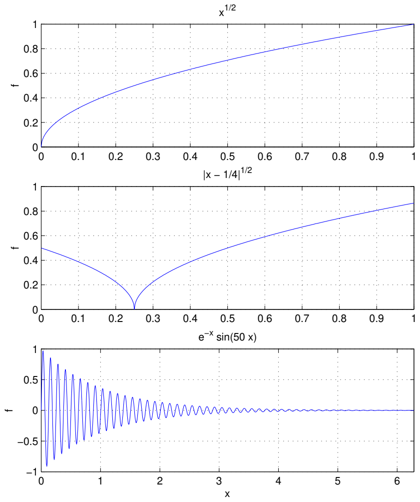
using the Trapezoidal rule, Simpson's rule and the Gauss-Legendre rule with $N = 2, 4, 8, 16, 32, 64$.

Solution

	Trapezoidal rule		*Simpson's rule*		*Gauss-Legendre rule*	
N	$Q_N(f)$	$E_N(f)$	$Q_N(f)$	$E_N(f)$	$Q_N(f)$	$E_N(f)$
2	0.6035533906	6.31e-02	0.6380711875	2.86e-02	0.6738873387	-7.22e-03
4	0.6432830462	2.34e-02	0.6565262648	1.01e-02	0.6678276454	-1.16e-03
8	0.6581302216	8.54e-03	0.6630792801	3.59e-03	0.6668355801	-1.69e-04
16	0.6635811969	3.09e-03	0.6653981886	1.27e-03	0.6666896315	-2.30e-05
32	0.6655589363	1.11e-03	0.6662181827	4.48e-04	0.6666696674	-3.00e-06
64	0.6662708114	3.96e-04	0.6665081031	1.59e-04	0.6666670504	-3.84e-07

Table: Quadrature rules for $\int_0^1 \sqrt{x}\, dx$

Examples of hard integrals



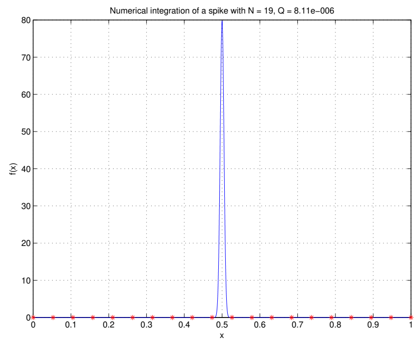
- Some difficult integrands: $\sqrt{x}$, $\sqrt{|x - 1/4|}$ and $e^{-x}\sin(50x)$

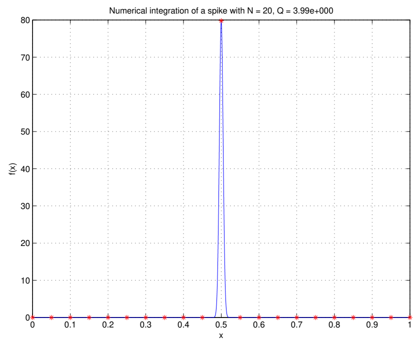
Difficult integrals cont

- Methods assume integrand f is sufficiently smooth on $[a, b]$
  - Trapezoidal rule $f \in C^2([a, b])$
  - Simpson's rule $f \in C^4([a, b])$
  - Gauss-Legendre rule $f \in C^{2N}([a, b])$
- Difficult: Derivative unbounded
  - Example: $f(x) = \sqrt{x}$ on $[0, b]$
  - Unbounded derivatives at 0
  - Change of variables: $x = y^2$
    - $\int_0^b \sqrt{x}dx = 2\int_0^{\sqrt{b}} y^2 dy$
- Difficult: Derivative discontinuity
  - Example: $f(x) = \sqrt{|x - 1/4|}$ on $[0, 1]$
  - Split integral to remove derivative discontinuity from $|\cdot|$
  - $\int_0^1 f(x)dx = \int_0^{\frac{1}{4}} \sqrt{1/4 - x}\,dx + \int_{\frac{1}{4}}^1 \sqrt{x - 1/4}\,dx$
  - Change of variables to remove square roots
- Difficult: Highly oscillatory
  - Example: $f(x) = e^{-x}\sin(50x)$
  - N sufficiently large or special method

Numerical integration can fail

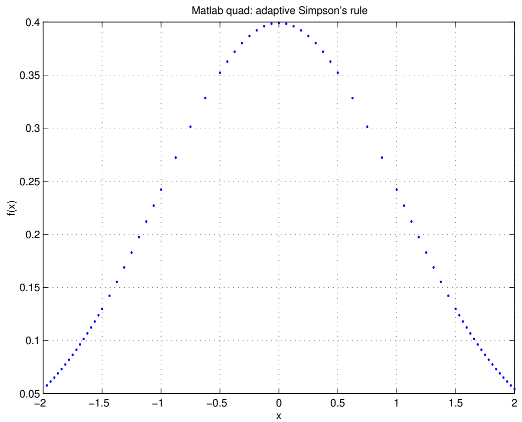
- Integrating a narrow spike: $I(f) = 1$
  - Underestimate integral if spike between nodes ($Q_{19}(f) \approx 8.11 \times 10^{-6}$)
  - Overestimate integral if node falls on spike ($Q_{20}(f) \approx 3.99$)
  - MATLAB script spike.m





Adaptive quadrature

- Use error estimates to add more nodes where error is largest
- MATLAB function `quad`



Integrals vs Differential equations

- Fundamental theorem of calculus

$$y(x) = \int_a^x f(t)\ dt = F(x) - F(a)$$

  where

$$f(t) = \frac{dF(t)}{dt} \iff F(t) = \int f(t)dt$$

- Differentiate wrt x

$$y'(x) = f(x), \quad x > a$$

- Initial condition

$$y(a) = 0$$

- Integration is equivalent to solving a single differential equation with appropriate initial condition