BLG 202E
Numerical Methods

Recitation 2

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CHP 10 – Polynomial Interpolation

Interpolation

We are given a collection of **data samples** $\{(x_i, y_i)\}_{i=0}^{n}$.

- The $\{x_i\}_{i=0}^{n}$ are called the **abscissae** (singular: **abscissa**), the $\{y_i\}_{i=0}^{n}$ are called the **data values**.
- Want to find a function $v(x)$ which can be used to estimate sampled function for $x \neq x_i$. **Interpolation**: $v(x_i) = y_i, \quad i = 0, 1, \ldots, n$.
- Why?
  - We often get discrete data from sensors or computation, but want information as if the function were not discretely sampled.
  - May need to plot, differentiate or integrate data trend.
  - May require an economical approximation for the data.

Interpolation

- In general, it is important to distinguish two stages in the interpolation process:
  - Constructing
  - Evaluating
- Why polynomial interpolation?
  - easy to construct and evaluate
  - easy to sum and multiply
  - easy to differentiate and integrate
  - have widely varying characteristics despite their simplicity

Monomial Interpolation

Consider a **linear** combination of linearly independent **basis functions** $\{\phi_j(x)\}$

$$v(x) = c_0\phi_0(x) + c_1\phi_1(x) + \cdots + c_n\phi_n(x) = \sum_{j=0}^{n} c_j\phi_j(x)$$

where c_j are the **interpolation coefficients** or **interpolation weights**.
Then the interpolation conditions yield

$$\underbrace{\begin{pmatrix} \phi_0(x_0) & \phi_1(x_0) & \phi_2(x_0) & \cdots & \phi_n(x_0) \\ \phi_0(x_1) & \phi_1(x_1) & \phi_2(x_1) & \cdots & \phi_n(x_1) \\ \vdots & \vdots & \vdots & & \vdots \\ \phi_0(x_n) & \phi_1(x_n) & \phi_2(x_n) & \cdots & \phi_n(x_n) \end{pmatrix}}_{\text{Vandermonde Matrix}} \underbrace{\begin{pmatrix} c_0 \\ c_1 \\ \vdots \\ c_n \end{pmatrix}}_{\text{Calculated Coefficients}} = \underbrace{\begin{pmatrix} y_0 \\ y_1 \\ \vdots \\ y_n \end{pmatrix}}_{\text{Data Values}}.$$

Monomial Interpolation

$$v(x) = p(x) = p_n(x) = \sum_{j=0}^{n} c_j \phi_j(x).$$

Choose

$$\phi_j(x) = x^j.$$

Then

$$v(x) = p(x) = p_n(x) = \sum_{j=0}^{n} c_j x^j.$$

- We wish to create a linear combination of our basis functions that best represents the original function.
- Choose basis functions as powers of x.
- Find coefficients c to form the linear combination.

Monomial Interpolation

- Coefficients (*c_j*) are not indicative of the interpolated function
- Problematic if data points are unevenly spaced
- The Vandermonde matrix (*X*) is often ill-conditioned
  - Nonsingular, unique interpolating polynomial
- The complexity is:
  - Constructed with Gaussian Elimination: $O((2/3)n^3)$
  - Evaluation in Horner Form: O(2n)

Monomial Interpolation Problem

- Find an interpolating polynomial with the monomial interpolation method.

x	0	1	-1	2	-2
f(x)	-5	-3	-15	39	-9

n+1 = 5 (Number of data points)
n = 4 (Max degree of polynomial)

Monomial Interpolation Solution

- Form the Vandermonde Matrix:

x	0	1	-1	2	-2
f(x)	-5	-3	-15	39	-9

Basis Functions

Points of Evaluation		$\emptyset_0(x) = 1$	$\emptyset_1(x) = x$	$\emptyset_2(x) = x^2$	$\emptyset_3(x) = x^3$	$\emptyset_4(x) = x^4$
	$x = 0$	1	0	0	0	0
	$x = 1$	1	1	1	1	1
	$x = -1$	1	-1	1	-1	1
	$x = 2$	1	2	4	8	16
	$x = -2$	1	-2	4	-8	16

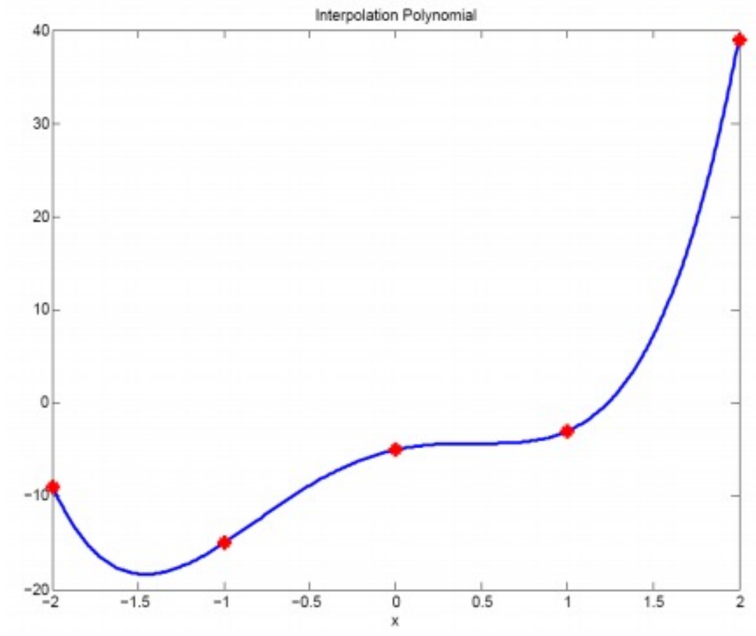
Monomial Interpolation Solution

- Solve the linear system:

$$\begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 2 & 4 & 8 & 16 \\ 1 & -2 & 4 & -8 & 16 \end{bmatrix} * \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix} = \begin{bmatrix} -5 \\ -3 \\ -15 \\ 39 \\ -9 \end{bmatrix} \Rightarrow \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix} = \begin{bmatrix} -5 \\ 4 \\ -7 \\ 2 \\ 3 \end{bmatrix}$$

The polynomial is: $v(x) = p_4(x) = -5 + 4x - 7x^2 + 2x^3 + 3x^4$

Monomial Interpolation Solution



x	0	1	-1	2	-2
f(x)	-5	-3	-15	39	-9

$$v(x) = p_4(x) = -5 + 4x - 7x^2 + 2x^3 + 3x^4$$

Lagrange Interpolation

In several ways, the opposite of monomials! Choose coefficients $c_j = y_j$.
For this define **Lagrange polynomials** $\phi_j(x) = L_j(x)$

$$\phi_j(x) = \frac{(x-x_0)\cdots(x-x_{j-1})(x-x_{j+1})\cdots(x-x_n)}{(x_j-x_0)\cdots(x_j-x_{j-1})(x_j-x_{j+1})\cdots(x_j-x_n)} = \prod_{\substack{i=0\\ i\neq j}}^{n} \frac{(x-x_i)}{(x_j-x_i)}.$$

Then

$$\phi_j(x_i) = \begin{cases} 0 & i \neq j \\ 1 & i = j, \end{cases}$$

so

$$p(x) = \sum_{j=0}^{n} y_j \phi_j(x).$$

$$\boxed{\psi(x) = \prod_{i=0}^{n}(x-x_i), \quad p(x) = \psi(x) \sum_{j=0}^{n} \frac{y_j w_j}{x-x_j}.}$$

Lagrange Interpolation

- Not as simple as monomial basis.
- The complexity is:
  - Construction: O(n^2)
  - Evaluation: O(n)
- Coefficients (c_j) indicative of data
  - Useful for function manipulation such as integration and differentiation
- Stable
  - Even if degree is large or abscissae spread apart

Lagrange Interpolation Problem

- Calculate f(4) using Lagrange polynomials of order 1 to 3 for the data given below:

x	1	2	3	5	7	8
f(x)	3	6	19	99	291	444

$$f(4) = ?$$

Lagrange Interpolation Solution

- FO using points x_0 = (3, 19) and x_1 = (5, 99) → (n = 1)
- $L_0(x) = \frac{x-x_1}{x_0-x_1} = \frac{x-5}{3-5}$
- $L_1(x) = \frac{x-x_0}{x_1-x_0} = \frac{x-3}{5-3}$

- $v(x) = \sum_{j=0}^{n} L_j(x) f\left(x_j\right) = L_0(x) f(x_0) + L_1\,(x) f(x_1) = \frac{19(x-5)}{3-5} + \frac{99(x-3)}{5-3}$

- $v(4) = \frac{19(4-5)}{3-5} + \frac{99(4-3)}{5-3} = 9.5 + 49.5 = 59$

Lagrange Interpolation Solution

- SO using points x_0 = (2, 6), x_1 = (3, 19) & x_2 = (5, 99) → (n = 2)
- $L_0(x) = \frac{x-x_1}{x_0-x_1}\frac{x-x_2}{x_0-x_2} = \frac{x-3}{2-3}\frac{x-5}{2-5}$
- $L_1(x) = \frac{x-x_0}{x_1-x_0}\frac{x-x_2}{x_1-x_2} = \frac{x-2}{3-2}\frac{x-5}{3-5}$
- $L_2(x) = \frac{x-x_0}{x_2-x_0}\frac{x-x_1}{x_2-x_1} = \frac{x-2}{5-2}\frac{x-3}{5-3}$
- $v(x) = \sum_{j=0}^{n} L_j(x)f\left(x_j\right) = L_0(x)f(x_0) + L_1\,(x)f(x_1) + L_2\,(x)f(x_2) =$
- $v(x) = 6 * \frac{x-3}{2-3}\frac{x-5}{2-5} + 19 * \frac{x-2}{3-2}\frac{x-5}{3-5} + 99 * \frac{x-2}{5-2}\frac{x-3}{5-3}$
- $v(4) = 6 * \frac{4-3}{2-3}\frac{4-5}{2-5} + 19 * \frac{4-2}{3-2}\frac{4-5}{3-5} + 99 * \frac{4-2}{5-2}\frac{4-3}{5-3} = -2 + 19 + 33 = 50$

Lagrange Interpolation Solution

- TO using points x_0 = (2, 6), x_1 = (3, 19), x_2 = (5, 99) & x_3 = (7, 291) → (n = 3)
- $L_0(x) = \frac{x-x_1}{x_0-x_1}\frac{x-x_2}{x_0-x_2}\frac{x-x_3}{x_0-x_3} = \frac{x-3}{2-3}\frac{x-5}{2-5}\frac{x-7}{2-7}$
- $L_1(x) = \frac{x-x_0}{x_1-x_0}\frac{x-x_2}{x_1-x_2}\frac{x-x_3}{x_1-x_3} = \frac{x-2}{3-2}\frac{x-5}{3-5}\frac{x-7}{3-7}$
- $L_2(x) = \frac{x-x_0}{x_2-x_0}\frac{x-x_1}{x_2-x_1}\frac{x-x_3}{x_2-x_3} = \frac{x-2}{5-2}\frac{x-3}{5-3}\frac{x-7}{5-7}$
- $L_3(x) = \frac{x-x_0}{x_3-x_0}\frac{x-x_1}{x_3-x_1}\frac{x-x_2}{x_3-x_2} = \frac{x-2}{7-2}\frac{x-3}{7-3}\frac{x-5}{7-5}$
- $v(x) = \sum_{j=0}^{n} L_j(x) f\left(x_j\right) = L_0(x)f(x_0) + L_1\,(x)f(x_1) + L_2\,(x)f(x_2) + L_3\,(x)f(x_3) =$
- $v(x) = 6 * \frac{x-3}{2-3}\frac{x-5}{2-5}\frac{x-7}{2-7} + 19 * \frac{x-2}{3-2}\frac{x-5}{3-5}\frac{x-7}{3-7} + 99 * \frac{x-2}{5-2}\frac{x-3}{5-3}\frac{x-7}{5-7} + 291 * \frac{x-2}{7-2}\frac{x-3}{7-3}\frac{x-5}{7-5}$
- $v(4) = 6 * \frac{4-3}{2-3}\frac{4-5}{2-5}\frac{4-7}{2-7} + 19 * \frac{4-2}{3-2}\frac{4-5}{3-5}\frac{4-7}{3-7} + 99 * \frac{4-2}{5-2}\frac{4-3}{5-3}\frac{4-7}{5-7} + 291 * \frac{4-2}{7-2}\frac{4-3}{7-3}\frac{4-5}{7-5} = 48$

Lagrange Interpolation Solution

- FO – f(4) = 59
- SO – f(4) = 50
- TO – f(4) = 48

- As long as we use higher orders, we get better and more accurate results.
- Third order is better than second, and second is better than first and so on…
- As we increase the number of terms in our calculations, the error decreases.

Newton’s Basis Interpolation

Newton basis functions

$$\phi_j(x) = \prod_{i=0}^{j-1}(x - x_i), \quad j = 0, 1, \ldots, n.$$

Leads to lower triangular matrix A .

- Wish to add **new data points without changing** the entire interpolant.
- We require:
  - New basis function cannot disturb prior interpolation:
    - **ϕj (xi) = 0 for i < j**.
  - Old basis function does not need information about new data values: ϕj(x) is independent of (xi, yi) for i > j.

Newton’s Basis Interpolation Problem

- Calculate f(4) using Newton’s Basis of order 3 for the data given below:

x	1	2	3	5	7	8
f(x)	3	6	19	99	291	444

$f(4) = ?$

Newton’s Basis Interpolation Solution

x	1	2	3	5	7	8
f(x)	3	6	19	99	291	444

- $x_0 = 2 , x_1 = 3, x_2 = 5\& \ x_3 = 7$
- $\emptyset_0(x) = 1$
- $\emptyset_1(x) = (x - 2)$
- $\emptyset_2(x) = (x - 2)(x - 3)$
- $\emptyset_3(x) = (x - 2)(x - 3)(x - 5)$

	$\emptyset_0(x)$	$\emptyset_1(x)$	$\emptyset_2(x)$	$\emptyset_3(x)$
x_0	1	0	0	0
x_1	1	1	0	0
x_2	1	3	6	0
x_3	1	5	20	40

Newton's Basis Interpolation Solution

x	1	2	3	5	7	8
f(x)	3	6	19	99	291	444

- $x_0 = 2\,, x_1 = 3, x_2 = 5\&\ x_3 = 7$

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 3 & 6 & 0 \\ 1 & 5 & 20 & 40 \end{bmatrix} * \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} 6 \\ 19 \\ 99 \\ 291 \end{bmatrix} \Rightarrow \begin{bmatrix} c_0 \\ c_1 \\ c_2 \\ c_3 \end{bmatrix} = \begin{bmatrix} 6 \\ 13 \\ 9 \\ 1 \end{bmatrix}$$

$$v(x) = \ p_3(x) = 6 + 13(x-2) + 9(x-2)(x-3) + (x-2)(x-3)(x-5)$$
$$v(4) = 6 + 13(4-2) + 9(4-2)(4-3) + (4-2)(4-3)(4-5) = 48$$

Newton's Divided Difference

Divided Differences.
Given points $x_0, x_1, \ldots, x_n$, for arbitrary indices $0 \le i < j \le n$, set

$$f[x_i] = f(x_i),$$
$$f[x_i, \ldots, x_j] = \frac{f[x_{i+1}, \ldots, x_j] - f[x_i, \ldots, x_{j-1}]}{x_j - x_i}.$$

i	x_i	$f[x_i]$	$f[x_{i-1}, x_i]$	$f[x_{i-2}, x_{i-1}, x_i]$	$\cdots$	$f[x_{i-n}, \ldots, x_i]$
0	x_0	$f(x_0)$				
1	x_1	$f(x_1)$	$\frac{f[x_1]-f[x_0]}{x_1-x_0}$			
2	x_2	$f(x_2)$	$\frac{f[x_2]-f[x_1]}{x_2-x_1}$	$f[x_0, x_1, x_2]$		
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\ddots$	
n	x_n	$f(x_n)$	$\frac{f[x_n]-f[x_{n-1}]}{x_n-x_{n-1}}$	$f[x_{n-2}, x_{n-1}, x_n]$	$\cdots$	$f[x_0, x_1, \ldots, x_n]$

The diagonal entries yield the coefficients $c_j = f[x_0, \ldots, x_j],\ j = 0, 1, \ldots, n$.

Newton’s Divided Difference Problem

- Construct the Newton Divided Difference Table and find the Newton Interpolation Polynomial for the following dataset:

i	x_i	$y_i = f(x_i)$
0	0	0
1	1	1
2	2	8
3	3	27
4	4	64

By observation, our function is actually $f(x) = x^3$

Newton’s Divided Difference Problem

i	x_i	$f[x_i]$	$f[x_{i-1}, x_i]$	…	…	…
0	0	0				
			$\frac{1-0}{1-0} = 1$			
1	1	1		$\frac{7-1}{2-0} = 3$		
			$\frac{8-1}{2-1} = 7$		$\frac{6-3}{3-0} = 1$	
2	2	8		$\frac{19-7}{3-1} = 6$		$\frac{1-1}{4-0} = 0$
			$\frac{27-8}{3-2} = 19$		$\frac{9-6}{4-1} = 1$	
3	3	27		$\frac{37-19}{4-2} = 9$		
			$\frac{64-27}{4-3} = 37$			
4	4	64				

$$v(x) = 0 + 1(x-0) + 3(x-0)(x-1) + 1(x-0)(x-1)(x-2) + 0\,(x-0)(x-1)(x-2)(x-3)$$
$$v(5) = 0 + 1(5-0) + 3(5-0)(5-1) + 1(5-0)(5-1)(5-2) + 0\,(5-0)(5-1)(5-2)(5-3)$$
$$v(5) = 0 + 5 + 3*5*4 + 1*5*4*3 + 0 = 125$$

Basis Comparison

Basis name	$\phi_j(x)$	construction cost	evaluation cost	selling feature
Monomial	x^j	$\frac{2}{3}n^3$	$2n$	simple
Lagrange	$L_j(x)$	n^2	$5n$	$c_j = y_j$ most stable
Newton	$\prod_{i=0}^{j-1}(x - x_i)$	$\frac{3}{2}n^2$	$2n$	adaptive

Error Analysis

- Assume that f is the function to be interpolated and $y_i = f(x_i),\ i = 0, 1, 2, \ldots, n$. Denote interpolant by $p_n(x)$. For any evaluation point x, want to estimate error

$$e_n(x) = f(x) - p_n(x)$$

  and see how it depends on the choice of n and the properties of f.
- Fixing $x \notin \{x_i\}_{i=0}^{n}$, pretend we are adding as new data point $(x, f(x))$.
- Using the properties of the Newton basis and divided differences,

$$f(x) = p_{n+1}(x) = p_n(x) + f[x_0, \ldots, x_n, x] \prod_{j=0}^{n} (x - x_j)$$

or, by rearranging,

$$e_n(x) = f(x) - p_n(x) = f[x_0, \ldots, x_n, x]\psi(x).$$

Divided Difference and Derivative

Theorem: Divided Difference and Derivative.
Let the function f be defined and have k bounded derivatives in an interval $[a,b]$ and let $z_0, z_1, \ldots, z_k$ be $k+1$ distinct points in $[a,b]$. Then there is a point $\zeta \in [a,b]$ such that

$$f[z_0, z_1, \ldots, z_k] = \frac{f^{(k)}(\zeta)}{k!}.$$

$$f[z_0, z_1, \ldots, z_k, z] = \frac{f^{(k+1)}(\xi)}{(k+1)!}$$

Error Analysis

- Let $a = \min_i x_i,\ b = \max_i x_i$ and assume $x \in [a,b]$ (otherwise $p_n(x)$ is "extrapolating")
- Relationship between divided differences and derivatives:

$$\exists \xi \in [a,b] \quad \text{such that} \quad f[x_0,\ldots,x_n,x] = \frac{f^{(n+1)}(\xi)}{(n+1)!}.$$

- So take upper bounds to find

$$|e_n(x)| \le \max_{t\in[a,b]} \frac{|f^{(n+1)}(t)|}{(n+1)!} \max_{s\in[a,b]} \left| \prod_{j=0}^{n} (s - x_j) \right| = \frac{\|f^{(n+1)}\|_\infty}{(n+1)!} \|\psi\|_\infty;$$

$$\|e_n\|_\infty \le \frac{\|f^{(n+1)}\|_\infty}{(n+1)!} (b-a)^{n+1}.$$

Error Analysis Problem

- $f(x) = \frac{1}{x}$ on $[2, 4]$ & $\{x_0 = 2, x_1 = 2.75, x_2 = 4\}$ (n = 2)
- $p(x) = \frac{x^2}{22} - \frac{35x}{88} + \frac{49}{44}$
- $f\left(\frac{1}{3}\right) = 0.33333$ & $p\left(\frac{1}{3}\right) = 0.32955$
- $e\left(\frac{1}{3}\right) = f\left(\frac{1}{3}\right) - p\left(\frac{1}{3}\right) = 0.003783$
- $f'(x) = \frac{-1}{x^2}, f''(x) = \frac{2}{x^3}, f'''(x) = \frac{-6}{x^4}$
- $e(x) = \frac{f'''(\xi)}{3!}(x - x_0)(x - x_1)(x - x_2) = \frac{-6\xi^{-4}}{3!}(x - 2)(x - 2.75)(x - 4)$
- Then we can bound e(x):
- $|e(x)| = \max\limits_{a \le \xi \le b} \frac{|-6\xi^{-4}|}{3!} \max\limits_{a \le x \le b} |(x - 2)(x - 2.75)(x - 4)|$
  - $\max \xi = 2$
  - $local \max x = \frac{7}{3}\left(y = \frac{25}{108}\right)$
  - $local \min x = \frac{7}{2}\left(y = -\frac{9}{16}\right)$ (We choose this one due to absolute value.)

$\boxed{\text{Our error is bounded by: } |e(x)| \le \left|-\frac{1}{16}\right| * \left|-\frac{9}{16}\right| = \frac{9}{256} \approx 0.0351}$

- **Distinguish between the terms data fitting, interpolation, and polynomial interpolation.**

- In interpolation we construct a curve through the data points. In doing so, we make the implicit assumption that the data points are accurate and distinct.
- Curve fitting is applied to data that contain scatter (noise), usually due to measurement errors. Here we want to find a smooth curve that approximates the data in some sense. Thus the curve does not necessarily hit the data points.
- In polynomial interpolation, the interpolant is a polynomial (the basis functions are polynomials as opposed to trigonometric functions for example).

- **What are basis functions?**

- In mathematics, a basis function is an element of a particular basis for a function space.
- Every function in the function space can be represented as a linear combination of basis functions, just as every vector in a vector space can be represented as a linear combination of basis vectors.

CHP 14 – Numerical Differentiation

Numerical Differentiation

- Given a function f(x) that is differentiable in the vicinity of a point x_0, it is often necessary to estimate the derivative f’(x) and higher derivatives using nearby values of f.

Deriving Formulas Using Taylor Series

- This is the most convenient, ad hoc approach.
- Start from Taylor's expansion, generally written for a small $h > 0$ as

$$\begin{aligned} f(x_0 \pm h) &= f(x_0) \pm hf'(x_0) + \frac{h^2}{2}f''(x_0) \pm \frac{h^3}{6}f'''(x_0) + \\ &+ \frac{h^4}{24}f^{(iv)}(x_0) \pm \frac{h^5}{120}f^{(v)}(x_0) + \frac{h^6}{720}f^{(vi)}(x_0) + \mathcal{O}(h^7). \end{aligned}$$

- Truncate this as needed and derive an expression for $f'(x_0)$.
- Simplest example is the forward difference of Example 1.2. Likewise, backward difference is obtained by writing $f(x_0 - h) = f(x_0) - hf'(x_0) + \frac{h^2}{2}f''(\xi)$, hence $f'(x_0)$ is approximated by $\frac{f(x_0)-f(x_0-h)}{h}$ with truncation error $\frac{h}{2}f''(\xi)$ for some $x_0 - h \le \xi \le x_0$.
- The forward and backward formulas are one-sided, two-point formulas with truncation error $\mathcal{O}(h)$, i.e., they are 1st order methods.

Forward Difference

Expanding $f(x)$ in a Taylor series about x_0 yields the **forward** and **backward** difference formulas, which both fall in the category of *one-sided* formulas.

For instance, letting $x = x_0 - h$ we have

$$f(x_0 - h) = f(x_0) - hf'(x_0) + \frac{h^2}{2} f''(\xi), \quad x_0 - h \le \xi \le x_0$$

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

The formula $\frac{f(x_0)-f(x_0-h)}{h}$ is first order accurate; i.e., it provides an approximation to $f'(x_0)$ such that the associated truncation error is $\mathcal{O}(h)$. This is the *backward difference formula*, since we use $x_0 - h$ as an argument for the formula, which can be thought of as proceeding backwards from the point we evaluate the derivative at, namely, x_0. The *forward* formula is the one derived in Example 1.2, and it reads $\frac{f(x_0+h)-f(x_0)}{h}$.

https://www.youtube.com/watch?v=ZJkGI5DZQv8

Three Point Central Differentiation

A **centered** formula for $f'(x_0)$ is obtained by expanding about $x = x_0$ at both $x = x_0 + h$ and $x = x_0 - h$, obtaining

$$f(x_0+h) = f(x_0) + hf'(x_0) + \frac{h^2}{2} f''(x_0) + \frac{h^3}{6} f'''(\xi_1),$$
$$f(x_0-h) = f(x_0) - hf'(x_0) + \frac{h^2}{2} f''(x_0) - \frac{h^3}{6} f'''(\xi_2).$$

Then subtracting the second from the first of these two expressions and solving for $f'(x_0)$ yields

$$f'(x_0) = \frac{f(x_0+h) - f(x_0-h)}{2h} - \frac{h^2}{6} f'''(\xi), \quad x_0 - h \leq \xi \leq x_0 + h.$$

The truncation error term is obtained from $\frac{h^2}{12}(f'''(\xi_1) + f'''(\xi_2))$ by using the Intermediate Value Theorem (see page 10) to find a common ξ between ξ_1 and ξ_2. This three-point formula (namely, the first term on the right-hand side) is second order accurate, so its accuracy order is higher than the order of the previous ones, although it also uses only two evaluations of f. However, the points are more spread apart than for the forward and backward formulas.

https://www.youtube.com/watch?v=giVVG64Mba8

Five Point Central Differentiation

Higher order approximations of the first derivative can be obtained by using more neighboring points. For instance, we derive a centered fourth order formula by writing

$$\begin{aligned}
f(x_0 \pm h) &= f(x_0) \pm h f'(x_0) + \frac{h^2}{2} f''(x_0) \pm \frac{h^3}{6} f'''(x_0) \\
&\quad + \frac{h^4}{24} f^{(iv)}(x_0) \pm \frac{h^5}{120} f^{(v)}(x_0) + \frac{h^6}{720} f^{(vi)}(x_0) + \mathcal{O}(h^7), \\
f(x_0 \pm 2h) &= f(x_0) \pm 2h f'(x_0) + 2h^2 f''(x_0) \pm \frac{8h^3}{6} f'''(x_0) \\
&\quad + \frac{16h^4}{24} f^{(iv)}(x_0) \pm \frac{32h^5}{120} f^{(v)}(x_0) + \frac{64h^6}{720} f^{(vi)}(x_0) + \mathcal{O}(h^7).
\end{aligned}$$

Subtracting the pair $f(x_0 \pm h)$ from each other and likewise for the pair $f(x_0 \pm 2h)$ leads to two centered second order approximations to $f'(x_0)$, with the truncation error for the first being four times smaller than for the second. (Can you see why without any further expansion?) Some straightforward algebra subsequently verifies that the formula

$$f'(x_0) \approx \frac{1}{12h}\left(f(x_0 - 2h) - 8f(x_0 - h) + 8f(x_0 + h) - f(x_0 + 2h)\right)$$

has the truncation error

$$e(h) = \frac{h^4}{30} f^{(v)}(\xi).$$

Differentiation Problem

- Compute forward difference approximation of O(h), central difference approximations of $O(h^2)$ and $O(h^4)$ for the first derivative of y = cos(x) at x = pi/4 using a value of h = pi/12. Estimate the true percent relative error for each approximation.

Analytical Solution & Function Values

- $\frac{dy}{dx} = -\sin(x)$
- $\left.\frac{dy}{dx}\right]_{\frac{\pi}{4}} = -\sin\left(\frac{\pi}{4}\right) = -0.707106$
- $y(x_{i-2}) = y\left(\frac{\pi}{4} - \frac{2\pi}{12}\right) = \cos\left(\frac{\pi}{12}\right) = 0.9659258$
- $y(x_{i-1}) = y\left(\frac{\pi}{4} - \frac{\pi}{12}\right) = \cos\left(\frac{\pi}{6}\right) = 0.8660254$
- $y(x_i) = y\left(\frac{\pi}{4}\right) = \cos\left(\frac{\pi}{4}\right) = 0.7071067$
- $y(x_{i+1}) = y\left(\frac{\pi}{4} + \frac{\pi}{12}\right) = \cos\left(\frac{\pi}{3}\right) = 0.5$
- $y(x_{i+2}) = y\left(\frac{\pi}{4} + \frac{2\pi}{12}\right) = \cos\left(\frac{5\pi}{12}\right) = 0.258819$

Forward Difference Differentiation

True Value: -0.7071068

x	f(x)
$x_{i-2} = \frac{\pi}{4} - \frac{2\pi}{12} = \frac{\pi}{12}$	0.9659258
$x_{i-1} = \frac{\pi}{4} - \frac{\pi}{12} = \frac{\pi}{6}$	0.8660254
$x_i = \frac{\pi}{4}$	0.7071067
$x_{i+1} = \frac{\pi}{4} + \frac{\pi}{12} = \frac{\pi}{3}$	0.5
$x_{i+2} = \frac{\pi}{4} + \frac{2\pi}{12} = \frac{5\pi}{12}$	0.258819

$$y'(x_i) = \frac{y(x_{i+1}) - y(x_i)}{h}$$

$$y'\left(\frac{\pi}{4}\right) = \frac{0.5 - 0.7071067}{0.2617993}$$

$$\boxed{y'\left(\frac{\pi}{4}\right) = -0.79108963}$$

The corresponding Error is:

$$\varepsilon_T = 100 \times \left|\frac{\text{True Value} - \text{Approx Value}}{\text{True Value}}\right|$$

$$\varepsilon_T = 100 \times \left|\frac{-0.707106 + 0.791089}{-0.707106}\right|$$

$$\boxed{\varepsilon_T = 11.8769\%}$$

Three Point Differentiation

True Value: -0.7071068

x	f(x)
$x_{i-2} = \frac{\pi}{4} - \frac{2\pi}{12} = \frac{\pi}{12}$	0.9659258
$x_{i-1} = \frac{\pi}{4} - \frac{\pi}{12} = \frac{\pi}{6}$	0.8660254
$x_i = \frac{\pi}{4}$	0.7071067
$x_{i+1} = \frac{\pi}{4} + \frac{\pi}{12} = \frac{\pi}{3}$	0.5
$x_{i+2} = \frac{\pi}{4} + \frac{2\pi}{12} = \frac{5\pi}{12}$	0.258819

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

$$y'\left(\frac{\pi}{4}\right) = \frac{0.5 - 0.8660254}{2 \times 0.2617993}$$

$$\boxed{y'\left(\frac{\pi}{4}\right) = -0.6990571}$$

The corresponding Error is:

$$\varepsilon_T = 100 \times \left| \frac{\text{True Value} - \text{Approx Value}}{\text{True Value}} \right|$$

$$\varepsilon_T = 100 \times \left| \frac{-0.707106 + 0.6990571}{-0.707106} \right|$$

$$\boxed{\varepsilon_T = 1.138407\%}$$

Five Point Differentiation

True Value: -0.7071068

x	f(x)
$x_{i-2} = \frac{\pi}{4} - \frac{2\pi}{12} = \frac{\pi}{12}$	0.9659258
$x_{i-1} = \frac{\pi}{4} - \frac{\pi}{12} = \frac{\pi}{6}$	0.8660254
$x_i = \frac{\pi}{4}$	0.7071067
$x_{i+1} = \frac{\pi}{4} + \frac{\pi}{12} = \frac{\pi}{3}$	0.5
$x_{i+2} = \frac{\pi}{4} + \frac{2\pi}{12} = \frac{5\pi}{12}$	0.258819

$$y'(x_i) = \frac{-y(x_{i+2}) + 8y(x_{i+1}) - 8y(x_{i-1}) + y(x_{i-2})}{12h}$$

$$y'\left(\frac{\pi}{4}\right) = \frac{-0.2588190 + 8 \times 0.5 - 8 \times 0.8660254 + 0.9659258}{12 \times 0.2617993}$$

$$\boxed{y'\left(\frac{\pi}{4}\right) = -0.70699696}$$

The corresponding Error is:

$$\varepsilon_T = 100 \times \left|\frac{\text{True Value} - \text{Approx Value}}{\text{True Value}}\right|$$

$$\varepsilon_T = 100 \times \left|\frac{-0.707106 + 0.70699696}{-0.707106}\right|$$

$$\boxed{\varepsilon_T = 0.015531\%}$$

Error Analysis

True Value: -0.7071068

x	f(x)
$x_{i-2} = \frac{\pi}{4} - \frac{2\pi}{12} = \frac{\pi}{12}$	0.9659258
$x_{i-1} = \frac{\pi}{4} - \frac{\pi}{12} = \frac{\pi}{6}$	0.8660254
$x_i = \frac{\pi}{4}$	0.7071067
$x_{i+1} = \frac{\pi}{4} + \frac{\pi}{12} = \frac{\pi}{3}$	0.5
$x_{i+2} = \frac{\pi}{4} + \frac{2\pi}{12} = \frac{5\pi}{12}$	0.258819

Method	Value	Error
Forward Difference (O(h))	-0.79108963	11.87696857 %
Three Point Central Difference ($O(h^2)$)	-0.69905703	1.13840705 %
Five Point Central Difference ($O(h^4)$)	-0.70699696	0.01531316 %

Unequally Spaced Data

- Use (n+1) points to fit an nth order polynomial and derivate that polynomial.
- $P_n(x) = y_0 L_0(x) + y_1 L_1(x) + \ldots + y_n L_n(x)$
  - The y values are constants. We only need to derivate the Li(x) functions.
- $P'_n(x) = y_0 L_0'(x) + y_1 L_1'(x) + \ldots + y_n L_n'(x)$
- $L_{j}(x) = \frac{(x-x_0)(x-x_1)\ldots(x-x_{(j-1)})(x-x_{(j+1)})\ldots(x-xn)}{(xj-x_0)(xj-x_1)\ldots(xj-x_{(j-1)})(xj-x_{(j+1)})\ldots(xj-xn)} = \frac{N}{D}$
- $L'_{j}(x) = \frac{N}{D} \sum_{\substack{i=0 \\ i \neq j}}^{n} \frac{1}{x - xi}$
- Then, we can calculate the derivative at values of x.

Unequally Spaced Data

x	10	12	13.75
f(x)	3.75	1.25	0

- $x_0 = 10, x_1 = 12, x_2 = 13.75, f'(11)$
- $L_0(x) = \frac{x-x_1}{x_0-x_1}\frac{x-x_2}{x_0-x_2} = \frac{x-12}{10-12}\frac{x-13.75}{10-13.75}$
- $L_1(x) = \frac{x-x_0}{x_1-x_0}\frac{x-x_2}{x_1-x_2} = \frac{x-10}{12-10}\frac{x-13.75}{12-13.75}$
- $L_2(x) = \frac{x-x_0}{x_2-x_0}\frac{x-x_1}{x_2-x_1} = \frac{x-10}{13.75-10}\frac{x-12}{13.75-12}$
- $P(x) = 3.75\frac{x-12}{10-12}\frac{x-13.75}{10-13.75} + 1.25\frac{x-10}{12-10}\frac{x-13.75}{12-13.75}$
- $P'(x) = 3.75\frac{2x-25.75}{7.5} + 1.25\frac{2x-23.75}{-3.5}$
- $\mathrm{f}'(11) \approx P'(11) = 3.75\frac{2*11-25.75}{7.5} + 1.25\frac{2*11-23.75}{-3.5} = -1.25$

Naïve Linear Estimate:

$$\boxed{\frac{y_1 - y_0}{x_1 - x_0} = \frac{12 - 10}{1.25 - 3.75} = -0.8}$$

Roundoff and Data Error

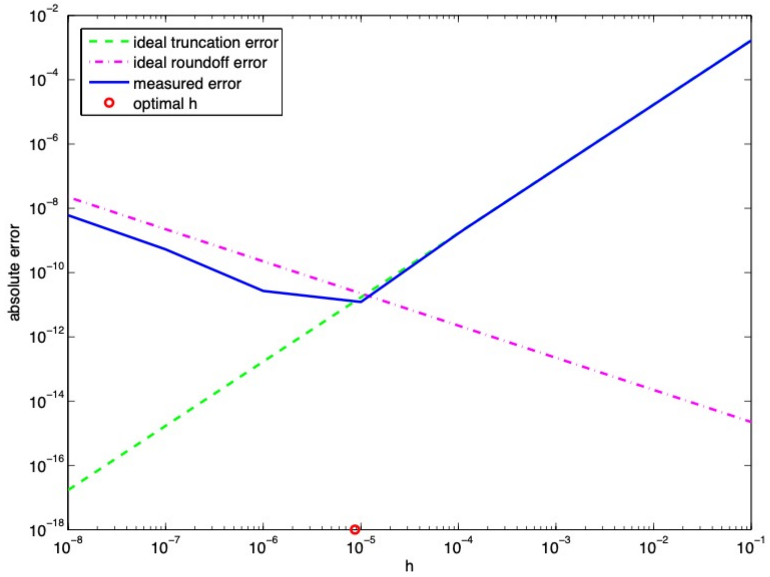
Consider the 2nd order method $f'(x_0) \simeq D_h = \frac{f(x_0+h)-f(x_0-h)}{2h}$.

- Denote $\mathrm{fl}(f(x)) \equiv \bar{f}(x) = f(x) + e_r(x), \quad |e_r(x)| \le \epsilon$, where ϵ depends on the **rounding unit**. Assuming exact arithmetic for simplicity, $\bar{D}_h = \frac{\bar{f}(x_0+h)-\bar{f}(x_0-h)}{2h}$.
- Obtain

$$\begin{aligned}
|\bar{D}_h - D_h| &= \left| \frac{\bar{f}(x_0+h)-\bar{f}(x_0-h)}{2h} - \frac{f(x_0+h)-f(x_0-h)}{2h} \right| \\
&= \left| \frac{e_r(x_0+h)-e_r(x_0-h)}{2h} \right| \\
&\le \left| \frac{e_r(x_0+h)}{2h} \right| + \left| \frac{e_r(x_0-h)}{2h} \right| \le \frac{\epsilon}{h}.
\end{aligned}$$

- So, if $|f'''(\xi)| \le M$ then

$$\begin{aligned}
|f'(x_0) - \bar{D}_h| &= |(f'(x_0) - D_h) + (D_h - \bar{D}_h)| \\
&\le |f'(x_0) - D_h| + |D_h - \bar{D}_h| \le \frac{h^2 M}{6} + \frac{\epsilon}{h}.
\end{aligned}$$



- "Theoretically optimal" h is where this bound is minimized: $h_* = (3\epsilon/M)^{1/3}$.

- **How does numerical differentiation differ from symbolic differentiation?**

- Symbolic differentiation finds the derivative of a formula with respect to a variable produces a formula as an output. In general, symbolic mathematics programs manipulate formulas to produce new formulas, rather than performing numeric calculations based on formulas.
- In numerical analysis, numerical differentiation describes algorithms for estimating the derivative of a mathematical function or function subroutine using values of the function and perhaps other knowledge about the function.

- **Define order of accuracy.**

- In numerical analysis, order of accuracy quantifies the rate of convergence of a numerical approximation of a differential equation to the exact solution.

$$\tilde{u}_h = \frac{f(h) - f(0)}{h}.$$

After Taylor expansion we get

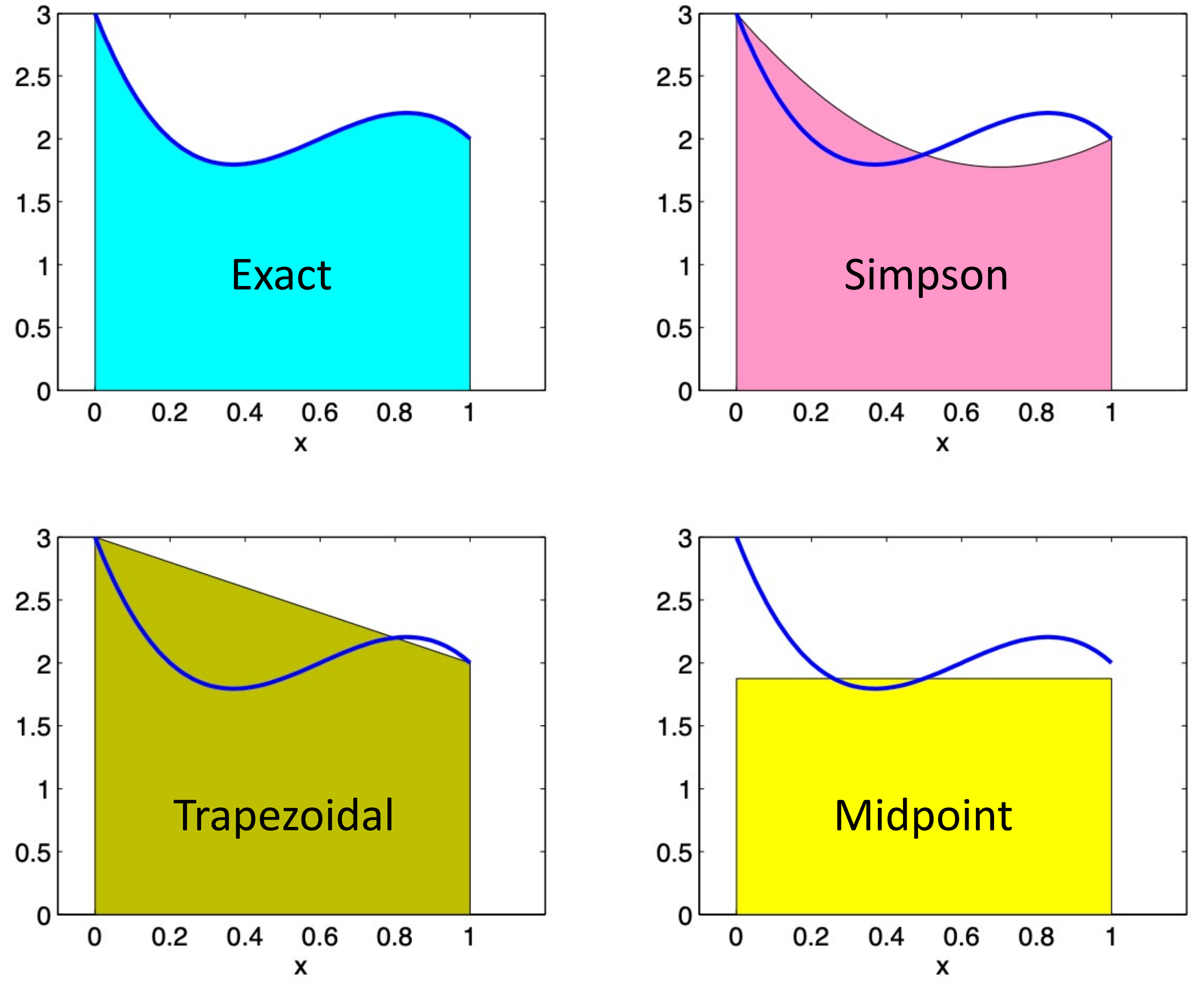
$$\tilde{u}_h - u = \frac{f(0) + hf'(0) + \frac{h^2}{2}f''(\xi) - f(0)}{h} - f'(0) = \frac{h}{2}f''(\xi)$$

- **What advantage does the formula derivation using Lagrange polynomial interpolation have over using Taylor expansions?**

- We are able to derive functions which have unequally spaced data using the Lagrange polynomial.

CHP 15 – Numerical Integration

Basic Integration Rules



Basic Quadrature Rules

Method	Formula	Error
Midpoint	$(b-a)f(\frac{a+b}{2})$	$\frac{f''(\xi_1)}{24}(b-a)^3$
Trapezoidal	$\frac{b-a}{2}[f(a)+f(b)]$	$-\frac{f''(\xi_2)}{12}(b-a)^3$
Simpson	$\frac{b-a}{6}[f(a)+4f(\frac{b+a}{2})+f(b)]$	$-\frac{f''''(\xi_3)}{90}(\frac{b-a}{2})^5$

Composite Quadrature Rules

Composite Quadrature Methods.
With $rh = b - a$, where r is a positive integer (must be even in the Simpson case), we have the formulas

$$\begin{aligned}\int_a^b f(x)dx &\approx \frac{h}{2}\left[f(a) + 2\sum_{i=1}^{r-1} f(a+ih) + f(b)\right], \quad \text{trapezoidal}\\ &\approx \frac{h}{3}\left[f(a) + 2\sum_{k=1}^{r/2-1} f(t_{2k}) + 4\sum_{k=1}^{r/2} f(t_{2k-1}) + f(b)\right], \quad \text{Simpson}\\ &\approx h\sum_{i=1}^{r} f(a + (i-1/2)h), \quad \text{midpoint.}\end{aligned}$$

Composite Quadrature Errors

Theorem: Quadrature Errors.
Let f be sufficiently smooth on $[a,b]$, and consider a composite method using a mesh $a = t_0 < t_1 < \cdots < t_r = b$ with $h_i = t_i - t_{i-1}$. Denote $h = \max_{1 \le i \le r} h_i$. In the case of the Simpson method assume that $h_{i+1} = h_i$ for all i odd.

Then the error in the composite trapezoidal method satisfies

$$|E(f)| \le \frac{\|f''\|_\infty}{12}(b-a)h^2,$$

the error in the composite midpoint method satisfies

$$|E(f)| \le \frac{\|f''\|_\infty}{24}(b-a)h^2,$$

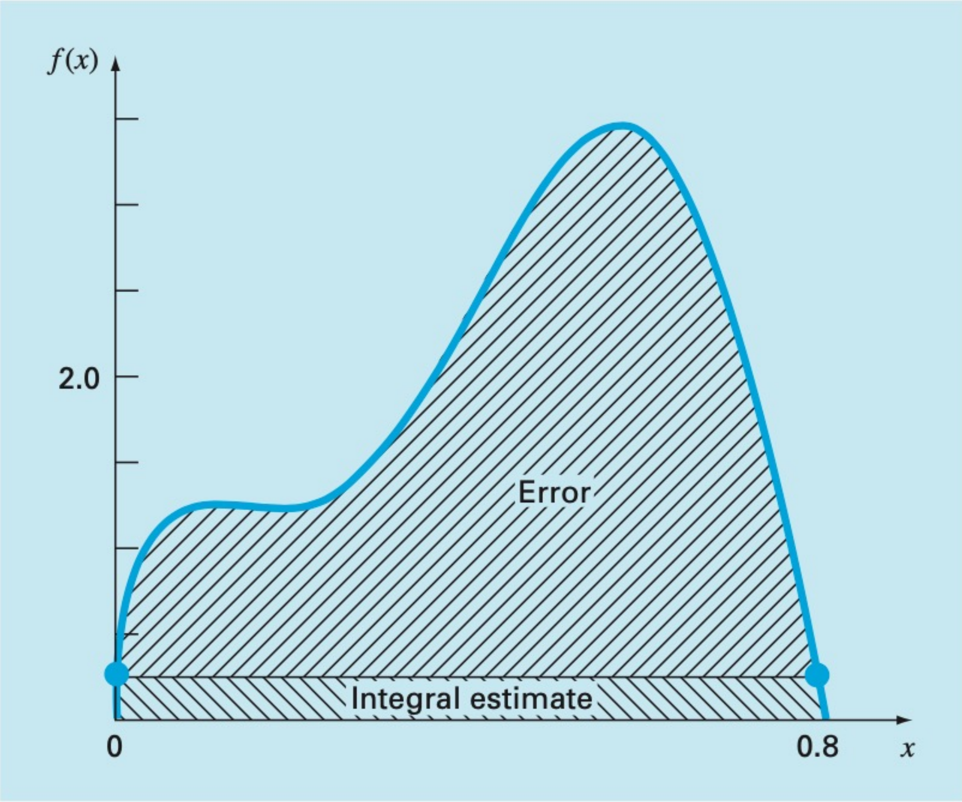
and the error in the composite Simpson method satisfies

$$|E(f)| \le \frac{\|f''''\|_\infty}{180}(b-a)h^4.$$

Trapezoidal Integration (Single)

True Value: 1.640533

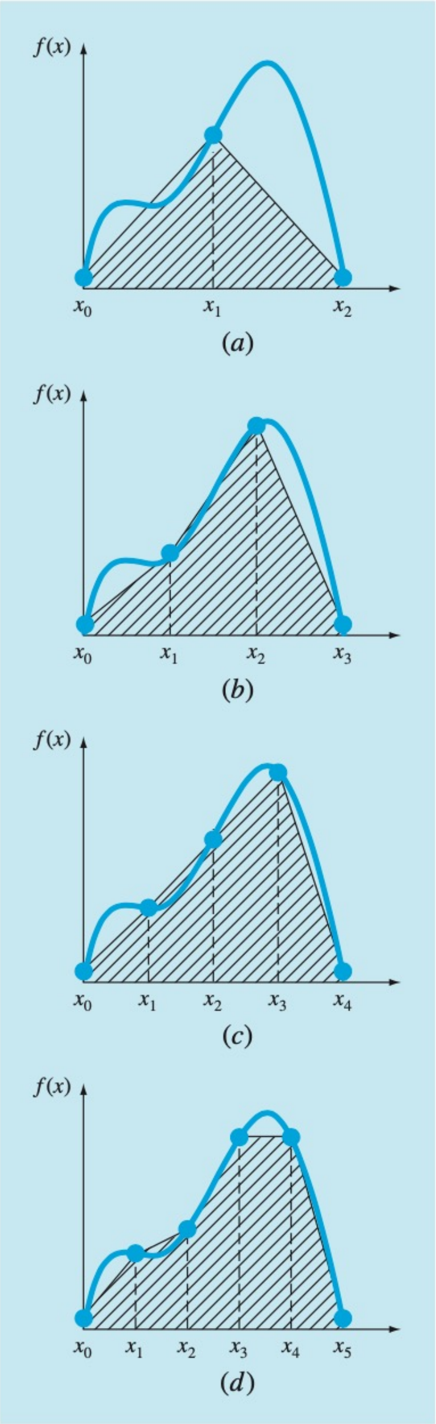
- $\int_0^{0.8} 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5 dx$
- $f(0) = 0.2 \,\&\, f(0.8) = 0.232$
- $I_{TRAP} = (0.8 - 0)\dfrac{0.2+0.232}{2} = 0.1728$
- $Error = 1.640533 - 0.1728 = 1.467722$
- $Error = 89.5\%$



Trapezoidal Integration (Composite)

$$\int_a^b f(x)dx \approx \frac{h}{2}[f(a) + 2f(t_1) + 2f(t_2) + \cdots + 2f(t_{r-1}) + f(b)].$$

$$I = \underbrace{(b - a)}_{\text{Width}} \underbrace{\frac{f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)}{2n}}_{\text{Average height}}$$



Trapezoidal Integration (Composite)

- $\int_{0}^{0.8} 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5 dx$
- $\mathrm{n} = 2 \;\&\; \mathrm{h} = 0.4$
- $f(0) = 0.2 \;\&\; f(0.4) = 2.456 \;\&\; f(0.8) = 0.232$
- $I_{TRAP} = (0.8 - 0)\dfrac{0.2 + 2*2.456 + 0.232}{2*2} = 1.0688$
- $Error = 1.640533 - 1.0688 = 0.57173$
- $Error = 34.9\%$

Trapezoidal Integration

n	h	I	ε_t (%)
2	0.4	1.0688	34.9
3	0.2667	1.3695	16.5
4	0.2	1.4848	9.5
5	0.16	1.5399	6.1
6	0.1333	1.5703	4.3
7	0.1143	1.5887	3.2
8	0.1	1.6008	2.4
9	0.0889	1.6091	1.9
10	0.08	1.6150	1.6

Midpoint Integration (Single)

True Value: 1.640533

- $\int_0^{0.8} 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5 dx$
- $f(0) = 0.2 \;\&\; f(0.4) = 2.456 \;\&\; f(0.8) = 0.232$
- $I_{MID} = (0.8 - 0)f\left(\frac{0.8+0}{2}\right) = 0.8f(0.4) = 0.8 * 2.456 = 1.9648$
- $Error = 1.640533 - 1.9648 = 0.324267$
- $Error = 19.8\%$

Simpson Method

$$I \cong \underbrace{(b-a)}_{\text{Width}} \underbrace{\frac{f(x_0) + 4f(x_1) + f(x_2)}{6}}_{\text{Average height}}$$

$$I \cong \underbrace{(b-a)}_{\text{Width}} \underbrace{\frac{f(x_0) + 4\sum_{i=1,3,5}^{n-1} f(x_i) + 2\sum_{j=2,4,6}^{n-2} f(x_j) + f(x_n)}{3n}}_{\text{Average height}}$$

Simpson Integration (Single)

True Value: 1.640533

- $\int_0^{0.8} 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5 dx$
- $f(0) = 0.2 \ \& \ f(0.4) = 2.456 \ \& \ f(0.8) = 0.232$
- $I_{SIM} = (0.8 - 0)\frac{0.2+4(2.456)+0.232}{6} = 1.367467$
- $Error = 1.640533 - 1.367467 = 0.2730667$
- $Error = 16.6\%$

Simpson Integration (Composite)

- $\int_0^{0.8} 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5 dx$
- $n = 4\ (h = 0.2)$
- $f(0) = 0.2\ \&\ f(0.2) = 1.288\ \&\ f(0.4) = 2.456\ \&\ f(0.6) = 3.464\ \&\ f(0.8) = 0.232$
- $I_{SIM} = (0.8 - 0)\dfrac{0.2+4(1.288+3.464)+2(2.456)+0.232}{12} = 1.623467$
- $Error = 1.640533 - 1.623467 = 0.017067$
- $Error = 1.04\ \%$

- **Define quadrature rule.**

- The basic idea of a quadrature rule is to replace the definite integral by a sum of the integrand evaluated at certain points (called quadrature points) multiplied by a number (called quadrature weights).

- **In what basic way is numerical integration easier than numerical differentiation?**
- Generally speaking, for humans (at least those humans who have taken a calculus course) it is easier to differentiate a given function than to integrate it: the recipes for differentiation are more automatic and require less ingenuity.
- For computers employing floating point arithmetic, however, there are certain aspects of inte- gration which make it in some sense *easier* to deal with than differentiation. Indeed, differentiation may be considered as a *roughing* operation whereas integration (finding the primitive function) is a *smoothing* operation.
- Differentiation is easier than integration analytically. It can be performed systematically on many very messy functions. However, differentiation makes a curve more jagged or the derivative might not exist, even when the function is continuous. Computing a derivative numerically is more unstable than integration.

- **Define a composite quadrature method.**

When using a quadrature rule to approximate $I(f)$ on some interval $[a, b]$, the error is proportional to h^r, where $h = b - a$ and r is some positive integer. Therefore, if the interval $[a, b]$ is large, it is advisable to divide $[a, b]$ into smaller intervals, use a quadrature rule to compute the integral of f on each subinterval, and add the results to approximate $I(f)$. Such a scheme is called a *composite quadrature rule.*