Part 6. Numerical Differentiation and Integration
Chapter 22. Integration of Equations

Lecture 22

Gauss Quadrature

22.4

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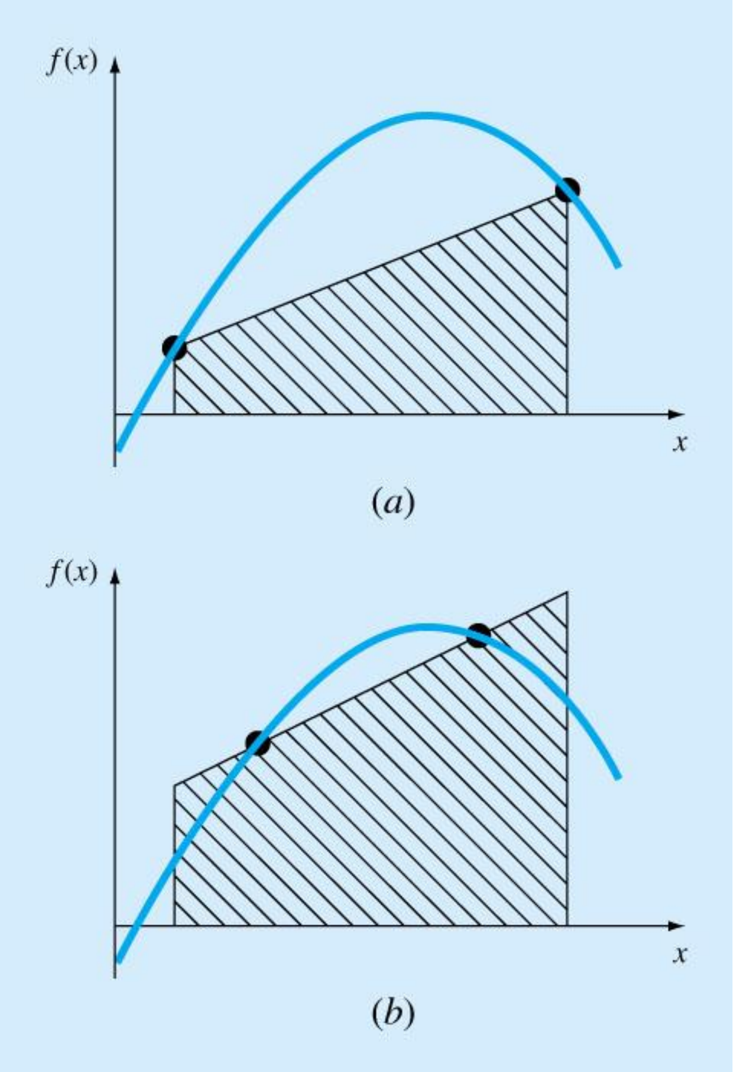
Gauss Quadrature

Features:

- Instead of two fixed points
- Choose points that balance positive and negative errors



Gauss Quadrature: 2-Point

The extension of Trapezoidal Rule is called the two-point Gauss Quadrature Rule or Gaussian Quadrature Rule

Method of undetermined coefficient for trapezoidal rule

is used for Gauss quadrature

$$I = \int_a^b f(x)dx \approx c_1 f(x_1) + c_2 f(x_2)$$

Gauss Quadrature: 2-Point

- Straight line pass through 2 intermediate points
- 4 unknowns : Two coefficient and two x-values in points 1 and 2.
- Third-order polynomial can be used to approximate f(x) and solve for coefficients and x-values

(see written notes)

Recall: Trapezoidal Rule

Trapezoidal Rule could be developed by the method of undetermined coefficients:

$$I = \int_a^b f(x)dx \approx c_1 f(a) + c_2 f(b)$$

$$= \frac{b-a}{2} f(a) + \frac{b-a}{2} f(b)$$

What if : the arguments of the function are not predetermined as a and b but as unknowns x_1 and x_2 ?

$$I = \int_a^b f(x)dx \approx c_1 f(x_1) + c_2 f(x_2)$$

Gauss Quadrature

The four unknowns x_1, x_2, c_1 and c_2 are found by assuming that the formula gives exact results for integrating a general third order polynomial,

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3.$$

$$\int_a^b f(x)dx = \int_a^b \left(a_0 + a_1 x + a_2 x^2 + a_3 x^3\right)dx$$

$$= \left[a_0 x + a_1 \frac{x^2}{2} + a_2 \frac{x^3}{3} + a_3 \frac{x^4}{4}\right]_a^b$$

$$= a_0(b-a) + a_1\left(\frac{b^2 - a^2}{2}\right) + a_2\left(\frac{b^3 - a^3}{3}\right) + a_3\left(\frac{b^4 - a^4}{4}\right)$$

Gauss Quadrature

$$\int_a^b f(x)dx = c_1\left(a_0 + a_1x_1 + a_2x_1{}^2 + a_3x_1{}^3\right) + c_2\left(a_0 + a_1x_2 + a_2x_2{}^2 + a_3x_2{}^3\right)$$

Equating Equations the two previous two expressions yield

$$a_0(b-a) + a_1\left(\frac{b^2 - a^2}{2}\right) + a_2\left(\frac{b^3 - a^3}{3}\right) + a_3\left(\frac{b^4 - a^4}{4}\right)$$

$$= c_1\left(a_0 + a_1x_1 + a_2x_1{}^2 + a_3x_1{}^3\right) + c_2\left(a_0 + a_1x_2 + a_2x_2{}^2 + a_3x_2{}^3\right)$$

$$= a_0(c_1 + c_2) + a_1(c_1x_1 + c_2x_2) + a_2\left(c_1x_1{}^2 + c_2x_2{}^2\right) + a_3\left(c_1x_1{}^3 + c_2x_2{}^3\right)$$

Gauss Quadrature

Since the constants a_0, a_1, a_2, a_3 are arbitrary

$$b - a = c_1 + c_2$$

$$\frac{b^2 - a^2}{2} = c_1 x_1 + c_2 x_2$$

$$\frac{b^3 - a^3}{3} = c_1 x_1{}^2 + c_2 x_2{}^2$$

$$\frac{b^4 - a^4}{4} = c_1 x_1{}^3 + c_2 x_2{}^3$$

Gauss Quadrature

The previous four simultaneous nonlinear Equations have only one acceptable solution,

$$x_1 = \left(\frac{b-a}{2}\right)\left(-\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2} \qquad x_2 = \left(\frac{b-a}{2}\right)\left(\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2}$$

$$c_1 = \frac{b-a}{2} \qquad c_2 = \frac{b-a}{2}$$

Gauss Quadrature

$$\int_a^b f(x)\ dx \approx c_1\ f\left(x_1\right)+c_2\ f\left(x_2\right)$$

$$=\frac{b-a}{2}\ f\left(\frac{b-a}{2}\ \left(-\frac{1}{\sqrt{3}}\right)+\ \frac{b+a}{2}\right)+\frac{b-a}{2}\ f\left(\frac{b-a}{2}\ \left(\frac{1}{\sqrt{3}}\right)+\frac{b+a}{2}\right)$$

Note that this derivation is more general with integral boundaries of a to b

For simplicity the integration limits can be converted (e.g. to -1 to 1, used in textbook)

Higher Point Gauss Quadrature

(n-point)

Gauss Quadrature: n-points

$$\int_a^b f(x)dx \approx c_1 f(x_1) + c_2 f(x_2) + c_3 f(x_3)$$

three-point Gauss Quadrature

The coefficients c_1, c_2, and c_3, and the functional arguments x_1, x_2, and x_3

Unknowns are found by assuming the formula gives exact expressions for

integrating a fifth order polynomial

$$\int_a^b \left(a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5\right)dx$$

General n-point rules would approximate the integral

$$\int_a^b f(x)dx \approx c_1 f(x_1) + c_2 f(x_2) + \ldots\ldots\ldots + c_n f(x_n)$$

Coefficients c and function arguments x used in Gauss Quadrature

In textbook, coefficients and arguments given for n-point Gauss Quadrature are given for integrals:

$$\int_{-1}^{1} g(x)dx \cong \sum_{i=1}^{n} c_i g(x_i)$$

Points	**Coefficients**	**Function Arguments**
2	$c_1 = 1.000000000$ $c_2 = 1.000000000$	$x_1 = -0.577350269$ $x_2 = 0.577350269$
3	$c_1 = 0.555555556$ $c_2 = 0.888888889$ $c_3 = 0.555555556$	$x_1 = -0.774596669$ $x_2 = 0.000000000$ $x_3 = 0.774596669$
4	$c_1 = 0.347854845$ $c_2 = 0.652145155$ $c_3 = 0.652145155$ $c_4 = 0.347854845$	$x_1 = -0.861136312$ $x_2 = -0.339981044$ $x_3 = 0.339981044$ $x_4 = 0.861136312$

Coefficients c and function arguments x used in Gauss Quadrature

Points	Coefficients	Function Arguments
5	$c_1 = 0.236926885$ $c_2 = 0.478628670$ $c_3 = 0.568888889$ $c_4 = 0.478628670$ $c_5 = 0.236926885$	$x_1 = -0.906179846$ $x_2 = -0.538469310$ $x_3 = 0.000000000$ $x_4 = 0.538469310$ $x_5 = 0.906179846$
6	$c_1 = 0.171324492$ $c_2 = 0.360761573$ $c_3 = 0.467913935$ $c_4 = 0.467913935$ $c_5 = 0.360761573$ $c_6 = 0.171324492$	$x_1 = -0.932469514$ $x_2 = -0.661209386$ $x_3 = -0.2386191860$ $x_4 = 0.2386191860$ $x_5 = 0.661209386$ $x_6 = 0.932469514$

Engineering Application of Numerical Integration

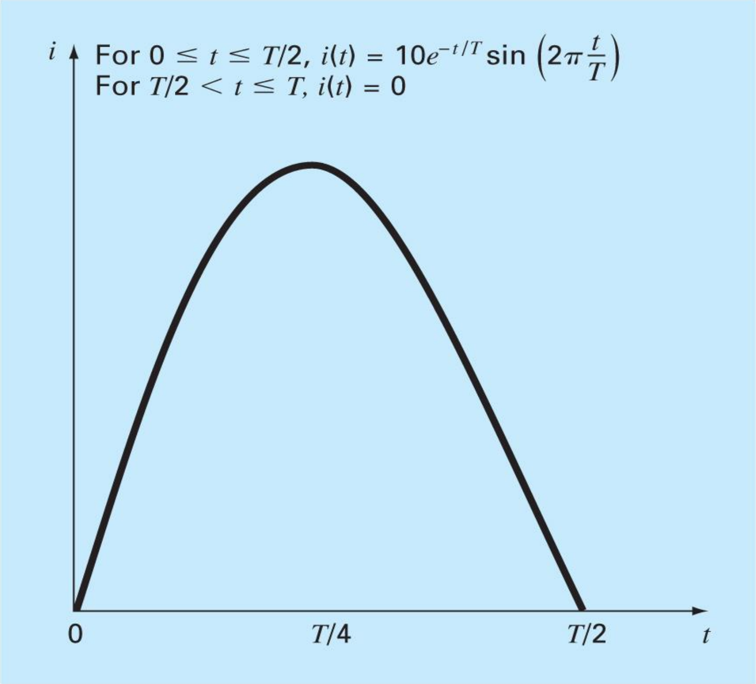
Example. RMS Current by Numerical Integration. The average value of an oscillating eclectic current over one period may be zero. For instance, if the current is i (t) = sin (2π/T), where T is period, the average value of this function is:

$$i = \frac{\int_0^T \sin\left(\frac{2\pi t}{T}\right) dt}{T - 0} = \frac{-\cos(2\pi) + \cos 0}{T} = 0$$

Despite zero result, current is capable of working and generating heat. This current has been characterized by engineers as RMS or root-mean-square current of shown waveform by:

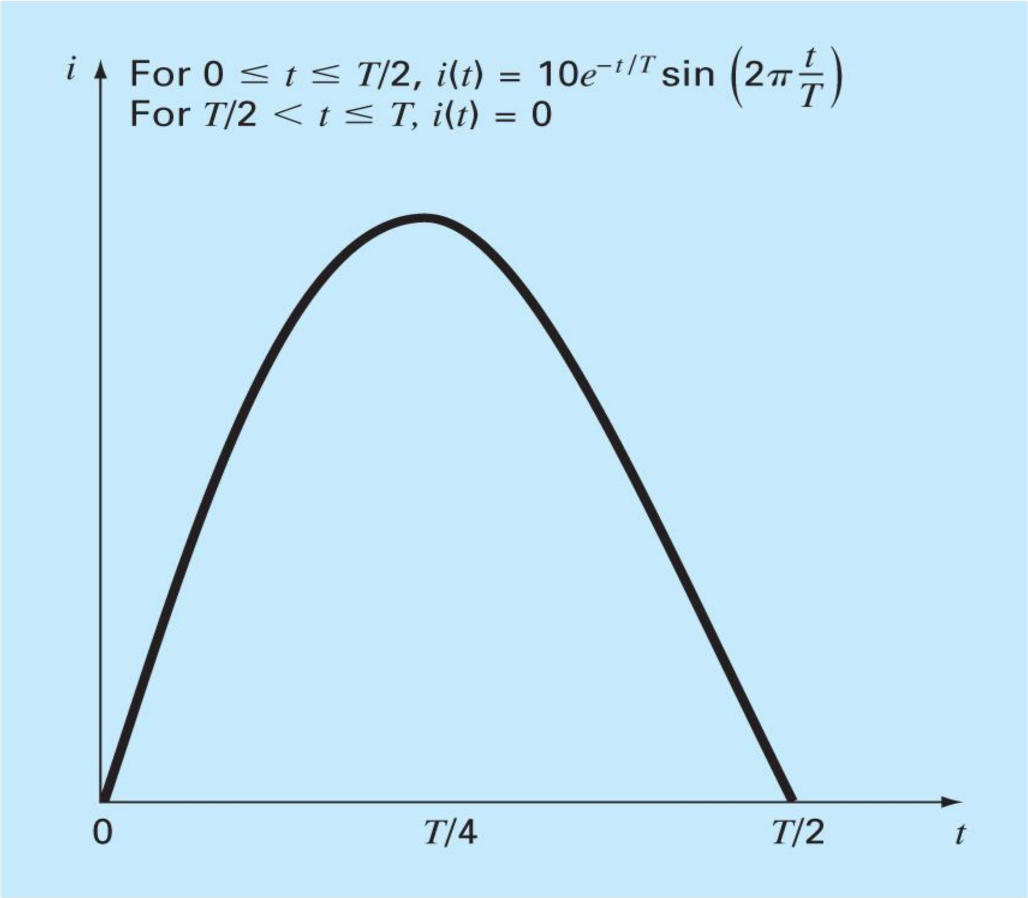
$$I_{RMS} = \sqrt{\frac{1}{T}\int_0^T i^2\,(t) dt}$$

Where i (t) is instantaneous current. What is the perspective of RMS current calculation using Trapezoidal rule, Simpson's rule, Romberg integration, and Gauss Quadrature for T=1 s.



A periodically varying electric current

A Periodically Varying Electric Current



This integral is evaluated for RMS current (T=1):

$$I = \int_0^{1/2} (10e^{-t} sin2\pi t)^2 dt$$

Trapezoidal and Simpson's Rule Application for RMS Current Calculation

Values for the integral calculated using various numerical schemes. The percent relative error ε_t is based on a true value of 15.41261.

Technique	Segments	Integral	ε_t (%)
Trapezoidal rule	1	0.0	100
	2	15.16327	1.62
	4	15.40143	0.0725
	8	15.41196	4.21×10^{-3}
	16	15.41257	2.59×10^{-4}
	32	15.41261	1.62×10^{-5}
	64	15.41261	1.30×10^{-6}
	128	15.41261	0
Simpson's 1/3 rule	2	20.21769	−31.2
	4	15.48082	−0.443
	8	15.41547	−0.0186
	16	15.41277	1.06×10^{-3}
	32	15.41261	0

Romberg Integration for RMS Current Calculation

$O(h^2)$	$O(h^4)$	$O(h^6)$	$O(h^8)$	$O(h^{10})$	$O(h^{12})$
0	20.21769	15.16503	15.41502	15.41261	15.41261
15.16327	15.48082	15.41111	15.41262	15.41261	
15.40143	15.41547	15.41225	15.41261		
15.41196	15.41277	15.41261			
15.41257	15.41262				
15.41261					

5th iteration

4th iteration

3rd iteration

2nd iteration

1st iteration

Sequence of Integral Estimate using Romberg integration

Gauss Quadrature for RMS Current Calculation

Results of using various-point Gauss quadrature formulas to approximate the integral.

Points	Estimate	ε_t (%)
2	11.9978243	22.1
3	15.6575502	−1.59
4	15.4058023	4.42×10^{-2}
5	15.4126391	-2.01×10^{-4}
6	15.4126109	-1.82×10^{-5}

RMS Current by Numerical Integration

- The numerically estimated integral is substituted in:

$$I_{RMS}= \sqrt{\frac{1}{T}\int_0^T i^2\,(t)dt}$$

- The result employed to guide other aspects of design and operations of the circuit.

Part 6. Numerical Differentiation and Integration
Chapter 23. Numerical Differentiation

Lecture 23

High Accuracy Differentiation Formulas

23.1

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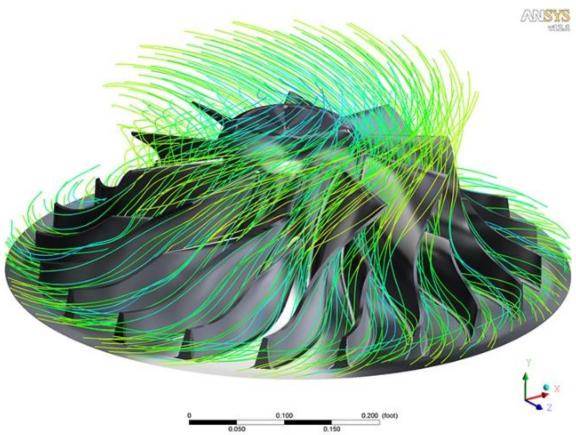
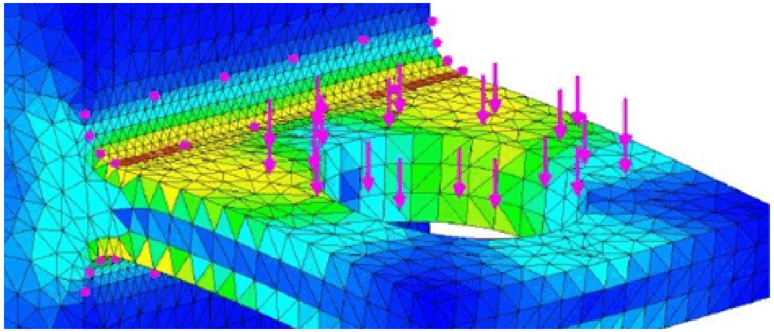
Learning Outcomes

- Understand the application of high-accuracy numerical differentiation formulas: Forward difference, Backward difference and Central difference

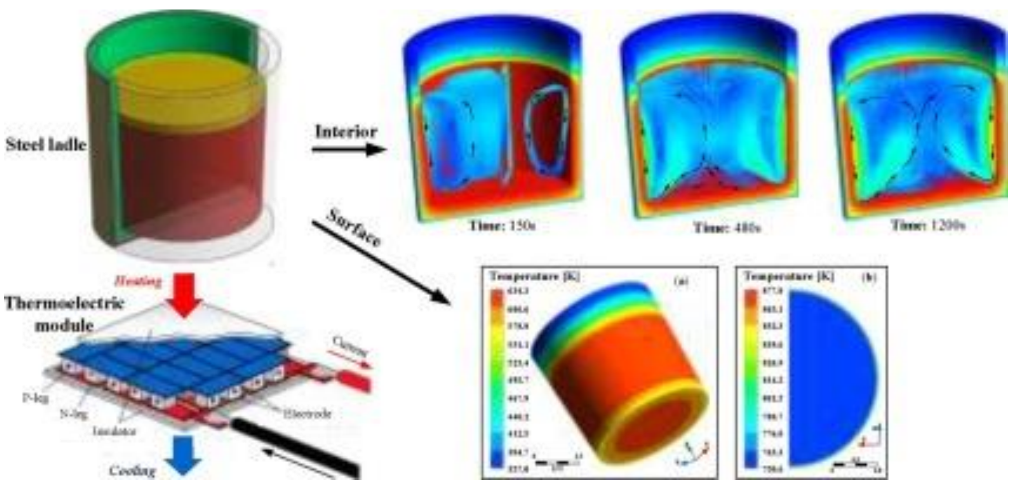
Numerical Differentiation Applications



Computational Fluid Dynamics
(Navier–Stokes Equations)



Finite Element Method



Heat Transfer

Dynamic Analysis of a Robot

High Accuracy Differentiation Formulas

- High-accuracy divided-difference formulas can be generated by including additional terms from the Taylor series expansion.

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2}h^2 + \cdots$$

$$f'(xi) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f''(x_i)}{2}h + O(h^2)$$

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + O(h)$$

$$f'(xi) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{2h^2}h + O(h^2)$$

$$f'(xi) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O(h^2)$$

High Accuracy Differentiation Formulas

- Inclusion of the 2nd derivative term has improved the accuracy to $O(h^2)$.

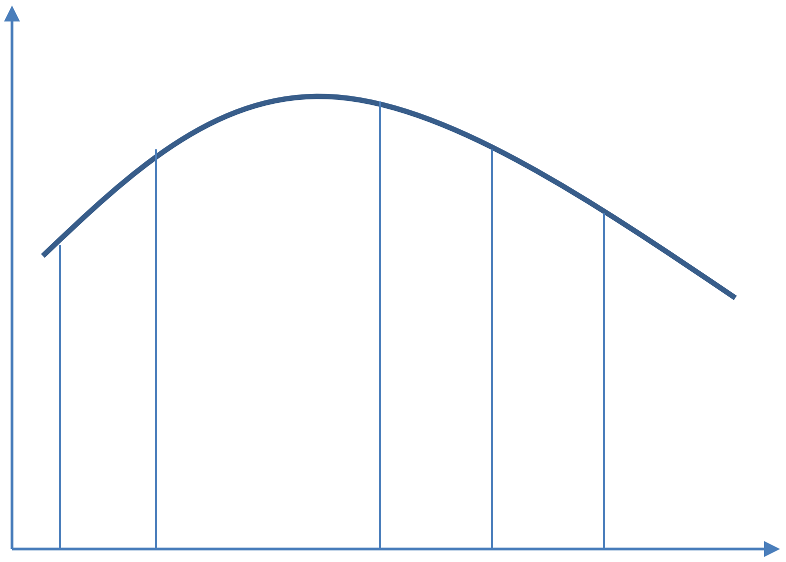
- Similar improved versions can be developed for the backward and centered formulas as well as for the approximations of the higher derivatives.

Approximating Derivatives of Functions

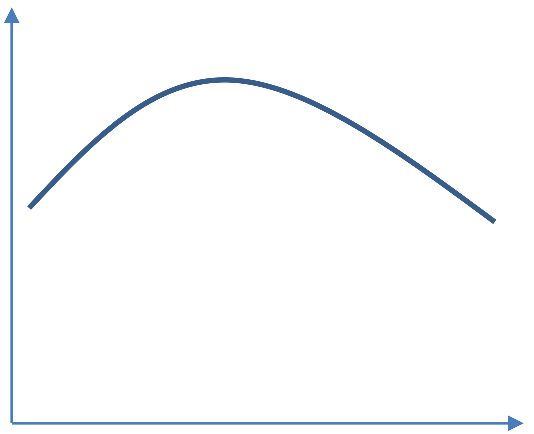
Uniform interval of ΔX

X_i arbitrary location

Goal: relate derivatives



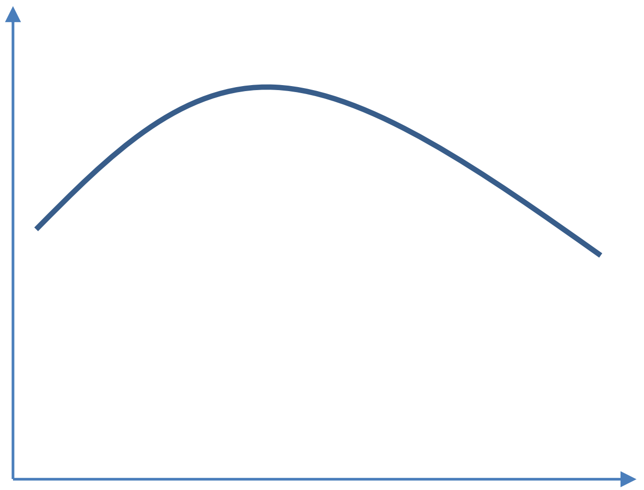
Forward Difference



Accuracy of Approximation Based on Taylor Series

$$f(x_{i+1}) = f(x_i) + \Delta x\, f'(x_i) + f''(x_i)\frac{\Delta x^2}{2!} + f'''(x_i)\frac{\Delta x^3}{3!} + \ldots$$

Backward Difference



Central Difference

$$f(x_{i+1}) = f(x_i) + \Delta x\, f'(x_i) + f''(x_i)\frac{\Delta x^2}{2!} + f'''(x_i)\frac{\Delta x^3}{3!} + \ldots$$

$$f(x_{i-1}) = f(x_i) - \Delta x\, f'(x_i) - f''(x_i)\frac{\Delta x^2}{2!} - f'''(x_i)\frac{\Delta x^3}{3!} + \ldots$$

Example. Find $\dfrac{df(0.5)}{dx}$ for

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2\ x$$

Example. If $\Delta x = 0.25$

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2\,x$$

x	$f(x)$	$f'(x)$	E
$x_{i-1} = 0.25$			
$x_i = 0.5$			
$x_{i+1} = 0.75$			

The 2nd Derivatives

Forward Difference

$$f(x_{i+2}) = f(x_i) + 2\Delta x\ f'(x_i) + f''(x_i)\frac{(2\Delta x)^2}{2!} + f'''(x_i)\frac{(2\Delta x)^3}{3!} + \ldots$$

$$f(x_{i+1}) = f(x_i) + \Delta x\ f'(x_i) + f''(x_i)\frac{\Delta x^2}{2!} + f'''(x_i)\frac{\Delta x^3}{3!} + \ldots$$

Higher Accuracy Approximations

Forward Difference

$$f(x_{i+2}) = f(x_i) + 2\Delta x\, f'(x_i) + f''(x_i)\frac{(2\Delta x)^2}{2!} + f'''(x_i)\frac{(2\Delta x)^3}{3!} + \ldots$$

$$f(x_{i+1}) = f(x_i) + \Delta x\, f'(x_i) + f''(x_i)\frac{\Delta x^2}{2!} + f'''(x_i)\frac{\Delta x^3}{3!} + \ldots$$

Summary of Forward Difference Equations (Fig. 23.1)

First Derivative	Error
$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_i)}{h}$	$O(h)$
$f'(x_i) = \dfrac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}$	$O(h^2)$
Second Derivative	
$f''(x_i) = \dfrac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2}$	$O(h)$
$f''(x_i) = \dfrac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2}$	$O(h^2)$
Third Derivative	
$f'''(x_i) = \dfrac{f(x_{i+3}) - 3f(x_{i+2}) + 3f(x_{i+1}) - f(x_i)}{h^3}$	$O(h)$
$f'''(x_i) = \dfrac{-3f(x_{i+4}) + 14f(x_{i+3}) - 24f(x_{i+2}) + 18f(x_{i+1}) - 5f(x_i)}{2h^3}$	$O(h^2)$
Fourth Derivative	
$f''''(x_i) = \dfrac{f(x_{i+4}) - 4f(x_{i+3}) + 6f(x_{i+2}) - 4f(x_{i+1}) + f(x_i)}{h^4}$	$O(h)$
$f''''(x_i) = \dfrac{-2f(x_{i+5}) + 11f(x_{i+4}) - 24f(x_{i+3}) + 26f(x_{i+2}) - 14f(x_{i+1}) + 3f(x_i)}{h^4}$	$O(h^2)$

Summary of Backward Difference Equations (Fig. 23.2)

First Derivative	Error
$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h}$$	$O(h)$
$$f'(x_i) = \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h}$$	$O(h^2)$
Second Derivative	
$$f''(x_i) = \frac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2}$$	$O(h)$
$$f''(x_i) = \frac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3})}{h^2}$$	$O(h^2)$
Third Derivative	
$$f'''(x_i) = \frac{f(x_i) - 3f(x_{i-1}) + 3f(x_{i-2}) - f(x_{i-3})}{h^3}$$	$O(h)$
$$f'''(x_i) = \frac{5f(x_i) - 18f(x_{i-1}) + 24f(x_{i-2}) - 14f(x_{i-3}) + 3f(x_{i-4})}{2h^3}$$	$O(h^2)$
Fourth Derivative	
$$f''''(x_i) = \frac{f(x_i) - 4f(x_{i-1}) + 6f(x_{i-2}) - 4f(x_{i-3}) + f(x_{i-4})}{h^4}$$	$O(h)$
$$f''''(x_i) = \frac{3f(x_i) - 14f(x_{i-1}) + 26f(x_{i-2}) - 24f(x_{i-3}) + 11f(x_{i-4}) - 2f(x_{i-5})}{h^4}$$	$O(h^2)$

Summary of Central Difference Equations (Fig. 23.3)

First Derivative | Error

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} \qquad O(h^2)$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h} \qquad O(h^4)$$

Second Derivative

$$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2} \qquad O(h^2)$$

$$f''(x_i) = \frac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2} \qquad O(h^4)$$

Third Derivative

$$f'''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + 2f(x_{i-1}) - f(x_{i-2})}{2h^3} \qquad O(h^2)$$

$$f'''(x_i) = \frac{-f(x_{i+3}) + 8f(x_{i+2}) - 13f(x_{i+1}) + 13f(x_{i-1}) - 8f(x_{i-2}) + f(x_{i-3})}{8h^3} \qquad O(h^4)$$

Fourth Derivative

$$f''''(x_i) = \frac{f(x_{i+2}) - 4f(x_{i+1}) + 6f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{h^4} \qquad O(h^2)$$

$$f''''(x_i) = \frac{-f(x_{i+3}) + 12f(x_{i+2}) - 39f(x_{i+1}) + 56f(x_i) - 39f(x_{i-1}) + 12f(x_{i-2}) - f(x_{i-3})}{6h^4} \qquad O(h^4)$$

Example. Find $\dfrac{df(0.5)}{dx}$ for

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2\ x$$

x	$f(x)$
$x_{i-2} = 0$	
$x_{i-1} = 0.25$	
$x_i = 0.5$	
$x_{i+1} = 0.75$	
$x_{i+2} = 1.0$	