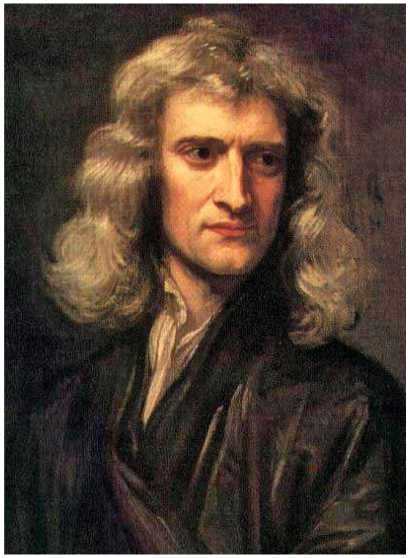
Numerical Integration and Differentiation

1. Function interpolation
2. Numerical integration
3. Numerical differentiation

Johannes Kepler
1610



Isaac Newton
1671

Carl Friedrich Gauss
1814

Numerical Integration and Differentiation

Function Interpolation

Function Interpolation

- The interpolation problem
  - » Given values of an unknown function $f(x)$ at values $x = x_0, x_1, \ldots, x_n$, find approximate values of $f(x)$ between these values
- Polynomial interpolation
  - » Find nth-order polynomial $p_n(x)$ that approximates the function $f(x)$ and provides exact agreement at the $n+1$ node points:

$$p_n(x_0) = f(x_0), \quad p_n(x_1) = f(x_1), \quad \cdots \quad p_n(x_n) = f(x_n)$$

  - » Can prove that the polynomial $p_n(x)$ is unique (see text)
  - » Interpolation: evaluate $p_n(x)$ for $x_0 \leq x \leq x_n$
  - » Extrapolation: evaluate $p_n(x)$ for $x_0 > x > x_n$

Motivation for Polynomial Interpolation

- Practical
  - » Polynomials are readily differentiated and integrated
  - » Polynomials are linearly parameterized

$$p_n(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_n x^n$$

- Theoretical – Weierstrass approximation theorem
  - » Any continuous function $f(x)$ can be approximated to arbitrary accuracy on an interval with a polynomial $p_n(x)$ of sufficiently high order:

$$\exists n \in I \ni \quad \left| f(x) - p_n(x) \right| < \beta \quad \forall x \in J : a \le x \le b$$

Lagrange Interpolation: Linear

- Linear interpolation
  - » Interpolate the two points $[x_0, f(x_0)]$, $[x_1, f(x_1)]$
- Lagrange polynomial

$$p_1(x) = L_0(x) f(x_0) + L_1(x) f(x_1) = \frac{x - x_1}{x_0 - x_1} f(x_0) + \frac{x - x_0}{x_1 - x_0} f(x_1)$$

$$p_1(x) = \left(\frac{f(x_1) - f(x_0)}{x_1 - x_0} \right) x + \left(\frac{x_1 f(x_0) - x_0 f(x_1)}{x_1 - x_0} \right) = ax + b$$

$$p_1(x_0) = f(x_0) \quad p_1(x_1) = f(x_1)$$

Lagrange Interpolation: Quadratic

- Quadratic interpolation
  - » Interpolate the three points $[x_0, f(x_0)]$, $[x_1, f(x_1)]$, $[x_2, f(x_2)]$
- Lagrange polynomial

$$p_2(x) = L_0(x)\, f(x_0) + L_1(x)\, f(x_1) + L_2(x)\, f(x_2) = ax^2 + bx + c$$

$$p_2(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2)$$

$$p_2(x_0) = f(x_0) \quad p_2(x_1) = f(x_1) \quad p_2(x_2) = f(x_2)$$

Lagrange Interpolation: Theory

- General case

$$f(x) \approx p_n(x) = \sum_{k=0}^{n} L_k(x) f(x_k) = \sum_{k=0}^{n} \frac{l_k(x)}{l_k(x_k)} f(x_k)$$

  » Formulas for Lagrange polynomials given in text

- Error estimate

  » If $f(x)$ has a continuous $(n+1)$-st derivative, then the polynomial approximation has the error:

$$\varepsilon_n(x) = f(x) - p_n(x) = (x - x_0)(x - x_1)\cdots(x - x_n)\frac{1}{(n+1)!}\frac{d^{n+1} f(t)}{dx^{n+1}}$$

  » The error is zero at the node points and small near the node points → more node points improve accuracy

  » The error may be large away from the node points → extrapolation is risky

Numerical Integration and Differentiation

Numerical Integration

Numerical Integration

- Definite integral

$$J=\int_a^b f(x)dx = F(b)-F(a)$$

  » Many problems do not admit analytical solution $F(x)$

  » Need numerical methods to evaluate integral

- Rectangular rule

  » Divide interval into n subintervals of equal length: $h=\dfrac{b-a}{n}$

  » Evaluate function at midpoint of each interval

$$J=\int_a^b f(x)dx \approx h[f(x_1^*)+f(x_2^*)+\cdots+f(x_n^*)]$$

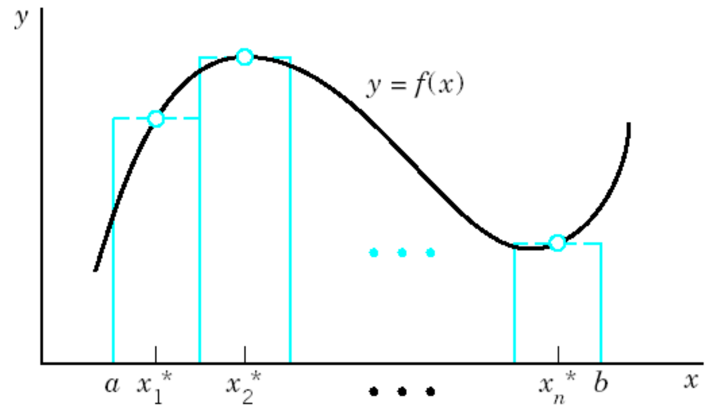


Fig. 438. Rectangular rule

Trapezoidal Rule

- Divide interval into *n* subintervals of equal length *h*
- Approximate integral by *n* trapezoids

$$J \approx \tfrac{1}{2}[f(a)+f(x_1)]h + \tfrac{1}{2}[f(x_1)+f(x_2)]h + \cdots + \tfrac{1}{2}[f(x_{n-1})+f(b)]h$$

$$J = [\tfrac{1}{2}f(a)+f(x_1)+\cdots+f(x_{n-1})+\tfrac{1}{2}f(b)]h$$

- Error estimate

$$KM_2 \le \varepsilon \le KM_2^* \qquad K = -\frac{b-a}{12}h^2$$

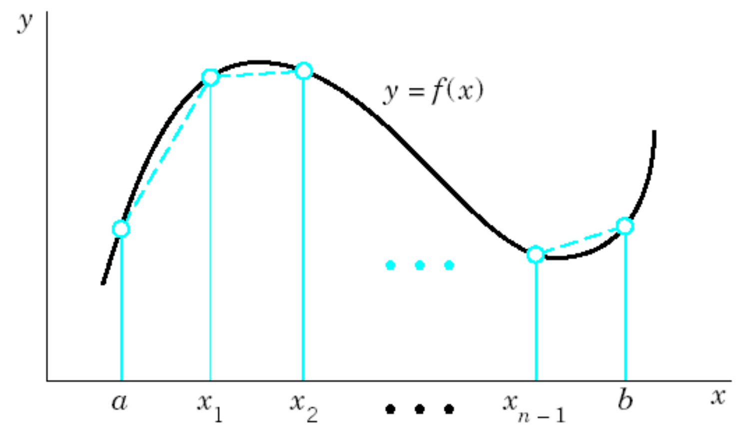


Fig. 439. Trapezoidal rule

  - » ε = difference between actual and approximate integrals
  - » M_2 = largest value of d^2f/dx^2 in the interval [*a*,*b*]
  - » M_2^* = smallest value of d^2f/dx^2 in the interval [*a*,*b*]

Simpson's Rule

- Divide interval into an even number $n = 2m$ subintervals of equal length h
- Evaluate function at endpoints of subintervals: a, x_1, x_2, …, x_{2m-1}, b
- Approximate function over two subintervals using Lagrange interpolation polynomial $p_2(x)$:

$$p_2(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2)$$

$$p_2(x) = \frac{(x-x_1)(x-x_2)}{2h^2} f(x_0) + \frac{(x-x_0)(x-x_2)}{-h^2} f(x_1) + \frac{(x-x_0)(x-x_1)}{2h^2} f(x_2)$$

- Define new variable

$$s \equiv \frac{x-x_1}{h} \quad \Rightarrow \quad p_2(s) = \tfrac{1}{2} s(s-1) f(x_0) - (s+1)(s-1) f(x_1) + \tfrac{1}{2}(s+1)sf(x_2)$$

Simpson's Rule cont.

- Perform integration over first two subintervals:

$$\int_{x_0}^{x_2} f(x)dx \approx \int_{x_0}^{x_2} p_2(x)dx = \int_{-1}^{1} p_2(s)hds = h\left[\tfrac{1}{3} f(x_0) + \tfrac{4}{3} f(x_1) + \tfrac{1}{3} f(x_2)\right]$$

- Sum integrals over all *m* intervals:

$$J \approx \frac{h}{3}[f(a) + 4f(x_1) + 2f(x_2) + \cdots + 2f(x_{2m-2}) + 4f(x_{2m-1}) + f(b)]$$

- Error bounds

$$CM_4 \le \varepsilon \le CM_4^* \quad C = -\frac{b-a}{180}h^4$$

» M_4 = largest value of d^4f/dx^4 in the interval [*a*,*b*]

» M_4^* = smallest value of d^4f/dx^4 in the interval [*a*,*b*]

Gaussian Quadrature

- Introduce new independent variable

$$t = \frac{2x-(a+b)}{b-a} \quad \Rightarrow \quad x:[a,b] \rightarrow t:[-1,1]$$

- Approximate integral

$$J = \int_a^b f(x)dx = \int_{-1}^{1} f(t)dt \approx \sum_{j=1}^{n} A_j f(t_j)$$

  - » Node points t_j not equally spaced
  - » A_j are the Gaussian weights
- Evaluating sum
  - » Select number of node points n
  - » Determine t_j as roots of nth-order Legendre polynomial
  - » Determine A_j using Lagrange interpolation polynomial

Gaussian Quadrature cont.

Table 19.7 **Gauss Integration: Nodes t_j and Coefficients A_j**

n	Nodes t_j	Coefficients A_j	Degree of Precision
2	−0.57735 02692 0.57735 02692	1 1	3
3	−0.77459 66692 0 0.77459 66692	0.55555 55556 0.88888 88889 0.55555 55556	5
4	−0.86113 63116 −0.33998 10436 0.33998 10436 0.86113 63116	0.34785 48451 0.65214 51549 0.65214 51549 0.34785 48451	7
5	−0.90617 98459 −0.53846 93101 0 0.53846 93101 0.90617 98459	0.23692 68851 0.47862 86705 0.56888 88889 0.47862 86705 0.23692 68851	9

- Example – third-order approximation

$$J = \int_a^b f(x)dx = \int_{-1}^{1} f(t)dt \approx A_1 f(t_1) + A_2 f(t_2) + A_3 f(t_3)$$

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Gaussian Quadrature Example

- Analytical solution

$$\int_1^5 e^{\frac{1}{2}x}\,dx = 2e^{\frac{1}{2}x}\Big|_1^5 = 21.067545$$

- Variable transformation

$$t = \frac{2x-(a+b)}{b-a} = \tfrac{1}{2}x - \tfrac{3}{2} \quad \Rightarrow \quad x = 2t+3$$

- Approximate solution

$$\int_1^5 e^{\frac{1}{2}x}\,dx \approx \int_{-1}^1 e^{\frac{1}{2}(2t+3)}\,2dt = 2\int_{-1}^1 e^{t+3/2}\,dt$$

$$\int_{-1}^1 e^{t+3/2}\,dt = (0.55555)e^{-0.77459+3/2} + (0.88889)e^{0+3/2} + (0.55555)e^{0.77459+3/2} = 10.533346$$

$$\int_1^5 e^{\frac{1}{2}x}\,dx \approx 2(10.533346) = 21.066691$$

- Approximation error = 4x10^{-3}%

Approximation Accuracy

- Degree of precision (*DP*)
  - » Maximum order of polynomial for which the integration formula provides an exact answer
- Trapezoidal rule
  - » Error $O(h^2)$
  - » $DP = 1$
  - » Perfect approximation only for linear functions
- Simpson's rule
  - » Error $O(h^4)$
  - » $DP = 3$
  - » Perfect approximation up to cubic functions
- Gaussian quadrature
  - » $DP = n\text{–}1$
  - » Perfect approximation possible for any polynomial function

Numerical Integration and Differentiation

In-class Exercise

Numerical Integration and Differentiation

Numerical Differentiation

Numerical Differentiation

- Introduction
  - » Often need to approximate derivatives to solve ODE models
  - » Numerical differentiation: approximate derivatives of a function using only functional values
  - » Can introduce large errors due to data noise and numerical inaccuracies
- Definition of derivative

$$\frac{df(x)}{dx} = \lim_{h\to 0} \frac{f(x+h) - f(x)}{h}$$

- Finite difference approximations

Forward $$\frac{df(x_j)}{dx} = \frac{f(x_{j+1}) - f(x_j)}{h}$$

Backward $$\frac{df(x_j)}{dx} = \frac{f(x_j) - f(x_{j-1})}{h}$$

Central $$\frac{df(x_j)}{dx} = \frac{f(x_{j+1}) - f(x_{j-1})}{2h}$$

Second-Order Finite Differences

- Forward difference

$$\frac{df(x_j)}{dx} = \frac{f(x_{j+1}) - f(x_j)}{h}$$

$$\frac{d^2 f(x_j)}{dx^2} = \frac{\dfrac{df(x_{j+1})}{dx} - \dfrac{df(x_j)}{dx}}{h}$$

$$= \frac{\dfrac{f(x_{j+2}) - f(x_{j+1})}{h} - \dfrac{f(x_{j+1}) - f(x_j)}{h}}{h}$$

$$= \frac{f(x_{j+2}) - 2f(x_{j+1}) + f(x_j)}{h^2}$$

- Analogous formulas for backward and central differences
- More accurate formulas can de derived by differentiating Lagrange interpolation polynomials

Lagrange Interpolation Polynomials

- Approximate $f(x)$ with Lagrange polynomial $p_2(x)$

$$f(x) \approx p_2(x) = \frac{(x-x_1)(x-x_2)}{2h^2} f(x_0) + \frac{(x-x_0)(x-x_2)}{-h^2} f(x_1) + \frac{(x-x_0)(x-x_1)}{2h^2} f(x_2)$$

- Compute derivative

$$\frac{df(x)}{dx} \approx \frac{dp_2(x)}{dx} = \frac{2x-x_1-x_2}{2h^2} f(x_0) - \frac{2x-x_0-x_2}{h^2} f(x_1) + \frac{2x-x_0-x_1}{2h^2} f(x_2)$$

- Evaluate at different x values

$$x = x_0 \quad \Rightarrow \quad \frac{df(x_0)}{dx} \approx \frac{1}{2h}[-3f(x_0) + 4f(x_1) - f(x_2)]$$

$$x = x_1 \quad \Rightarrow \quad \frac{df(x_1)}{dx} \approx \frac{1}{2h}[-f(x_0) + f(x_2)]$$

$$x = x_2 \quad \Rightarrow \quad \frac{df(x_2)}{dx} \approx \frac{1}{2h}[f(x_0) - 4f(x_1) + 3f(x_2)]$$