Numerical Methods - Numerical Integration & Differentiation

Y. K. Goh

Universiti Tunku Abdul Rahman

2013

Outline

1. Numerical Integration
   - Basic Numerical Integration
   - Newton-Cotês Rules
   - Romberg Integration
   - Gaussian Quadrature
   - Adaptive Quadrature Methods

2. Numerical Differentiation
   - Finite Differences
   - Richardson's Extrapolation

Outline

1. Numerical Integration
   - Basic Numerical Integration
   - Newton-Cotês Rules
   - Romberg Integration
   - Gaussian Quadrature
   - Adaptive Quadrature Methods

2. Numerical Differentiation
   - Finite Differences
   - Richardson's Extrapolation

Definite Integral and Numerical Integration

- The main focus of the remaining of this chapter is to evaluate the definite integral $I = \int_a^b f(x)\,dx$ numerically.

Definition (Definite integral)

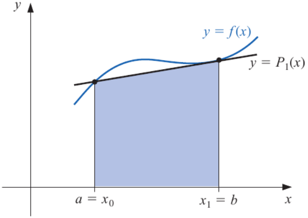
The definite integral of a function $f(x)$ over the interval $[a, b]$ that partitioned into $a = x_0 < x_1 < \cdots < x_n = b$ is defined as the limit of its Riemann sum:

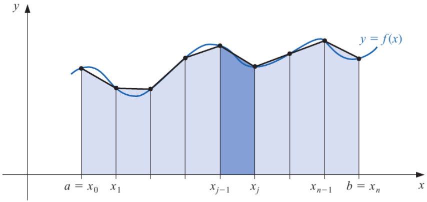
$$\int_a^b f(x)\,dx = \lim_{\Delta x_i \to 0} \sum f(z_i)\Delta x_i, \quad \Delta x_i = x_{i+1} - x_i, z_i \in [x_i, x_{i+1}].$$

- Numerical integration or quadrature formulae are all based on adding up the appropriate combinations of integrands at the partition of points within the range of integration to achieve the best accuracy for the least number of function evaluations.
- Quadrature is a historical term for computation of a univariate definite integral.

Trapezoid Rule

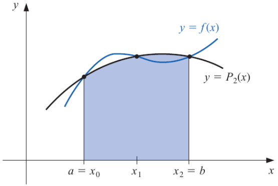
- Basic trapezoid rule :
$$\int_a^b f(x)\,dx = \frac{h}{2}[f(a)+f(b)] - \frac{1}{12}h^3 f''(\xi),$$ where $h = b-a, \xi \in [a,b]$.
- Composite trapezoid rule:
$$\int_a^b f(x)\,dx = \sum_{i=0}^{n-1} \frac{h}{2}[f(x_i)+f(x_{i+1})] - \frac{1}{12}(b-a)h^2 f''(\xi),$$ where the interval $[a,b]$ is uniformly partitioned into $a = x_0 < x_1 < \cdots < x_n = b$, ie $x_i = a + ih, i \geq n$ and $h = (b-a)/n$.

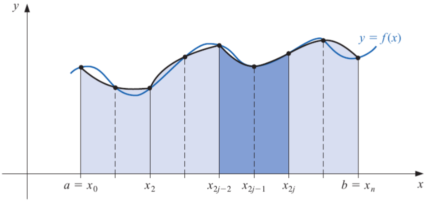




Simpson's Rule

- Basic Simpson's rule :
$$\int_a^b f(x)\,dx = \frac{h}{3}[f(x_0)+4f(x_1)+f(x_2)] - \frac{1}{90}h^5 f^{(4)}(\xi),$$ where
$h=(b-a)/2, \xi \in [a,b], x_0 = a, x_1 = a+h, x_2 = b.$
- Composite Simpson' rule:
$$\int_a^b f(x)\,dx = \frac{h}{3}\left[f(x_0) + 2\sum_{i=1}^{(n/2)-1} f(x_{2i}) + 4\sum_{i=1}^{n/2} f(x_{2i-1}) + f(x_n)\right] -$$
$\frac{1}{180}(b-a)h^4 f^{(4)}(\xi)$, where the interval $[a,b]$ is uniformly partitioned into $a = x_0 < x_1 < \cdots < x_n = b$, $h = (b-a)/n$ and n is **even**.





Example: Trapezoid Rule and Simpson's Rule

Example

Let $I = \displaystyle\int_1^2 \frac{1}{x^3}\, dx$.

1. Calculate the exact value for I. [**ANS:** $I = \frac{3}{8} = 0.37500.$]
2. Use the basic trapezoid rule to estimate I and compute the error.
   [**ANS:** $h = 1, I \approx \frac{1}{2}[f(1) + f(2)] = 0.56250.$ Error $= 0.18750.$]
3. Use the composite trapezoid rule with 4 partitions to estimate I and compute the error.
   [**ANS:** $h = 0.25, I \approx \frac{0.25}{2}[f(1) + 2f(1.25) + 2f(1.5) + 2f(1.75) + f(2)] = 0.38935.$ Error $= 0.01434.$]
4. Use the basic Simpson's rule with two partition to estimate I and compute the error.
   [**ANS:** $h = 0.5, I \approx \frac{0.5}{3}[f(1) + 4f(1.5) + f(2)] = 0.38503.$ Error $= 0.01003$]
5. Use the composite Simpson's rule with 4 partitions to estimate I and compute the error.
   [**ANS:** $h = 0.25, I \approx \frac{0.25}{3}[f(1) + 4f(1.25) + 2f(1.5) + 4f(1.75) + f(2)] = 0.37600.$ Error $= 0.00100.$]

Example: Trapezoid Rule and Simpson's Rule

Example

How many subintervals are needed to approximate $\displaystyle\int_1^2 \frac{1}{x^3}\,dx$ with error not exceed 10^{-5} by using a (i) composite trapezoid rule, and (ii) composite Simpson's rule?

ANSWER:

- Composite trapezoid rule:
  - The error formula : $-\frac{b-a}{12}h^2 f''(\xi)$
  - $f''(x) = \frac{12}{x^5}$, for $\xi \in [1, 2]$, $|f''(\xi)| \le 12$.
  - Thus, the maximum error will not greater than h^2.
  - To have error less than 10^{-5}, $h^2 \le 10^{-5}$, or $h \le 0.003162$.
  - $h = (b-a)/n \le 0.003162$ implies $n \ge 316.23$, ie 317 or more partitions will certainly produce the desirable accuracy.
- Composite Simpson's rule:
  - The error formula : $-\frac{b-a}{180}h^4 f^{(4)}(\xi)$
  - $f^{(4)}(x) = \frac{360}{x^7}$, for $\xi \in [1, 2]$, $|f^{(4)}(\xi)| \le 360$.
  - Thus, the maximum error will not greater than $2h^4$.
  - $2h^4 = 2/n^4 \le 10^{-5}$ implies $n \ge 21.147$, ie at most 22 partitions needed.

Outline

1. Numerical Integration
   - Basic Numerical Integration
   - Newton-Cotês Rules
   - Romberg Integration
   - Gaussian Quadrature
   - Adaptive Quadrature Methods
2. Numerical Differentiation
   - Finite Differences
   - Richardson's Extrapolation

Newton-Cotês Rules (Closed)

- The Newton-Cotês quadrature formulas are obtained by approximating the $f(x)$ by interpolating polynomials. Let $f_0 = f(x_0), f_1 = f(x_1)$ and so on.
- **Trapezoid Rule:**

$$\int_{x_0}^{x_1} f(x)\,dx = \frac{1}{2}h[f_0 + f_1] - \frac{1}{12}h^3 f''(\xi)$$

- **Simpson's $\frac{1}{3}$ Rule:**

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{1}{3}h[f_0 + 4f_1 + f_2] - \frac{1}{90}h^5 f^{(4)}(\xi)$$

- **Simpson's $\frac{3}{8}$ Rule:**

$$\int_{x_0}^{x_3} f(x)\,dx = \frac{3}{8}h[f_0 + 3f_1 + 3f_2 + f_3] - \frac{3}{80}h^5 f^{(4)}(\xi)$$

- **Boole's Rule:**

$$\int_{x_0}^{x_4} f(x)\,dx = \frac{2}{45}h[7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4] - \frac{8}{945}h^7 f^{(6)}(\xi)$$

Newton-Cotês Rules (Opened)

- The quadrature rules are closed when the values of $f(x)$ at the end points are involve in the integration. Otherwise they are opened.
- **Midpoint Rule**
$$\int_{x_0}^{x_2} f(x)\,dx = 2hf_1 + \frac{1}{24}h^3 f''(\xi)$$
- **Two-Point Newton-Cotês Open Rule**
$$\int_{x_0}^{x_3} f(x)\,dx = \frac{3}{2}h[f_1 + f_2] + \frac{1}{4}h^3 f''(\xi)$$
- **Three-Point Newton-Cotês Open Rule**
$$\int_{x_0}^{x_4} f(x)\,dx = \frac{4}{3}h[2f_1 - f_2 + 2f_3] + \frac{28}{90}h^5 f^{(4)}(\xi)$$
- **Four-Point Newton-Cotês Open Rule**
$$\int_{x_0}^{x_5} f(x)\,dx = \frac{5}{24}h[11f_1 + f_2 + f_3 + 11f_4] + \frac{95}{144}h^5 f^{(4)}(\xi)$$

Outline

1. Numerical Integration
   - Basic Numerical Integration
   - Newton-Cotês Rules
   - Romberg Integration
   - Gaussian Quadrature
   - Adaptive Quadrature Methods
2. Numerical Differentiation
   - Finite Differences
   - Richardson's Extrapolation

Romberg Integration

- Consider the composite trapezoid rule
$$I = \int_a^b f(x)\,dx = \sum_{i=0}^{n-1} \frac{h}{2}[f(x_i) + f(x_{i+1})] - \frac{1}{12}(b-a)h^2 f''(\xi)$$
- Alternatively, the trapezoid rule could be writen in a Euler-Maclaurin form of
$$I = \int_a^b f(x)\,dx = \sum_{i=0}^{n-1} \frac{h}{2}[f(x_i) + f(x_{i+1})] + a_2h^2 + a_4h^4 + a_6h^6 + \ldots, \text{ or}$$
$$I = \int_a^b f(x)\,dx = R^{(0)}(h) + a_2h^2 + a_4h^4 + a_6h^6 + \ldots.$$
- Apply the Richardson's extrapolation by subdivide the interval into half and eliminate a_2, we get $I = [\frac{4}{3}R^{(0)}(h/2) - \frac{1}{3}R^{(0)}(h)] + a_4h^4/4 + \ldots$.
- Now $R^{(1)}(h) = \frac{4}{3}R^{(0)}(h/2) - \frac{1}{3}R^{(0)}(h)$ is a better approximation to I with error of the order $O(h^4)$.
- We could continue to eliminate the error terms of $O(h^4)$, $O(h^6), \ldots,$ to get $R^{(2)}(h) = \frac{16}{15}R^{(1)}(h/2) - \frac{1}{15}R^{(1)}(h)$, $R^{(3)}(h) = \frac{64}{63}R^{(2)}(h/2) - \frac{1}{63}R^{(2)}(h)$, and so on.

Romberg Integration

- Define $R_{n,0} = R^{(0)}(h/2^n)$ and use the Richardson's formula

$$R_{n,m} = R_{n,m-1} + \frac{1}{4^m - 1}(R_{n,m-1} - R_{n-1,m-1}),$$

then the previous approximation could be summarised as:

$$\begin{aligned}
R^{(0)}(h) &= \sum_{i=0}^{n-1} \frac{h}{2}[f(x_i) + f(x_{i+1})] &=& \quad R_{0,0} = \sum_{i=0}^{n-1} \frac{h}{2}[f(x_i) + f(x_{i+1})] \\
R^{(1)}(h) &= \frac{4}{3}R^{(0)}(h/2) - \frac{1}{3}R^{(0)}(h) &\Longrightarrow& \quad R_{1,1} = R_{1,0} + \frac{1}{3}[R_{1,0} - R_{0,0}] \\
R^{(2)}(h) &= \frac{16}{15}R^{(1)}(h/2) - \frac{1}{15}R^{(1)}(h) &\Longrightarrow& \quad R_{2,2} = R_{2,1} + \frac{1}{15}[R_{2,1} - R_{1,1}] \\
R^{(3)}(h) &= \frac{64}{63}R^{(2)}(h/2) - \frac{1}{63}R^{(2)}(h) &\Longrightarrow& \quad R_{3,3} = R_{3,2} + \frac{1}{63}[R_{3,2} - R_{2,2}]
\end{aligned}$$

Romberg Integration

m	$O(h^2)$	$O(h^4)$	$O(h^6)$		$O(h^{2N})$
0	$R_{0,0}$				
1	$R_{1,0}$	$R_{1,1}$			
2	$R_{2,0}$	$R_{2,1}$	$R_{2,2}$		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	
N	$R_{N,0}$	$R_{N,1}$	$R_{N,2}$	$\dots$	$R_{N,N}$

Outline

Gaussian Quadrature

- The Newton-Cotês formulas are derived by integrating the interpolating polynomials over a equally spaced (uniformly distributed) nodes for $f(x)$.
- It is not always optimal to use the equally spaced nodes, and if this restriction is relaxed and with appropriate weighting coefficients, we come to an approach called Gaussian quadrature.
- The idea of Gaussian quadrature is to fixed the number of nodes N, and select the weight w_i and position of the nodes x_i, so that

$$I = \int_a^b f(x)\,dx \approx \sum_{i=1}^{N} w_i f(x_i)$$

  is best accuracy possible.
- For simplicity, we will discuss Gaussian quadrature for $I = \int_{-1}^{1} f(x)\,dx$ and it is easy to extend to a more general interval $[a, b]$ by change of variable $x' = \frac{a+b}{2} + \frac{b-a}{2}x$.

Two-point Gauss-Legendre Quadrature

- The two-point Gauss-Legendre quadrature is of the form
  $I = \int_{-1}^{1} f(x)\,dx \approx w_1 f(x_1) + w_2 f(x_2)$.
- Let assume that the two-point quadrature will give exact result for any cubic polynomial, $f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$.
- We will setup 4 equations to determine the four unknowns w_1, w_2, x_1 and x_2.
- Since integration is additive, it is suffice to require the quadrature to be exact for $f(x) = 1, x, x^2$ and x^3. Thus,

$$
\begin{aligned}
f(x) = 1 \quad &: \quad \int_{-1}^{1} 1\,dx = 2 = w_1 + w_2 \\
f(x) = x \quad &: \quad \int_{-1}^{1} x\,dx = 0 = w_1 x_1 + w_2 x_2 \\
f(x) = x^2 \quad &: \quad \int_{-1}^{1} x^2\,dx = \frac{2}{3} = w_1 x_1^2 + w_2 x_2^2 \\
f(x) = x^3 \quad &: \quad \int_{-1}^{1} x^3\,dx = 0 = w_1 x_1^3 + w_2 x_2^3
\end{aligned}
$$

Gauss-Legendre Quadrature

- Solve the system of nonlinear equations, we get $w_1 = w_2 = 1$ and $-x_1 = x_2 = \frac{1}{\sqrt{3}}$.

Theorem (Two-Point Gauss-Legendre Rule)

If f is continous on $[-1, 1]$, then

$$\int_{-1}^{1} f(x)\,dx \approx G_2(f) = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

Example

Evaluate $\int_{-1}^{1} \frac{1}{x+2}$ numerically with two-point Gauss-Legendre rule.
ANS:

- Exact solution : $\ln(3) - \ln(1) \approx 1.09861.$
- Gauss-Legendre : $G_2(f) = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) = 1.09091.$
- Trapezoid rule : $\frac{2}{2}[f(-1) + f(1)] = 1.33333.$
- Simpson's rule : $\frac{1}{3}[f(-1) + 4f(0) + f(1)] = 1.11111.$

- A general N-point Gauss-Legendre rule is exact for evaluating integral of polynomial of degree $< 2N-1$:

$$G_N(f) = w_1 f(x_1) + w_2 f(x_2) + \cdots + w_N f(x_N) + E_N(f).$$

- The values of the nodes x_i and weights w_i are given by the following table

N	Nodes x_i	Weight w_i	Truncation error $E_N(f)$
2	$\pm\frac{1}{\sqrt{3}}$	1	$\frac{1}{135} f^{(4)}(\xi)$
3	$\pm\sqrt{\frac{3}{5}}$ 0	$\frac{5}{9}$ $\frac{8}{9}$	$\frac{1}{15750} f^{(6)}(\xi)$
4	$\pm\sqrt{\frac{1}{7}(3-4\sqrt{\frac{3}{10}})}$ $\pm\sqrt{\frac{1}{7}(3+4\sqrt{\frac{3}{10}})}$	$\frac{1}{2}+\frac{1}{12}\sqrt{\frac{10}{3}}$ $\frac{1}{2}-\frac{1}{12}\sqrt{\frac{10}{3}}$	$\frac{1}{3472875} f^{(8)}(\xi)$

Outline

1. Numerical Integration
   - Basic Numerical Integration
   - Newton-Cotês Rules
   - Romberg Integration
   - Gaussian Quadrature
   - Adaptive Quadrature Methods

2. Numerical Differentiation
   - Finite Differences
   - Richardson's Extrapolation

Adaptive Quadrature Methods

- In an adaptive scheme, the partition of $[a, b]$ is not pre-detemined.
- Instead, $[a, b]$ is subdivided into two subintervals on every iteration and test if the desirable accuracy is obtained.
- Adaptive algorithm procedure for $I = \int_a^b f(x)\,dx$ with accuracy ϵ:
  - If basic quadrature rule $S(a, b)$ is less than ϵ than stop.
  - Otherwise, subdivide $[a, b]$ into two equal intervals
  - evaluate quadratures on both intervals
  - test if each of quadratures is less than $\epsilon/2$
  - if yes, than stop; otherwise further subdivide the subinterval again and repeat.
- We will illustrate the adaptive scheme based on Simpson's rule.

Simpson's Adaptive Scheme

- Write $I = \int_a^b f(x)\,dx = S(a,b) + E(a,b)$, where $S(a,b) = \frac{1}{3}h[f(a) + 4f(a+h) + f(b)]$ and $E(a,b) = -\frac{1}{90}h^5 f^{(4)}(\xi_0)$.
- First approximation,
$$I = S^{(1)} + E^{(1)}, \tag{1}$$
where $S^{(1)} = S(a,b)$ and $E^{(1)} = E(a,b)$.
- Then half the interval for next approximation:
$$I = S^{(2)} + E^{(2)}, \tag{2}$$
where $S^{(2)} = S(a,a+h) + S(a+h,b)$.
- The new error term, $E^{(2)} = -\frac{1}{90}(h/2)^5 f^{(4)}(\xi_1) - \frac{1}{90}(h/2)^5 f^{(4)}(\xi_2)$.
- Assuming $f^{(4)}(\xi_i), i = 0,1,2$ do not change too much throughout $[a,b]$, then $E^{(2)} = \frac{1}{16}[-\frac{1}{90}h^5 f^{(4)}(\xi_0)] = \frac{1}{16}E^{(1)}$.
- Eq.(1) - Eq.(2) gives, $S^{(2)} - S^{(1)} = E^{(1)} - E^{(2)} = 15E^{(2)}$
- Thus, if $|E^{(2)}| = \frac{1}{15}|S^{(2)} - S^{(1)}| < \epsilon$ then $I = \frac{16}{15}S^{(2)} - \frac{1}{15}S^{(1)}$ and stop.
- Otherwise, split $[a,b]$ into $[a,a+h]$ and $[a+h,b]$ and test if both intervals with accuracy $\epsilon/2$.

Outline

1. Numerical Integration
   - Basic Numerical Integration
   - Newton-Cotês Rules
   - Romberg Integration
   - Gaussian Quadrature
   - Adaptive Quadrature Methods
2. Numerical Differentiation
   - Finite Differences
   - Richardson's Extrapolation

Outline

First Derivative

- Formula for numerical derivatives are important in numerical solutions of boundary value problems.
- Often this involves calculating derivatives of a function f that its value is only known at a few points $(x_0, f(x_0)), \dots, (x_n, f(x_n))$.
- Naively, we could use the definition of the derivative $f'(x_0) = \lim_{h\to 0} \dfrac{f(x_0+h) - f(x_0)}{h}$ of the function f at point x_0, and thus a simple approximation to $f'(x_0)$ is $f'(x_0) \approx \dfrac{f(x_0+h) - f(x_0)}{h}$.
- However this obvious approximation suffer from:
  - round-off error of substracting two quantities that are nearly equal.
  - truncation error of $|-\frac{1}{2}hf''(\xi)|$ that will present even if the calculation are performed with infinite precision.
- Note that the naive approximation of $f'(x_0)$ and its truncation error could be "derived" from the Taylor's theorem $f(x_0+h) = f(x_0) + hf'(x_0) + \frac{1}{2}h^2 f''(\xi(x_0))$.

First Derivative (Example)

Example

Let $f(x) = \cos x$ find $f'(\frac{\pi}{4})$, with $h = 0.1$ and 0.01. Calculate the corresponding absolute errors.

ANSWER :

- $f'(\frac{\pi}{4}) \approx \dfrac{f(\frac{\pi}{4}+h) - f(\frac{\pi}{4})}{h}$.
- For $h = 0.1$, $f'(\frac{\pi}{4}) \approx \dfrac{0.6329813067 - 0.7071067812}{0.1} = -0.7412547451$.
- For $h = 0.01$, $f'(\frac{\pi}{4}) \approx \dfrac{0.7000004762 - 0.7071067812}{0.1} = -0.7106305006$.
- For $h = 0.1$ case, absolute errors $= |-0.7412547451 - (-\sin(\pi/4))| = 0.0341$.
- For $h = 0.01$ case, absolute errors $= |-0.7106305006 - (-\sin(\pi/4))| = 0.00352$.

First Derivative (Example)

Example

Let $f(x) = \exp(x)$ and $x_0 = 1$. The following figure shows the secant lines for $h = 0.25, 0.5, 0.75$ and 1.0.

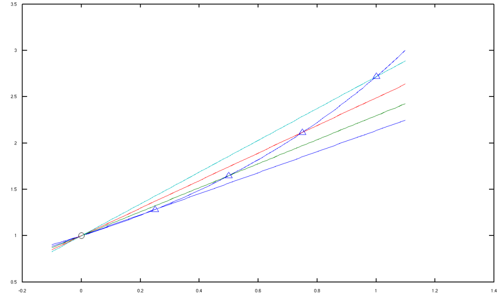


Figure: Several secant lines for $y = e^x$.

Also, MATLAB code : `nm05_error.m` illustrate the fact that it is not always smaller h gives better approximation.

Formula for First Derivative

- Taylor's series for $f(x_0+h)$ and $f(x_0-h)$ with $h>0$:

$$
\begin{aligned}
f(x_0+h) &= f(x_0) + hf'(x_0) + \frac{1}{2!}h^2 f''(x_0) + \frac{1}{3!}h^3 f'''(x_0) + \ldots \\
f(x_0-h) &= f(x_0) - hf'(x_0) + \frac{1}{2!}h^2 f''(x_0) - \frac{1}{3!}h^3 f'''(x_0) + \ldots
\end{aligned}
$$

Definition (Forward difference formula)

Forward difference formula : $f'(x_0) = \dfrac{f(x_0+h)-f(x_0)}{h} - \dfrac{1}{2}hf''(\xi)$.

Definition (Backward difference formula)

Backward difference formula : $f'(x_0) = \dfrac{f(x_0)-f(x_0-h)}{h} - \dfrac{1}{2}hf''(\xi)$.

Definition (Central difference formula)

Central difference formula : $f'(x_0) = \dfrac{f(x_0+h)-f(x_0-h)}{2h} - \dfrac{1}{6}h^2f'''(\xi)$.

Formula for First Derivatives (Example)

Example

Find $f'(x)$ for the following data set $(x, f(x))$ by using the forward / backward / center difference formula, given that $f(x) = \tan(x)$

ANSWER :

x	$f(x)$	$f'(x)$			
		Exact Value	Forward Diff.	Backward Diff.	Center Diff.
2.1	-1.70985	3.9236	3.3602	-	-
2.2	-1.37382	2.8874	2.5461	3.3602	2.9532
2.3	-1.11921	2.2526	2.0320	2.5461	2.2890
2.4	-0.91601	1.8391	1.6899	2.0320	1.8610
2.5	-0.74702	1.5580	1.4543	1.6899	1.5721
2.6	-0.60160	1.3619	-	1.4543	-

Second Derivatives

Definition (Central difference formula)

Central difference formula :

$$f''(x_0) = \frac{f(x_0+h) - 2f(x_0) + f(x_0-h)}{h^2} - \frac{1}{12}h^2 f'''(\xi).$$

Example

Let $f(x) = \cos x$, estimate $f''(\frac{\pi}{4})$ with $h = 0.01$ with the center difference formulat and calculate the corresponding absolute error.

ANSWER :

- $f''(\pi/4) \approx \dfrac{f(\pi/4+h) - 2f(\pi/4) + f(\pi/4-h)}{h^2} = -0.7071008887.$
- Absolute error $= |-0.707100888650558 + \cos(\pi/4)| = 5.89 \times 10^{-6}$.

Outline

1. Numerical Integration
   - Basic Numerical Integration
   - Newton-Cotês Rules
   - Romberg Integration
   - Gaussian Quadrature
   - Adaptive Quadrature Methods
2. Numerical Differentiation
   - Finite Differences
   - Richardson's Extrapolation

- From Taylor's series

$$f(x+h) = \sum_{k=0}^{\infty} \frac{h^k}{k!} f^{(k)}(x)$$

$$f(x-h) = \sum_{k=0}^{\infty} \frac{(-1)^k h^k}{k!} f^{(k)}(x)$$

- Substracting and rearrange yields

$$\begin{aligned} f'(x) &= \frac{1}{2h}[f(x+h) - f(x-h)] - [\frac{1}{3!}h^2 f'''(x) + \frac{1}{5!}h^4 f^{(5)}(x) + \dots] \\ &\equiv \varphi(h) + a_2 h^2 + a_4 h^4 + \dots \end{aligned}$$

- Let $L = \varphi(h) + a_2 h^2 + a_4 h^4 + \dots$ and replace h with $\frac{h}{2}$, then $L = \varphi(h/2) + a_2 h^2/4 + a_4 h^4/16 + \dots$
- Eliminating a_2 and obtain

$$L = \frac{4}{3}\varphi(h/2) - \frac{1}{3}\varphi(h) - a_4 h^4/4 + \dots$$

which is a better approximation of $f'(x)$ with error of order $O(h^4)$.

Richardson's Extrapolation (Cont.)

- The Richardson's method could be applied repeatedly to eliminate $a_4, a_6, \ldots$ to get higher accuracy.
- Let denote $D(n,0) = \varphi(h/2^n) \quad (n \geq 0)$ which gives the first approximation to $f'(x)$.
- A generalised Richardson's formula for approximation of order $O(h^{2(m+1)})$

$$D(n,m) = D(n,m-1) + (4^m - 1)^{-1}[D(n,m-1) - D(n-1,m-1)].$$

Example

Let $f(x) = xe^x$. By using the center difference and Richardson's extrapolation, find approximation of order $O(h^2), O(h^4)$, and $O(h^6)$ for $f'(2.0)$ with $h = 0.2$.

ANSWER :

- The approximations required are $D(0,0), D(1,1), D(2,2)$.
- $D(0,0) = 22.414160, D(1,0) = 22.228786, D(2,0) = 22.182564$
- $D(1,1) = D(1,0) + \frac{1}{3}[D(1,0) - D(0,0)] = 22.166995, D(2,1) = 22.167157$
- $D(2,2) = D(2,1) + \frac{1}{15}[D(2,1) - D(1,1)] = 22.167168.$

THE END