

Introduction to Numerical Differentiation and Interpolation

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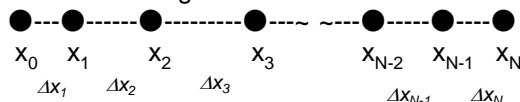
Introduction

- Interpolation is the use of a discrete set of data points $(x_k, y_k, k = 0, \dots, N)$ to approximate the value of $y(x)$ for some x that is not in the data set
- Numerical differentiation is the approximation of derivatives from a similar set of data
 - Often used as part more complex problems such as numerical solution of differential equations
 - Link: Derivatives of interpolation polynomials can be used as approximation to derivatives
- Looks at basic ideas in each topic

Finite Difference Grids

- Subdivide region into discrete points
- Spacing between the points may be uniform or non-uniform
- Example: grid for $x_{\min} \leq x \leq x_{\max}$ with $N+1$ nodes numbered from zero to N
- Initial node value, $x_0 = x_{\min}$
- Final grid node value, $x_N = x_{\max}$
- Nodal spacing $\Delta x_i = x_i - x_{i-1}$ ($i = 1, N$)
- Uniform spacing, $h = \Delta x_i = (x_{\max} - x_{\min})/N$
- $N+1$ nodes give N spaces

Finite Difference Grids II

- Non-uniform grid illustrated below
- 
- Use the following notation to represent the value of a function $f(x)$ at $x = x_i$
 - $f(x)$ at $x = x_i$ is represented as $f(x_i)$ or f_i
 - For **uniform grids**, all $\Delta x_i = x_{i+1} - x_i = h = \text{constant}$ so $x_i = x_0 + ih$ and $f_i = f(x_0 + ih)$

Derivative Expressions

- Obtain from differentiating interpolation polynomials or from Taylor series
- Series expansion for $f(x)$ about $x = a$

$$f(x) = f(a) + \frac{df}{dx}\bigg|_{x=a} (x-a) + \frac{1}{2!} \frac{d^2 f}{dx^2}\bigg|_{x=a} (x-a)^2 + \frac{1}{3!} \frac{d^3 f}{dx^3}\bigg|_{x=a} (x-a)^3 + \dots$$

- Note: $d^0 f/dx^0 = f$ and $0! = 1$
- What is error from truncating series?

$$f(x) = \sum_{n=0}^{\infty} \frac{1}{n!} \frac{d^n f}{dx^n}\bigg|_{x=a} (x-a)^n$$

Truncation Error

- If we truncate series after m terms

$$f(x) = \underbrace{\sum_{n=0}^m \frac{1}{n!} \frac{d^n f}{dx^n}\bigg|_{x=a} (x-a)^n}_{\text{Terms used}} + \underbrace{\sum_{n=m+1}^{\infty} \frac{1}{n!} \frac{d^n f}{dx^n}\bigg|_{x=a} (x-a)^n}_{\text{Truncation error, } \epsilon_m}$$

- Can write truncation error as single term at unknown location, ξ , (derivation based on the theorem of the mean)

$$\epsilon_m = \sum_{n=m+1}^{\infty} \frac{1}{n!} \frac{d^n f}{dx^n}\bigg|_{x=a} (x-a)^n = \frac{1}{(m+1)!} \frac{d^{m+1} f}{dx^{m+1}}\bigg|_{x=\xi} (x-a)^{m+1}$$

Derivative Expressions

- Look at finite-difference grid with equal spacing: $h = \Delta x$ so $x_k = x_0 + kh$; $f_k = f(x_k)$
- Taylor series about $x = x_i$ gives $f(x_i + kh) = f[x_0 + (i+k)h] = f_{i+k}$ in terms of $f(x_i) = f_i$

$$f(x_i + kh) = f(x_i) + \frac{df}{dx}\bigg|_{x=x_i} kh + \frac{1}{2!} \frac{d^2 f}{dx^2}\bigg|_{x=x_i} (kh)^2 + \frac{1}{3!} \frac{d^3 f}{dx^3}\bigg|_{x=x_i} (kh)^3 + \dots$$

$$x = x_i + kh \quad a = x_i \quad x - a = kh$$

- Compact derivative notation

$$f'_i = \frac{df}{dx}\bigg|_{x=x_i} \quad f''_i = \frac{d^2 f}{dx^2}\bigg|_{x=x_i} \quad \dots \quad f^{(n)}_i = \frac{d^n f}{dx^n}\bigg|_{x=x_i}$$

More Derivative Notation

- Use subscript to indicate location of derivatives at different points
 - Similar to notation that $f(x_i + kh) = f_{i+k}$ which is equivalent to $f[x_0 + (i+k)h] = f_{i+k}$
 - Expand results from previous slide to indicate different locations

$$f'_i = \frac{df}{dx}\bigg|_{x=x_i} \quad f''_i = \frac{d^2 f}{dx^2}\bigg|_{x=x_i} \quad \dots \quad f^{(n)}_i = \frac{d^n f}{dx^n}\bigg|_{x=x_i}$$

$$f'_{i+k} = \frac{df}{dx}\bigg|_{x=x_i+kh} \quad f''_{i+k} = \frac{d^2 f}{dx^2}\bigg|_{x=x_i+kh} \quad \dots \quad f^{(n)}_{i+k} = \frac{d^n f}{dx^n}\bigg|_{x=x_i+kh}$$

Derivative Expressions II

- Combine all definitions for compact series notation

$$f(x_i + kh) = f(x_i) + \frac{df}{dx}\bigg|_{x=x_i} kh + \frac{1}{2!} \frac{d^2 f}{dx^2}\bigg|_{x=x_i} (kh)^2 + \frac{1}{3!} \frac{d^3 f}{dx^3}\bigg|_{x=x_i} (kh)^3 + \dots$$

$$f_{i+k} = f_i + f'_i kh + \frac{f''_i (kh)^2}{2!} + \frac{f'''_i (kh)^3}{3!} + \dots$$

- Use this formula to get expansions for various grid locations about $x = x_i$ and use results to get derivative expressions

Derivative Expressions III

- Apply general equation for $k = 1$ and $k = -1$

$$f_{i+k} = f_i + f'_i kh + \frac{f''_i (kh)^2}{2!} + \frac{f'''_i (kh)^3}{3!} + \dots$$

$$f_{i+1} = f_i + f'_i h + \frac{f''_i h^2}{2!} + \frac{f'''_i h^3}{3!} + \dots$$

$$f_{i-1} = f_i - f'_i h + \frac{f''_i h^2}{2!} - \frac{f'''_i h^3}{3!} + \dots$$

$$f'_i = \frac{f_{i+1} - f_i}{h} - \frac{f''_i h}{2!} + \frac{f'''_i h^2}{3!} - \dots = \frac{f_{i+1} - f_i}{h} + Ah \quad \text{Forward}$$

$$f'_i = \frac{f_i - f_{i-1}}{h} + \frac{f''_i h}{2!} - \frac{f'''_i h^2}{3!} + \dots = \frac{f_i - f_{i-1}}{h} + Bh \quad \text{Backward}$$

Derivative Expressions IV

- Subtract f_{i+1} and f_{i-1} expressions

$$f_{i+1} = f_i + f'_i h + \frac{f''_i h^2}{2!} + \frac{f'''_i h^3}{3!} + \dots$$

$$f_{i-1} = f_i - f'_i h + \frac{f''_i h^2}{2!} - \frac{f'''_i h^3}{3!} + \dots$$

$$f_{i+1} - f_{i-1} = 2f'_i h + \frac{2f'''_i h^3}{3!} + \frac{2f^{(5)}_i h^5}{5!} + \dots$$

$$f'_i = \frac{f_{i+1} - f_{i-1}}{2h} - \frac{f'''_i h^2}{3!} + \frac{f^{(5)}_i h^4}{5!} - \dots = \frac{f_{i+1} - f_{i-1}}{2h} + Ah^2$$

- Result called central difference expression

Order of the Error

- Forward and backward derivative have error term that is proportional to h
- Central difference error is proportional to h^2
- Error proportional to h^n called n^{th} order
- Reducing step size by a factor of α reduces n^{th} order error by α^n

$$\epsilon_2 \approx \epsilon_1 \left(\frac{h_2}{h_1} \right)^n$$

Order of the Error Notation

- Write the error term for nth error term as $O(h^n)$
 - Big oh notation, O, denotes order
 - Recognizes that factor multiplying h^n may change slightly with h because ξ location of truncation error might change

First order forward First order backward

$$f'_i = \frac{f_{i+1} - f_i}{h} + O(h) \qquad f'_i = \frac{f_i - f_{i-1}}{h} + O(h)$$

Second order central $f'_i = \frac{f_{i+1} - f_{i-1}}{2h} + O(h^2)$

Higher Order Derivatives

- Add f_{i+1} and f_{i-1} expressions

$$f_{i+1} = f_i + f'_i h + \frac{f''_i h^2}{2!} + \frac{f'''_i h^3}{3!} + \dots$$

$$f_{i-1} = f_i - f'_i h + \frac{f''_i h^2}{2!} - \frac{f'''_i h^3}{3!} + \dots$$

$$f_{i+1} + f_{i-1} = 2f_i + 2\frac{f''_i h^2}{2!} + \frac{2f'''_i h^4}{4!} + \frac{2f^{(4)}_i h^6}{6!} + \dots$$

$$f''_i = \frac{f_{i+1} + f_{i-1} - 2f_i}{h^2} - \frac{f'''_i h^2}{3!} - \frac{f^{(4)}_i h^4}{5!} - \dots = \frac{f_{i+1} + f_{i-1} - 2f_i}{h^2} + O(h^2)$$

- f'' is second-order, central difference expression for second derivative

Higher Order Directional

- We can get higher order derivative expressions at the expense of more computations
- Get second order forward and backward derivative expressions from previous results and f_{i+2} and f_{i-2} , respectively
- Combine f_{i+2} and f_{i-2} equations with previous expressions for f_{i+1} and f_{i-1} to eliminate first order error term

Specific Taylor Series

General equation $f_{i+k} = f_i + f'_i kh + \frac{f''_i (kh)^2}{2!} + \frac{f'''_i (kh)^3}{3!} + \dots$

$k = 2$ $f_{i+2} = f_i + 2f'_i h + 4\frac{f''_i h^2}{2!} + 8\frac{f'''_i h^3}{3!} + \dots$

$k = -2$ $f_{i-2} = f_i - 2f'_i h + 4\frac{f''_i h^2}{2!} - 8\frac{f'''_i h^3}{3!} + \dots$

$k = 3$ $f_{i+3} = f_i + 3f'_i h + 9\frac{f''_i h^2}{2!} + 27\frac{f'''_i h^3}{3!} + \dots$

$k = -3$ $f_{i-3} = f_i - 3f'_i h + 9\frac{f''_i h^2}{2!} - 27\frac{f'''_i h^3}{3!} + \dots$

Second Order Forward

- Subtract $4f_{i+1}$ from f_{i+2} to eliminate h^2 term

$$f_{i+2} - 4f_{i+1} = \left[f_i + 2f'_i h + 4f''_i \frac{h^2}{2} + 8f'''_i \frac{h^3}{6} + \dots \right]$$

$$-4 \left[f_i + f'_i h + f''_i \frac{h^2}{2} + f'''_i \frac{h^3}{6} + \dots \right]$$

$$f_{i+2} - 4f_{i+1} + 3f_i = -2hf'_i + 4f'''_i \frac{h^3}{6} + \dots$$

$$f'_i = \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2h} + \frac{f'''_i h^2}{3} + \dots$$

Second order error, $O(h^2)$

Second Order Backwards

- Add $4f_{i-1}$ to $-f_{i-2}$ to eliminate h^2 term

$$-f_{i-2} + 4f_{i-1} = - \left[f_i - 2f'_i h + 4f''_i \frac{h^2}{2} - 8f'''_i \frac{h^3}{6} + \dots \right]$$

$$+4 \left[f_i - f'_i h + f''_i \frac{h^2}{2} - f'''_i \frac{h^3}{6} + \dots \right]$$

$$-f_{i-2} + 4f_{i-1} - 3f_i = -2hf'_i + 4f'''_i \frac{h^3}{6} + \dots$$

$$f'_i = \frac{-f_{i-2} + 4f_{i-1} - 3f_i}{2h} + \frac{f'''_i h^2}{3} + \dots$$

Second order error, $O(h^2)$

Other Derivative Expressions

- Can continue in this fashion
 - Write Taylor series for f_{i+1} , f_{i-1} , f_{i+2} , f_{i-2} , f_{i+3} , f_{i-3} , etc.
 - Create linear combinations with factors that eliminate desired terms
 - Eliminate f_i term to obtain central difference
 - Keep only terms in f_k with $k \geq i$ for forward difference expressions
 - Keep only terms in f_k with $k \leq i$ for backward difference expressions
 - See results on pages 514 and 515 of Rao

Derivative Expressions

$$f'_i = \frac{f_{i+1} - f_i}{h} + O(h)$$

$$f'_i = \frac{f_i - f_{i-1}}{h} + O(h)$$

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

$$f'_i = \frac{f_{i-2} - 4f_{i-1} + 3f_i}{2h} + O(h^2)$$

$$f'_i = \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2h} + O(h^2)$$

Note order of derivative, order of error, and direction (forward vs. backward)

$$f''_i = \frac{f_{i+1} + f_{i-1} - 2f_i}{h^2} + O(h^2)$$

Example Problem

- Use a second-order central-difference expression to estimate $d[\sin(x)]/dx|_{x=0}$ using $h = 0.1$
- What is the correct finite-difference expression?

$$f'_i = \frac{f_{i+1} - f_{i-1}}{2h} + O(h^2)$$
- What are f_{i+1} and f_{i-1} ?
 - Recall definition $f_{i+k} = f(x_i + kh)$
 - Using f'_i expression for derivative at $x = 0$ means that $f'_i = f'(x_i)$ must be f' at $x_i = 0$

Example Problem Continued

- If $x_i = 0$ what are f_{i+1} and f_{i-1} ?
 - Recall definition $f_{i+k} = f(x_i + kh)$
 - If $x_i = 0$, $x_{i+1} = x_i + (1)h = 0 + h = h = 0.1$ and $x_{i-1} = x_i + (-1)h = 0 - h = -h = -0.1$
- $$f'_i = \frac{f_{i+1} - f_{i-1}}{2h} = \frac{\sin(0+h) - \sin(0-h)}{2h}$$
- $$= \frac{\sin(0.1) - \sin(-0.1)}{2(0.1)} = 0.998334$$
- $d[\sin(x)]/dx|_{x=0} = \cos(x)|_{x=0} = 1$ so error is $|1 - 0.998334| = 1.667 \times 10^{-3}$

Repeat Example for $h = 0.01$

- Here we have the same expression we derived previously, $f'(0) = [\sin(h) - \sin(-h)]/(2h)$, but $h = 0.01$
- The result is now

$$f'_i = \frac{f_{i+1} - f_{i-1}}{2h} = \frac{\sin(0+h) - \sin(0-h)}{2h}$$

$$= \frac{\sin(0.01) - \sin(-0.01)}{2(0.01)} = 0.999983$$

Previous result: for $h = 0.1$, error = 1.667×10^{-3}
- Here error is $|1 - 0.9999833| = 1.667 \times 10^{-5}$
- Reducing h by 0.1 reduces error by 0.1^2 for second-order error

General Result

- In a finite-difference expression
- With an error of order n ($\epsilon \approx Ah^n$)
- Reducing the step size h by a factor α
- Should reduce the error by a factor α^n

Exercise

- Find the second derivatives of e^x at $x = 0$ for $h = .1$ and $h = .01$ (equation below)
- Compare to exact results $de^x/dx|_{x=0} = d^2e^x/dx^2|_{x=0} = e^x|_{x=0} = e^0 = 1$
- Estimate order of numerical results from equation $\epsilon_2 \approx \epsilon_1 \left(\frac{h_2}{h_1}\right)^n \Rightarrow n \approx \frac{\ln(\epsilon_2/\epsilon_1)}{\ln(h_2/h_1)}$
- Possible quiz question similar to this one

$$f_i'' = \frac{f_{i+1} + f_{i-1} - 2f_i}{h^2} + O(h^2)$$

Roundoff Error

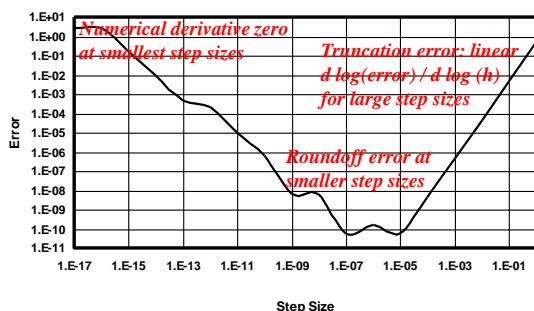
- Possible in derivative expressions from subtracting close differences
- Example $f(x) = e^x$: $f'(x) \approx (e^{x+h} - e^{x-h})/(2h)$ and error at $x = 1$ is $(e^{1+h} - e^{1-h})/(2h) - e^1$

$$E = \frac{3.004166 - 2.722815}{2(0.1)} - 2.718282 = 4.5 \times 10^{-3}$$

$$E = \frac{2.7185536702 - 2.7180100139}{2(0.0001)} - 2.718281828459 = 4.5 \times 10^{-9}$$

$$E = \frac{2.71828210028724 - 2.71828155660388}{2(0.0000001)} - 2.718281828 = 5.9 \times 10^{-9}$$

Figure 2-1. Effect of Step Size on Error



Difference Expressions

- Forward differences for constant h
 - General definition: $\Delta f_k = f_{k+1} - f_k$
 - Second order definition: $\Delta^2 f_k = \Delta(\Delta f) = \Delta(f_{k+1} - f_k) = \Delta f_{k+1} - \Delta f_k = (f_{k+2} - f_{k+1}) - (f_{k+1} - f_k) = f_{k+2} - 2f_{k+1} + f_k$
 - Can you show that the following is correct? $\Delta^3 f_k = f_{k+3} - 3f_{k+2} + 3f_{k+1} - f_k$
 - In general, $\Delta^n f_k = \Delta^{n-1} f_{k+1} - \Delta^{n-1} f_k$

Difference Expressions II

- Backward differences for constant h
 - General definition: $\nabla f_k = f_k - f_{k-1}$
 - Second order definition: $\nabla^2 f_k = \nabla(\nabla f) = \nabla(f_k - f_{k-1}) = \nabla f_k - \nabla f_{k-1} = (f_k - f_{k-1}) - (f_{k-1} - f_{k-2}) = f_k - 2f_{k-1} + f_{k-2}$
 - Can you show that the following is correct? $\nabla^3 f_k = f_k - 3f_{k-1} + 3f_{k-2} - f_{k-3}$
 - In general, $\nabla^n f_k = \nabla^{n-1} f_k - \nabla^{n-1} f_{k-1}$

Difference Expressions III

- Central differences for constant h
 - General definition: $\delta f_k = f_{k+1/2} - f_{k-1/2}$
 - Second order definition: $\delta^2 f_k = \delta(\delta f) = \delta(f_{k+1/2} - f_{k-1/2}) = \delta f_{k+1/2} - \delta f_{k-1/2} = (f_{k+1} - f_k) - (f_k - f_{k-1}) = f_{k+1} - 2f_k + f_{k-1}$
 - Can you show that the following is correct? $\delta^3 f_k = f_{k+3/2} - 3f_{k+1/2} + 3f_{k-1/2} - f_{k-3/2}$
 - General recursion formula for odd and even deltas: Odd: $\delta^{2n+1} f_{k+1/2} = \delta^{2n} f_{k+1} - \delta^{2n} f_k$
Even: $\delta^{2n} f_k = \delta^{2n-1} f_{k+1/2} - \delta^{2n-1} f_{k-1/2}$

Interpolation

- Start with N data pairs x_i, y_i
- Find a function (usually a polynomial) that can be used for interpolation
 - N data points give polynomial order $N - 1$
- **Basic rule:** the interpolation polynomial must fit all points exactly
- Denote the polynomial as $p(x)$
- The **basic rule is that $p(x_i) = y_i$**
- Many different forms

Interpolation Data Example

| | |
|----|-----|
| x | y |
| 0 | 0 |
| 10 | 10 |
| 20 | 30 |
| 30 | 60 |
| 40 | 100 |
| 50 | 150 |

- Here we have six data pairs
- Example problem: What is the value of y when $x = 34$?
- Can use different numbers of data pairs from 2 to 6
- For polynomial $p(x)$, the **basic rule is that $p(x_i) = y_i$**
 - E.g. $p(20) = 30$
 - What is $p(40)$?

$p(40) = 100$

Newton Polynomials

- $p(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + a_3(x - x_0)(x - x_1)(x - x_2) + \dots + a_n(x - x_0)(x - x_1)(x - x_2) \dots (x - x_{n-1})$
 - $n+1$ data points required for n^{th} order polynomial*
- Terms with factors of $x - x_i$ are zero when $x = x_i$
 - Use this and rule that $p(x_i) = y_i$ to find a_i
- $a_0 = y_0, a_1 = (y_1 - y_0) / (x_1 - x_0)$
- $y_2 = a_0 + a_1(x_2 - x_0) + a_2(x_2 - x_0)(x_2 - x_1)$
 - Solve for a_2 using results for a_0 and a_1

Newton Polynomials II

- $y_2 = a_0 + a_1(x_2 - x_0) + a_2(x_2 - x_0)(x_2 - x_1)$
- $$a_2 = \frac{y_2 - a_0 - a_1(x_2 - x_0)}{(x_2 - x_0)(x_2 - x_1)} = \frac{y_2 - y_0 - \frac{y_1 - y_0}{x_1 - x_0}(x_2 - x_0)}{(x_2 - x_0)(x_2 - x_1)}$$
- Could continue in this fashion to determine coefficients from data
- Use alternative scheme – not derived here – known as divided difference table to compute a_k from same data

Divided Difference Table

- Enter data on x_i and y_i in rows of table skipping one row between entries
- Start with y_i data as zeroth divided difference
- First divided difference, $F_i = (y_{i+1} - y_i) / (x_{i+1} - x_i)$
 - Second (or later) divided difference is difference of first (or later) differences
 - a_i coefficients are initial divided differences

Zeroth difference Divided Difference Table

| | | | | | |
|-------|-------|---|---|---|-------------------------|
| x_0 | y_0 | $\leftarrow a_0$ | <i>First difference</i> | <i>Second difference</i> | <i>Third difference</i> |
| | | $F_0 = \frac{y_1 - y_0}{x_1 - x_0}$ | $\leftarrow a_1$ | | |
| x_1 | y_1 | | $S_0 = \frac{F_1 - F_0}{x_2 - x_0}$ | $\leftarrow a_2$ | |
| | | $F_1 = \frac{y_2 - y_1}{x_2 - x_1}$ | | $T_0 = \frac{S_1 - S_0}{x_3 - x_0}$ | |
| x_2 | y_2 | | $S_1 = \frac{F_2 - F_1}{x_3 - x_1}$ | $\uparrow a_3$ | |
| | | $F_2 = \frac{y_3 - y_2}{x_3 - x_2}$ | | | |
| x_3 | y_3 | $F_k = \frac{y_{k+1} - y_k}{x_{k+1} - x_k}$ | $S_k = \frac{F_{k+1} - F_k}{x_{k+2} - x_k}$ | $T_k = \frac{S_{k+1} - S_k}{x_{k+3} - x_k}$ | |

Divided Difference Example

| | | | | |
|----|-----|---|---|---|
| 0 | 0 | $\leftarrow a_0$ | | |
| | | $F_0 = \frac{10-0}{10-0} = 1$ | $\leftarrow a_1$ | |
| 10 | 10 | | $S_0 = \frac{3-1}{20-0} = .1$ | $\leftarrow a_2$ |
| | | $F_1 = \frac{40-10}{20-10} = 3$ | | $T_0 = \frac{.15-.1}{30-0} = \frac{1}{600}$ |
| 20 | 40 | | $S_1 = \frac{6-3}{30-10} = .15$ | $\uparrow a_3$ |
| | | $F_2 = \frac{100-40}{30-20} = 6$ | | |
| 30 | 100 | $F_k = \frac{y_{k+1} - y_k}{x_{k+1} - x_k}$ | $S_k = \frac{F_{k+1} - F_k}{x_{k+2} - x_k}$ | $T_k = \frac{S_{k+1} - S_k}{x_{k+3} - x_k}$ |

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Divided Difference Example II

- Divided difference table gives $a_0 = 0$, $a_1 = 1$, $a_2 = .1$, and $a_3 = 1/600$
- Polynomial $p(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + a_3(x - x_0)(x - x_1)(x - x_2)$
 $= 0 + 1(x - 0) + 0.1(x - 0)(x - 10) + (1/600)(x - 0)(x - 10)(x - 20) = x + 0.1x(x - 10) + (1/600)x(x - 10)(x - 20)$
- Check $p(30) = 30 + .1(30)(20) + (1/600)(30)(20)(10) = 30 + 60 + 10 = 100$ (Correct!)

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Divided Difference Exercise

- Look at previous divided difference example
- Add new data point
- Determine interpolation coefficients
- Add new data point at x_4, y_4
- Determine divided difference all new divided difference terms out to fourth difference

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What is F_3 ?

| | | | | |
|-------|-------|-------------------------------------|-------------------------------------|-------------------------------------|
| x_1 | y_1 | | $S_0 = \frac{F_1 - F_0}{x_2 - x_0}$ | $\leftarrow a_2$ |
| | | $F_1 = \frac{y_2 - y_1}{x_2 - x_1}$ | | $T_0 = \frac{S_1 - S_0}{x_3 - x_0}$ |
| x_2 | y_2 | | $S_1 = \frac{F_2 - F_1}{x_3 - x_1}$ | $\uparrow a_3$ |
| | | $F_2 = \frac{y_3 - y_2}{x_3 - x_2}$ | | |
| x_3 | y_3 | | | |
| | | | | |
| x_4 | y_4 | | | |

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What is S_2 ?

| | | | | |
|-------|-------|-------------------------------------|-------------------------------------|-------------------------------------|
| x_1 | y_1 | | $S_0 = \frac{F_1 - F_0}{x_2 - x_0}$ | $\leftarrow a_2$ |
| | | $F_1 = \frac{y_2 - y_1}{x_2 - x_1}$ | | $T_0 = \frac{S_1 - S_0}{x_3 - x_0}$ |
| x_2 | y_2 | | $S_1 = \frac{F_2 - F_1}{x_3 - x_1}$ | $\uparrow a_3$ |
| | | $F_2 = \frac{y_3 - y_2}{x_3 - x_2}$ | | |
| x_3 | y_3 | | | |
| | | $F_3 = \frac{y_4 - y_3}{x_4 - x_3}$ | | |
| x_4 | y_4 | | | |

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What is T_1 ?

| | | | | |
|-------|-------|-------------------------------------|-------------------------------------|-------------------------------------|
| x_1 | y_1 | | $S_0 = \frac{F_1 - F_0}{x_2 - x_0}$ | $\leftarrow a_2$ |
| | | $F_1 = \frac{y_2 - y_1}{x_2 - x_1}$ | | $T_0 = \frac{S_1 - S_0}{x_3 - x_0}$ |
| x_2 | y_2 | | $S_1 = \frac{F_2 - F_1}{x_3 - x_1}$ | $\uparrow a_3$ |
| | | $F_2 = \frac{y_3 - y_2}{x_3 - x_2}$ | | |
| x_3 | y_3 | | $S_2 = \frac{F_3 - F_2}{x_4 - x_2}$ | |
| | | $F_3 = \frac{y_4 - y_3}{x_4 - x_3}$ | | |
| x_4 | y_4 | | | |

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Find Fourth Divided Difference

| | | | | |
|-------|-------|-------------------------------------|--|--|
| x_1 | y_1 | | $S_0 = \frac{F_1 - F_0}{x_2 - x_1} \leftarrow a_2$ | |
| | | $F_1 = \frac{y_2 - y_1}{x_2 - x_1}$ | | $T_0 = \frac{S_1 - S_0}{x_3 - x_1} \leftarrow a_3$ |
| x_2 | y_2 | | $S_1 = \frac{F_2 - F_1}{x_3 - x_2}$ | $\uparrow a_3$ |
| | | $F_2 = \frac{y_3 - y_2}{x_3 - x_2}$ | | $T_1 = \frac{S_2 - S_1}{x_4 - x_2} \leftarrow a_4$ |
| x_3 | y_3 | | $S_2 = \frac{F_3 - F_2}{x_4 - x_3}$ | |
| | | $F_3 = \frac{y_4 - y_3}{x_4 - x_3}$ | | |
| x_4 | y_4 | | | |

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Solution

| | | | |
|-------------------------------------|--|--|--|
| | $S_0 = \frac{F_1 - F_0}{x_2 - x_1} \leftarrow a_2$ | | |
| $F_1 = \frac{y_2 - y_1}{x_2 - x_1}$ | | $T_0 = \frac{S_1 - S_0}{x_3 - x_1} \leftarrow a_3$ | |
| | $S_1 = \frac{F_2 - F_1}{x_3 - x_2}$ | | $R_0 = \frac{T_1 - T_0}{x_4 - x_1} \leftarrow a_4$ |
| $F_2 = \frac{y_3 - y_2}{x_3 - x_2}$ | | $T_1 = \frac{S_2 - S_1}{x_4 - x_2}$ | $\uparrow a_4$ |
| | $S_2 = \frac{F_3 - F_2}{x_4 - x_3}$ | | |
| $F_3 = \frac{y_4 - y_3}{x_4 - x_3}$ | | | |

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Divided Difference Pattern

- Get general formula for code with $D(m,k)$ as m^{th} value of k^{th} divided difference
- Initial y_m data are the "zeroth" divided difference, $D(m,0)$
- First divided difference, $F_m = (y_{m+1} - y_m) / (x_{m+1} - x_m)$ is $D(m,1) = [D(m+1,0) - D(m,0)] / (x_{m+1} - x_m)$
- Second divided difference, S_m is $D(m,2) = (F_{m+1} - F_m) / (x_{m+2} - x_m) = [D(m+1,1) - D(m,1)] / (x_{m+2} - x_m)$

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Divided Difference Pattern II

- From previous slide we see that $D(m,k)$ is m^{th} value of k^{th} divided difference
- We want code to from interpolating polynomial for N data points (0 to $N-1$)
- We start by setting zeroth difference as initial data, i.e.: $D(m,0) = y_m$
- If we continue formulas for different divided differences we will see that the following formula is true
- $D(m,k) = [D(m+1,k-1) - D(m,k-1)] / (x_{m+k} - x_m)$

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Divided Difference Code

```

For m = 0 To N 'N+1 data points
  D(m, 0) = y(m) 'zeroth diff
Next m
For k = 1 To N
  For m = 0 To N - k
    D(m, k) = (D(m + 1, k - 1) - _
              D(m, k - 1)) / _
              (x(m + k) - x(m))
  Next m
Next k

```

- $D(m,k)$ is m^{th} value of k^{th} divided difference

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Using Code in Excel

- Arrays imported from Excel set input range to variant (lower bound = 1)
- ```

Sub model(xIn as Range)
 Dim x as Variant
 Dim rows as Long, cols as Long
 x = xIn
 rows = Ubound(x,1)
 cols = Ubound(x,2)

```
- Have to revise code to handle this array or copy array into one-dimensional array with lower bound of zero

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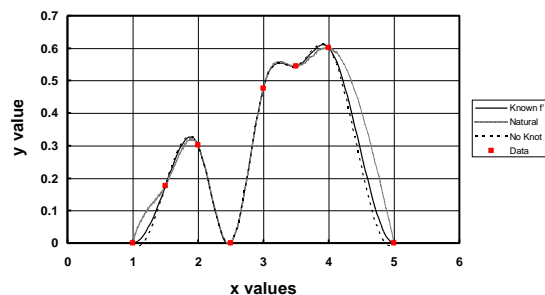
## Constant Step Size

- Divided differences work for equal or unequal step size in  $x$
- If  $\Delta x = h$  is a constant we have simpler results
  - $F_k = \Delta y_k / h = (y_{k+1} - y_k) / h$
  - $S_k = \Delta^2 y_k / 2h^2 = (y_{k+2} - 2y_{k+1} + y_k) / 2h^2$
  - $T_k = \Delta^3 y_k / 6h^3 = (y_{k+3} - 3y_{k+2} + 3y_{k+1} - y_k) / 6h^3$
  - $\Delta^n y_k$  is called the  $n^{\text{th}}$  forward difference
  - Can also define backwards and central differences

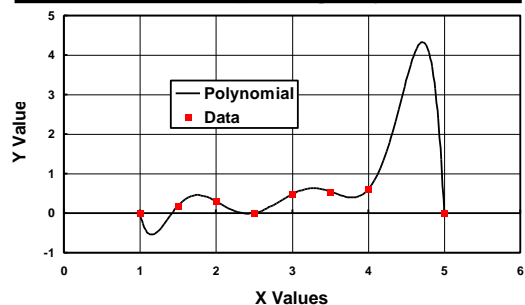
## Interpolation Approaches

- When we have  $N$  data points how do we interpolate among them?
  - Order  $N-1$  polynomial not good choice
  - Use piecewise polynomials of lower order (linear or quadratic)
  - Can match first and or higher derivatives where piecewise polynomials join
  - Cubic splines are piecewise cubic polynomials that match first and second derivatives (as well as values)

## Cubic Spline Interpolation



## Newton Interpolating Polynomial



## Polynomial Applications

- Data interpolation
- Approximation functions in numerical quadrature and solution of ODEs
- Basis functions for finite element methods
- Can obtain equations for numerical differentiation
- Statistical curve fitting (not discussed here) usually used in practice

## Fifth Quiz Results

- Maximum possible score: 25
- Number of students: 22
- Mean score: 13.3
- Median score: 15.5
- Standard deviation: 7.3
- Grade distribution:
 

|    |    |    |    |    |    |    |
|----|----|----|----|----|----|----|
| 2  | 2  | 3  | 3  | 4  | 6  | 7  |
| 12 | 14 | 15 | 15 | 16 | 16 | 17 |
| 17 | 17 | 20 | 21 | 23 | 23 | 24 |

## Quiz Five Comments

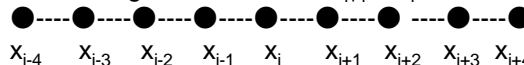
- When left side is the same, can solve both right sides at same time
- Watch roundoff in calculator
- Learn to use numbers without symbols to represent equations
- Cannot use iteration unless array is diagonally dominant
- Quiz six moved from this Wednesday to next Wednesday

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## Uniform Grids

- Uniform grid notation:  $h = x_{i+1} - x_i$



- Formulas with terms  $f_i$  represent  $f(x_i)$
- Equations like the following

$$f'_i = \frac{f_{i-2} - 4f_{i-1} + 3f_i}{2h} + O(h^2) \quad f'_i = \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2h} + O(h^2)$$

- Give the derivative at  $x = x_i$  in terms of  $f$  values,  $f_i = f(x_i)$  at grid locations  $x_i$

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