

# Numerical Analysis and Computing

## Lecture Notes #5 — Interpolation and Polynomial Approximation

### Divided Differences, and Hermite Interpolatory Polynomials

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#5 Interpolation and Polynomial Approximation — (1/40)

## Outline

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  - Representing Polynomials
  - Divided Differences
  - Different forms of Divided Difference Formulas
- 2 Polynomial Approximation, Higher Order Matching
  - Osculating Polynomials
  - Hermite Interpolatory Polynomials
  - Computing Hermite Interpolatory Polynomials
- 3 Beyond Hermite Interpolatory Polynomials

#5 Interpolation and Polynomial Approximation — (2/40)

## Recap and Lookahead

### Previously:

Neville's Method to successively generate higher degree polynomial approximations **at a specific point**. — If we need to compute the polynomial at many points, we have to re-run Neville's method for each point.  $\mathcal{O}(n^2)$  operations/point.

Algorithm: Neville's Method

To evaluate the polynomial that interpolates the  $n + 1$  points  $(x_i, f(x_i))$ ,  $i = 0, \dots, n$  at the point  $x$ :

1. Initialize  $Q_{i,0} = f(x_i)$ .
2. FOR  $i = 1 : n$   
  FOR  $j = 1 : i$   
    
$$Q_{i,j} = \frac{(x - x_{i-j})Q_{i,j-1} - (x - x_i)Q_{i-1,j-1}}{x_i - x_{i-j}}$$
  
  END  
END
3. Output the  $Q$ -table.

#5 Interpolation and Polynomial Approximation — (3/40)

## Recap and Lookahead

### Next:

Use divided differences to *generate the polynomials\* themselves*.

\* The coefficients of the polynomials. Once we have those, we can quickly (remember Horner's method?) compute the polynomial in any desired points.  $\mathcal{O}(n)$  operations/point.

Algorithm: Horner's Method

Input: Degree  $n$ ; coefficients  $a_0, a_1, \dots, a_n$ ;  $x_0$

Output:  $y = P(x_0)$ ,  $z = P'(x_0)$ .

1. Set  $y = a_n$ ,  $z = a_n$
2. For  $j = (n - 1), (n - 2), \dots, 1$   
  Set  $y = x_0 y + a_j$ ,  $z = x_0 z + y$
3. Set  $y = x_0 y + a_0$
4. Output  $(y, z)$
5. End program

#5 Interpolation and Polynomial Approximation — (4/40)

## Representing Polynomials

If  $P_n(x)$  is the  $n^{\text{th}}$  degree polynomial that agrees with  $f(x)$  at the points  $\{x_0, x_1, \dots, x_n\}$ , then we can (for the appropriate constants  $\{a_0, a_1, \dots, a_n\}$ ) write:

$$P_n(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + \dots \\ \dots + a_n(x - x_0)(x - x_1) \dots (x - x_{n-1})$$

Note that we can evaluate this “Horner-style,” by writing

$$P_n(x) = a_0 + (x - x_0)(a_1 + (x - x_1)(a_2 + \dots \\ \dots + (x - x_{n-2})(a_{n-1} + a_n(x - x_{n-1}))))),$$

so that each step in the Horner-evaluation consists of a subtraction, a multiplication, and an addition.

## Finding the Constants $\{a_0, a_1, \dots, a_n\}$

“Just Algebra”

Given the relation

$$P_n(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + \dots \\ \dots + a_n(x - x_0)(x - x_1) \dots (x - x_{n-1})$$

at  $x_0$ :  $a_0 = P_n(x_0) = f(x_0)$ .

at  $x_1$ :  $f(x_0) + a_1(x_1 - x_0) = P_n(x_1) = f(x_1)$

$$\Rightarrow a_1 = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

at  $x_2$ :  $a_2 = \frac{f(x_2) - f(x_0)}{(x_2 - x_0)(x_2 - x_1)} - \frac{f(x_1) - f(x_0)}{(x_2 - x_0)(x_1 - x_0)}$ .

This gets massively ugly fast! — We need some nice clean notation!

## Sir Isaac Newton to the Rescue: Divided Differences

### Zeroth Divided Difference:

$$f[x_i] = f(x_i).$$

### First Divided Difference:

$$f[x_i, x_{i+1}] = \frac{f[x_{i+1}] - f[x_i]}{x_{i+1} - x_i}$$

### Second Divided Difference:

$$f[x_i, x_{i+1}, x_{i+2}] = \frac{f[x_{i+1}, x_{i+2}] - f[x_i, x_{i+1}]}{x_{i+2} - x_i}$$

### $k^{\text{th}}$ Divided Difference:

$$f[x_i, x_{i+1}, \dots, x_{i+k}] = \frac{f[x_{i+1}, x_{i+2}, \dots, x_{i+k}] - f[x_i, x_{i+1}, \dots, x_{i+k-1}]}{x_{i+k} - x_i}$$

## The Constants $\{a_0, a_1, \dots, a_n\}$ — Revisited

We had

at  $x_0$ :  $a_0 = P_n(x_0) = f(x_0)$ .

at  $x_1$ :  $f(x_0) + a_1(x_1 - x_0) = P_n(x_1) = f(x_1)$

$$\Rightarrow a_1 = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

at  $x_2$ :  $a_2 = \frac{f(x_2) - f(x_0)}{(x_2 - x_0)(x_2 - x_1)} - \frac{f(x_1) - f(x_0)}{(x_2 - x_0)(x_1 - x_0)}$ .

Clearly:

$$a_0 = f[x_0], \quad a_1 = f[x_0, x_1].$$

We may suspect that  $a_2 = f[x_0, x_1, x_2]$ , that is indeed so (a “little bit” of careful algebra will show it), and in general

$$a_k = f[x_0, x_1, \dots, x_k].$$

## Algebra: Chasing down $a_2 = f[x_0, x_1, x_2]$

$$\begin{aligned}
 a_2 &= \frac{f(x_2) - f(x_0)}{(x_2 - x_0)(x_2 - x_1)} - \frac{f(x_1) - f(x_0)}{(x_2 - x_1)(x_1 - x_0)} \\
 &= \frac{(f(x_2) - f(x_0))(x_1 - x_0) - (f(x_1) - f(x_0))(x_2 - x_0)}{(x_2 - x_0)(x_2 - x_1)(x_1 - x_0)} \\
 &= \frac{(x_1 - x_0)f(x_2) - (x_2 - x_0)f(x_1) + (x_2 - x_0 - x_1 + x_0)f(x_0)}{(x_2 - x_0)(x_2 - x_1)(x_1 - x_0)} \\
 &= \frac{(x_1 - x_0)f(x_2) - (x_1 - x_0 + x_2 - x_1)f(x_1) + (x_2 - x_1)f(x_0)}{(x_2 - x_0)(x_2 - x_1)(x_1 - x_0)} \\
 &= \frac{(x_1 - x_0)(f(x_2) - f(x_1)) - (x_2 - x_1)(f(x_1) - f(x_0))}{(x_2 - x_0)(x_2 - x_1)(x_1 - x_0)} \\
 &= \frac{(f(x_2) - f(x_1))}{(x_2 - x_0)(x_2 - x_1)} - \frac{(f(x_1) - f(x_0))}{(x_2 - x_0)(x_1 - x_0)} \\
 &= \frac{f[x_1, x_2]}{x_2 - x_0} - \frac{f[x_0, x_1]}{x_2 - x_0} = f[x_0, x_1, x_2] \quad (!!!)
 \end{aligned}$$

## Newton's Interpolatory Divided Difference Formula

Hence, we can write

$$P_n(x) = f[x_0] + \sum_{k=1}^n \left[ f[x_0, \dots, x_k] \prod_{m=0}^{k-1} (x - x_m) \right].$$

$$\begin{aligned}
 P_n(x) &= f[x_0] + \\
 & f[x_0, x_1](x - x_0) + \\
 & f[x_0, x_1, x_2](x - x_0)(x - x_1) + \\
 & f[x_0, x_1, x_2, x_3](x - x_0)(x - x_1)(x - x_2) + \dots
 \end{aligned}$$

This expression is known as **Newton's Interpolatory Divided Difference Formula**.

## Computing the Divided Differences (by table)

x	f(x)	1st Div. Diff.	2nd Div. Diff.
$x_0$	$f[x_0]$		
$x_1$	$f[x_1]$	$f[x_0, x_1] = \frac{f[x_1] - f[x_0]}{x_1 - x_0}$	
$x_2$	$f[x_2]$	$f[x_1, x_2] = \frac{f[x_2] - f[x_1]}{x_2 - x_1}$	$f[x_0, x_1, x_2] = \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0}$
$x_3$	$f[x_3]$	$f[x_2, x_3] = \frac{f[x_3] - f[x_2]}{x_3 - x_2}$	$f[x_1, x_2, x_3] = \frac{f[x_2, x_3] - f[x_1, x_2]}{x_3 - x_1}$
$x_4$	$f[x_4]$	$f[x_3, x_4] = \frac{f[x_4] - f[x_3]}{x_4 - x_3}$	$f[x_2, x_3, x_4] = \frac{f[x_3, x_4] - f[x_2, x_3]}{x_4 - x_2}$
$x_5$	$f[x_5]$	$f[x_4, x_5] = \frac{f[x_5] - f[x_4]}{x_5 - x_4}$	$f[x_3, x_4, x_5] = \frac{f[x_4, x_5] - f[x_3, x_4]}{x_5 - x_3}$

**Note:** The table can be extended with three *3rd* divided differences, two *4th* divided differences, and one *5th* divided difference.

## Algorithm: Computing the Divided Differences

Algorithm: Newton's Divided Differences

Given the points  $(x_i, f(x_i))$ ,  $i = 0, \dots, n$ .

Step 1: Initialize  $F_{i,0} = f(x_i)$ ,  $i = 0, \dots, n$

Step 2:

```

FOR i = 1 : n
  FOR j = 1 : i
     $F_{i,j} = \frac{F_{i,j-1} - F_{i-1,j-1}}{x_i - x_{i-j}}$ 
  END
END

```

Result: The diagonal,  $F_{i,i}$  now contains  $f[x_0, \dots, x_i]$ .

## A Theoretical Result: Generalization of the Mean Value Theorem

Theorem (Generalized Mean Value Theorem)

Suppose that  $f \in C^n[a, b]$  and  $\{x_0, \dots, x_n\}$  are distinct number in  $[a, b]$ . Then  $\exists \xi \in (a, b)$  :

$$f[x_0, \dots, x_n] = \frac{f^{(n)}(\xi)}{n!}.$$

For  $n = 1$  this is exactly the *Mean Value Theorem*...

So we have extended to MVT to higher order derivatives!

What is the theorem telling us?

- *Newton's  $n^{\text{th}}$  divided difference is in some sense an approximation to the  $n^{\text{th}}$  derivative of  $f$ .*

## Newton vs. Taylor...

Using Newton's Divided Differences...

$$P_n^N(x) = f[x_0] + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1) + f[x_0, x_1, x_2, x_3](x - x_0)(x - x_1)(x - x_2) + \dots$$

Using Taylor expansion

$$P_n^T(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2!} f''(x_0)(x - x_0)^2 + \frac{1}{3!} f'''(x_0)(x - x_0)^3 + \dots$$

It makes sense that the divided differences are approximating the derivatives in some sense!

## Simplification: Equally Spaced Points

When the points  $\{x_0, \dots, x_n\}$  are equally spaced, *i.e.*

$$h = x_{i+1} - x_i, \quad i = 0, \dots, n - 1,$$

we can write  $x = x_0 + sh$ ,  $x - x_k = (s - k)h$  so that

$$P_n(x) = P_n(x_0 + sh) = \sum_{k=0}^n s(s-1)\dots(s-k+1)h^k f[x_0, \dots, x_k].$$

Using the binomial coefficients,  $\binom{s}{k} = \frac{s(s-1)\dots(s-k+1)}{k!}$  —

$$P_n(x_0 + sh) = f[x_0] + \sum_{k=1}^n \binom{s}{k} k! h^k f[x_0, \dots, x_k].$$

This is **Newton's Forward Divided Difference Formula**.

## Notation, Notation, Notation...

Another form, **Newton's Forward Difference Formula** is constructed by using the forward difference operator  $\Delta$ :

$$\Delta f(x_n) = f(x_{n+1}) - f(x_n)$$

using this notation:

$$f[x_0, x_1] = \frac{f(x_1) - f(x_0)}{x_1 - x_0} = \frac{1}{h} \Delta f(x_0).$$

$$f[x_0, x_1, x_2] = \frac{1}{2h} \left[ \frac{\Delta f(x_1) - \Delta f(x_0)}{h} \right] = \frac{1}{2h^2} \Delta^2 f(x_0).$$

$$f[x_0, \dots, x_k] = \frac{1}{k! h^k} \Delta^k f(x_0).$$

Thus we can write **Newton's Forward Difference Formula**

$$P_n(x_0 + sh) = f[x_0] + \sum_{k=1}^n \binom{s}{k} \Delta^k f(x_0).$$

## Notation, Notation, Notation... Backward Formulas

If we reorder  $\{x_0, x_1, \dots, x_n\} \rightarrow \{x_n, \dots, x_1, x_0\}$ , and define the backward difference operator  $\nabla$ :

$$\nabla f(x_n) = f(x_n) - f(x_{n-1}),$$

we can define the backward divided differences:

$$f[x_n, \dots, x_{n-k}] = \frac{1}{k! h^k} \nabla^k f(x_n).$$

We write down **Newton's Backward Difference Formula**

$$P_n(x) = f[x_n] + \sum_{k=1}^n (-1)^k \binom{-s}{k} \nabla^k f(x_n),$$

where

$$\binom{-s}{k} = (-1)^k \frac{s(s+1)\cdots(s+k-1)}{k!}.$$

## Forward? Backward? I'm Confused!!!

x	f(x)	1st Div. Diff.	2nd Div. Diff.
x <sub>0</sub>	f[x <sub>0</sub> ]		
x <sub>1</sub>	f[x <sub>1</sub> ]	$f[x_0, x_1] = \frac{f[x_1] - f[x_0]}{x_1 - x_0}$	
x <sub>2</sub>	f[x <sub>2</sub> ]	$f[x_1, x_2] = \frac{f[x_2] - f[x_1]}{x_2 - x_1}$	$f[x_0, x_1, x_2] = \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0}$
x <sub>3</sub>	f[x <sub>3</sub> ]	$f[x_2, x_3] = \frac{f[x_3] - f[x_2]}{x_3 - x_2}$	$f[x_1, x_2, x_3] = \frac{f[x_2, x_3] - f[x_1, x_2]}{x_3 - x_1}$
x <sub>4</sub>	f[x <sub>4</sub> ]	$f[x_3, x_4] = \frac{f[x_4] - f[x_3]}{x_4 - x_3}$	$f[x_2, x_3, x_4] = \frac{f[x_3, x_4] - f[x_2, x_3]}{x_4 - x_2}$
x <sub>5</sub>	f[x <sub>5</sub> ]	$f[x_4, x_5] = \frac{f[x_5] - f[x_4]}{x_5 - x_4}$	$f[x_3, x_4, x_5] = \frac{f[x_4, x_5] - f[x_3, x_4]}{x_5 - x_3}$

**Forward:** The fwd div. diff. are the top entries in the table.

**Backward:** The bwd div. diff. are the bottom entries in the table.

## Forward? Backward? — Straight Down the Center!

The Newton formulas works best for points close to the edge of the table; if we want to approximate  $f(x)$  close to the center, we have to work some more...

x	f(x)	1st Div. Diff.	2nd Div. Diff.	3rd Div. Diff.	4th Div. Diff.
x <sub>-2</sub>	f[x <sub>-2</sub> ]				
x <sub>-1</sub>	f[x <sub>-1</sub> ]	$f[x_{-2}, x_{-1}]$	$f[x_{-2}, x_{-1}, x_0]$		
x <sub>0</sub>	f[x <sub>0</sub> ]	$f[x_{-1}, x_0]$	$f[x_{-1}, x_0, x_1]$	$f[x_{-2}, x_{-1}, x_0, x_1]$	$f[x_{-2}, x_{-1}, x_0, x_1, x_2]$
x <sub>1</sub>	f[x <sub>1</sub> ]	$f[x_0, x_1]$	$f[x_0, x_1, x_2]$	$f[x_{-1}, x_0, x_1, x_2]$	$f[x_{-1}, x_0, x_1, x_2, x_3]$
x <sub>2</sub>	f[x <sub>2</sub> ]	$f[x_1, x_2]$	$f[x_1, x_2, x_3]$		
x <sub>3</sub>	f[x <sub>3</sub> ]	$f[x_2, x_3]$			

We are going to construct **Stirling's Formula** — a scheme using **centered differences**. In particular we are going to use the **blue** (centered at  $x_0$ ) entries, and averages of the **red** (straddling the  $x_0$  point) entries.

## Stirling's Formula — Approximating at Interior Points

Assume we are trying to approximate  $f(x)$  close to the interior point  $x_0$ :

$$P_n(x) = P_{2m+1}(x) = f[x_0] + sh \frac{f[x_{-1}, x_0] + f[x_0, x_1]}{2} + s^2 h^2 f[x_{-1}, x_0, x_1] + s(s^2 - 1) h^3 \frac{f[x_{-2}, x_{-1}, x_0, x_1] + f[x_{-1}, x_0, x_1, x_2]}{2} + s^2 (s^2 - 1) h^4 f[x_{-2}, x_{-1}, x_0, x_1, x_2] + \dots + s^2 (s^2 - 1) \cdots (s^2 - (m-1)^2) h^{2m} f[x_{-m}, \dots, x_m] + s(s^2 - 1) \cdots (s^2 - m^2) h^{2m+1} \frac{f[x_{-m-1}, \dots, x_m] + f[x_{-m}, \dots, x_{m+1}]}{2}$$

If  $n$  is odd (can be written as  $2m + 1$ ), otherwise delete the last two lines.

## Summary: Divided Difference Formulas

Newton's Interpolatory Divided Difference Formula

$$P_n(x) = f[x_0] + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1) + f[x_0, x_1, x_2, x_3](x - x_0)(x - x_1)(x - x_2) + \dots$$

Newton's Forward Divided Difference Formula

$$P_n(x_0 + sh) = f[x_0] + \sum_{k=1}^n \binom{s}{k} h^k f[x_0, \dots, x_k]$$

Newton's Backward Difference Formula

$$P_n(x) = f[x_n] + \sum_{k=1}^n (-1)^k \binom{-s}{k} \nabla^k f(x_n)$$

Reference: Binomial Coefficients

$$\binom{s}{k} = \frac{s(s-1)\cdots(s-k+1)}{k!}, \quad \binom{-s}{k} = (-1)^k \frac{s(s+1)\cdots(s+k-1)}{k!}$$

## Homework #4

<http://webwork.sdsu.edu>

- Will open on 09/24/2014 at 09:30am PDT.
- Will close no earlier than 10/3/2014 at 09:00pm PDT.

## Combining Taylor and Lagrange Polynomials

A **Taylor polynomial of degree  $n$**  matches the function and its first  $n$  derivatives at one point.

A **Lagrange polynomial of degree  $n$**  matches the function values at  $n + 1$  points.

**Question:** Can we combine the ideas of Taylor and Lagrange to get an interpolating polynomial that matches both the function values and some number of derivatives at multiple points?

**Answer:** To our euphoric joy, such polynomials exist! They are called **Osculating Polynomials**.

**The Concise Oxford Dictionary:**

**Osculate 1.** (arch. or joc.) kiss. **2.** (Biol., of species, etc.) be related through intermediate species etc., have common characteristics *with* another or with each other. **3.** (Math., of curve or surface) have contact of higher than first order with, meet at three or more coincident points.

## Osculating Polynomials

In Painful Generality

Given  $(n + 1)$  distinct points  $\{x_0, x_1, \dots, x_n\} \in [a, b]$ , and non-negative integers  $\{m_0, m_1, \dots, m_n\}$ .

**Notation:** Let  $m = \max\{m_0, m_1, \dots, m_n\}$ .

The **osculating polynomial approximation** of a function  $f \in C^m[a, b]$  at  $x_i$ ,  $i = 0, 1, \dots, n$  is the polynomial (of lowest possible order) that agrees with

$$\{f(x_i), f'(x_i), \dots, f^{(m_i)}(x_i)\} \text{ at } x_i \in [a, b], \forall i.$$

The degree of the osculating polynomial is **at most**

$$M = n + \sum_{i=0}^n m_i.$$

In the case where  $m_i = 1, \forall i$  the polynomial is called a **Hermite Interpolatory Polynomial**.

If  $f \in C^1[a, b]$  and  $\{x_0, x_1, \dots, x_n\} \in [a, b]$  are distinct, the unique polynomial of least degree ( $\leq 2n + 1$ ) agreeing with  $f(x)$  and  $f'(x)$  at  $\{x_0, x_1, \dots, x_n\}$  is

$$\mathbf{H}_{2n+1}(\mathbf{x}) = \sum_{j=0}^n \mathbf{f}(x_j) \mathbf{H}_{n,j}(\mathbf{x}) + \sum_{j=0}^n \mathbf{f}'(x_j) \hat{\mathbf{H}}_{n,j}(\mathbf{x}),$$

where

$$H_{n,j}(x) = [1 - 2(x - x_j)L'_{n,j}(x_j)] L_{n,j}^2(x)$$

$$\hat{H}_{n,j}(x) = (x - x_j)L_{n,j}^2(x),$$

and  $L_{n,j}(x)$  are our old friends, the **Lagrange coefficients**:

$$L_{n,j}(x) = \prod_{i=0, i \neq j}^n \frac{x - x_i}{x_j - x_i}.$$

Further, if  $f \in C^{2n+2}[a, b]$ , then for some  $\xi(x) \in [a, b]$

$$f(x) = H_{2n+1}(x) + \frac{\prod_{i=0}^n (x - x_i)^2}{(2n + 2)!} f^{(2n+2)}(\xi(x)).$$

**Recall:**  $L_{n,j}(x_i) = \delta_{i,j} = \begin{cases} 0, & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases}$  ( $\delta_{i,j}$  is Kronecker's delta).

It follows that when  $i \neq j$ :  $H_{n,j}(x_i) = \hat{H}_{n,j}(x_i) = 0$ .

When  $i = j$ :  $\begin{cases} H_{n,j}(x_j) = [1 - 2(x_j - x_j)L'_{n,j}(x_j)] \cdot 1 = 1 \\ \hat{H}_{n,j}(x_j) = (x_j - x_j)L_{n,j}^2(x_j) = 0. \end{cases}$

Thus,  $\mathbf{H}_{2n+1}(\mathbf{x}_j) = \mathbf{f}(\mathbf{x}_j)$ .

$$\begin{aligned} H'_{n,j}(x) &= [-2L'_{n,j}(x_j)]L_{n,j}^2(x) + [1 - 2(x - x_j)L'_{n,j}(x_j)] \cdot 2L_{n,j}(x)L'_{n,j}(x) \\ &= L_{n,j}(x) [-2L'_{n,j}(x_j)L_{n,j}(x) + [1 - 2(x - x_j)L'_{n,j}(x_j)] \cdot 2(x)L'_{n,j}(x)] \end{aligned}$$

Since  $L_{n,j}(x)$  is a factor in  $H'_{n,j}(x)$ :  $H'_{n,j}(x_i) = 0$  when  $i \neq j$ .

Proof, continued...

$$\begin{aligned} H'_{n,j}(x_j) &= [-2L'_{n,j}(x_j)] \underbrace{L_{n,j}^2(x_j)}_1 \\ &+ [1 - 2 \underbrace{(x_j - x_j)}_0] \underbrace{L'_{n,j}(x_j)}_1 \cdot 2 \underbrace{L_{n,j}(x_j)}_1 \underbrace{L'_{n,j}(x_j)}_1 \\ &= -2L'_{n,j}(x_j) + 1 \cdot 2 \cdot L'_{n,j}(x_j) = 0 \end{aligned}$$

i.e.  $\mathbf{H}'_{n,j}(\mathbf{x}_i) = \mathbf{0}$ ,  $\forall i$ .

$$\begin{aligned} \hat{H}'_{n,j}(x) &= L_{n,j}^2(x) + 2(x - x_j)L_{n,j}(x)L'_{n,j}(x) \\ &= L_{n,j}(x) [L_{n,j}(x) + 2(x - x_j)L'_{n,j}(x)] \end{aligned}$$

If  $i \neq j$ :  $\hat{H}'_{n,j}(x_i) = 0$ , since  $L_{n,j}(x_i) = \delta_{i,j}$ .

If  $i = j$ :  $\hat{H}'_{n,j}(x_j) = 1 \cdot [1 + 2(x_j - x_j)L'_{n,j}(x_j)] = 1$ .

Hence,  $\mathbf{H}'_{2n+1}(\mathbf{x}_i) = \mathbf{f}'(\mathbf{x}_i)$ ,  $\forall i$ .  $\square$

Uniqueness Proof

- Assume there is a second polynomial  $G(x)$  (of degree  $\leq 2n + 1$ ) interpolating the same data.
- Define  $R(x) = H_{2n+1}(x) - G(x)$ .
- Then by construction  $R(x_i) = R'(x_i) = 0$ , i.e. all the  $x_i$ 's are zeros of multiplicity at least 2.
- This can only be true if  $R(x) = q(x) \prod_{i=0}^n (x - x_i)^2$ , for some  $q(x)$ .
- If  $q(x) \not\equiv 0$  then the degree of  $R(x)$  is  $\geq 2n + 2$ , which is a contradiction.
- Hence  $q(x) \equiv 0 \Rightarrow R(x) \equiv 0 \Rightarrow H_{2n+1}(x)$  is unique.  $\square$

## Main Use of Hermite Interpolatory Polynomials

One of the primary applications of Hermite Interpolatory Polynomials is the development of **Gaussian quadrature** for numerical integration. (To be revisited later this semester.)

The most commonly seen Hermite interpolatory polynomial is the cubic one, which satisfies

$$\begin{aligned} H_3(x_0) &= f(x_0), & H_3'(x_0) &= f'(x_0) \\ H_3(x_1) &= f(x_1), & H_3'(x_1) &= f'(x_1). \end{aligned}$$

it can be written explicitly as

$$\begin{aligned} H_3(x) &= \left[1 + 2 \frac{x-x_0}{x_1-x_0}\right] \left[\frac{x_1-x}{x_1-x_0}\right]^2 f(x_0) + (x-x_0) \left[\frac{x_1-x}{x_1-x_0}\right]^2 f'(x_0) \\ &+ \left[1 + 2 \frac{x_1-x}{x_1-x_0}\right] \left[\frac{x-x_0}{x_1-x_0}\right]^2 f(x_1) + (x-x_1) \left[\frac{x-x_0}{x_1-x_0}\right]^2 f'(x_1). \end{aligned}$$

It appears in some optimization algorithms (see Math 693a, *linesearch algorithms*.)

## Computing from the Definition is Tedious!

However, there is good news: we can re-use the algorithm for **Newton's Interpolatory Divided Difference Formula** with some modifications in the initialization.

We "double" the number of points, *i.e.* let

$$\{y_0, y_1, \dots, y_{2n+1}\} = \{x_0, x_0 + \epsilon, x_1, x_1 + \epsilon, \dots, x_n, x_n + \epsilon\}$$

Set up the divided difference table (up to the first divided differences), and let  $\epsilon \rightarrow 0$  (formally), and identify:

$$f'(x_i) = \lim_{\epsilon \rightarrow 0} \frac{f[x_i + \epsilon] - f[x_i]}{\epsilon},$$

to get the table [*next slide*]...

## Hermite Interpolatory Polynomial using Modified Newton Divided Differences

y	f(x)	1st Div. Diff.	2nd Div. Diff.	3rd Div. Diff.
$y_0 = x_0$	$f[y_0]$			
$y_1 = x_0$	$f[y_1]$	$f[y_0, y_1] = f'(y_0)$	$f[y_0, y_1, y_2]$	$f[y_0, y_1, y_2, y_3]$
$y_2 = x_1$	$f[y_2]$	$f[y_1, y_2]$	$f[y_1, y_2, y_3]$	$f[y_1, y_2, y_3, y_4]$
$y_3 = x_1$	$f[y_3]$	$f[y_2, y_3] = f'(y_2)$	$f[y_2, y_3, y_4]$	$f[y_2, y_3, y_4, y_5]$
$y_4 = x_2$	$f[y_4]$	$f[y_3, y_4]$	$f[y_3, y_4, y_5]$	$f[y_3, y_4, y_5, y_6]$
$y_5 = x_2$	$f[y_5]$	$f[y_4, y_5] = f'(y_4)$	$f[y_4, y_5, y_6]$	$f[y_4, y_5, y_6, y_7]$
$y_6 = x_3$	$f[y_6]$	$f[y_5, y_6]$	$f[y_5, y_6, y_7]$	$f[y_5, y_6, y_7, y_8]$
$y_7 = x_3$	$f[y_7]$	$f[y_6, y_7] = f'(y_6)$	$f[y_6, y_7, y_8]$	$f[y_6, y_7, y_8, y_9]$
$y_8 = x_4$	$f[y_8]$	$f[y_7, y_8]$	$f[y_7, y_8, y_9]$	
$y_9 = x_4$	$f[y_9]$	$f[y_8, y_9] = f'(y_8)$		

## $H_3(x)$ revisited...

Old notation

$$\begin{aligned} H_3(x) &= \left[1 + 2 \frac{x-x_0}{x_1-x_0}\right] \left[\frac{x_1-x}{x_1-x_0}\right]^2 f(x_0) + \left[1 + 2 \frac{x_1-x}{x_1-x_0}\right] \left[\frac{x-x_0}{x_1-x_0}\right]^2 f(x_1) \\ &+ (x-x_0) \left[\frac{x_1-x}{x_1-x_0}\right]^2 f'(x_0) + (x-x_1) \left[\frac{x-x_0}{x_1-x_0}\right]^2 f'(x_1). \end{aligned}$$

Divided difference notation

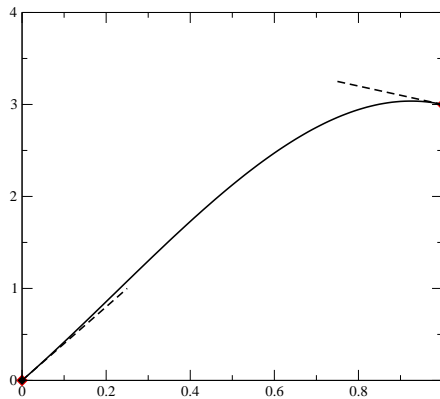
$$\begin{aligned} H_3(x) &= f(x_0) + f'(x_0)(x-x_0) + f[x_0, x_0, x_1](x-x_0)^2 \\ &+ f[x_0, x_0, x_1, x_1](x-x_0)^2(x-x_1). \end{aligned}$$

Or with the  $y$ 's...

$$\begin{aligned} H_3(x) &= f(y_0) + f'(y_0)(x-y_0) + f[y_0, y_1, y_2](x-y_0)(x-y_1) \\ &+ f[y_0, y_1, y_2, y_3](x-y_0)(x-y_1)(x-y_2). \end{aligned}$$



## $H_3(x)$ Example



$$x_0 = 0, \quad x_1 = 1$$

$$f(x_0) = 0, \quad f'(x_0) = 4, \quad f(x_1) = 3, \quad f'(x_1) = -1$$

$$H_3(x) = 4x - x^2 - 3x^2(x - 1)$$

## $H_3(x)$ Example — Not Very Pretty Computations

### Example

```

x0 = 0; x1 = 1;           % This is the data
fv0 = 0; fpv0 = 4;
fv1 = 3; fpv1 = -1;

y0 = x0; f0=fv0;         % Initializing the table
y1 = x0; f1=fv0;
y2 = x1; f2=fv1;
y3 = x1; f3=fv1;

f01 = fpv0;              % First divided differences
f12 = (f2-f1)/(y2-y1);
f23 = fpv1;

f012 = (f12-f01)/(y2-y0); % Second divided differences
f123 = (f23-f12)/(y3-y1);

f0123 = (f123-f012)/(y3-y0); % Third divided difference
x=(0:0.01:1)';
H3 = f0 + f01*(x-y0) + f012*(x-y0).*(x-y1) + ...
     f0123*(x-y0).*(x-y1).*(x-y2);
    
```

## Algorithm: Hermite Interpolation

### Algorithm: Hermite Interpolation, Part #1

Given the data points  $(x_i, f(x_i), f'(x_i))$ ,  $i = 0, \dots, n$ .

Step 1: FOR  $i=0:n$

$$y_{2i} = x_i, \quad Q_{2i,0} = f(x_i), \quad y_{2i+1} = x_i, \quad Q_{2i+1,0} = f(x_i)$$

$$Q_{2i+1,1} = f'(x_i)$$

IF  $i > 0$

$$Q_{2i,1} = \frac{Q_{i,0} - Q_{i-1,0}}{y_{2i} - y_{2i-1}}$$

END

END

## Algorithm: Hermite Interpolation

### Algorithm: Hermite Interpolation, Part #2

Step 2: FOR  $i = 2 : (2n + 1)$

FOR  $j = 2 : i$

$$Q_{i,j} = \frac{Q_{i,j-1} - Q_{i-1,j-1}}{y_i - y_{i-j}}$$

END

END

Result:  $q_i = Q_{i,i}$ ,  $i = 0, \dots, 2n + 1$  now contains the coefficients for

$$H_{2n+1}(x) = q_0 + \sum_{k=1}^{2n+1} \left[ q_k \prod_{j=0}^{k-1} (x - y_j) \right].$$

So far we have seen the osculating polynomials of order 0 — the Lagrange polynomial, and of order 1 — the Hermite interpolatory polynomial.

It turns out that generating osculating polynomials of higher order is fairly straight-forward; — and we use Newton’s divided differences to generate those as well.

Given a set of points  $\{x_k\}_{k=0}^n$ , and  $\{f^{(\ell)}(x_k)\}_{k=0, \ell=0}^{n, \ell_k}$ ; *i.e.* the function values, as well as the first  $\ell_k$  derivatives of  $f$  in  $x_k$ . (Note that we can specify a different number of derivatives in each point.)

Set up the Newton-divided-difference table, and put in  $(\ell_k + 1)$  duplicate entries of each point  $x_k$ , as well as its function value  $f(x_k)$ .

Run the computation of Newton’s divided differences as usual; with the following exception:

Whenever a zero-denominator is encountered — *i.e.* the divided difference for that entry cannot be computed due to duplication of a point — use a derivative instead. For  $m^{\text{th}}$  divided differences, use  $\frac{1}{m!} f^{(m)}(x_k)$ .

On the next slide we see the setup for two point in which two derivatives are prescribed.

y	f(x)	1st Div. Diff.	2nd Div. Diff.	3rd Div. Diff.
$y_0 = x_0$	$f[y_0]$			
$y_1 = x_0$	$f[y_1]$	$f[y_0, y_1] = f'(x_0)$		
$y_2 = x_0$	$f[y_2]$	$f[y_1, y_2] = f'(x_0)$	$f[y_0, y_1, y_2] = \frac{1}{2} f''(x_0)$	
$y_3 = x_1$	$f[y_3]$	$f[y_2, y_3]$	$f[y_1, y_2, y_3]$	$f[y_0, y_1, y_2, y_3]$
$y_4 = x_1$	$f[y_4]$	$f[y_3, y_4] = f'(x_1)$	$f[y_2, y_3, y_4]$	$f[y_1, y_2, y_3, y_4]$
$y_5 = x_1$	$f[y_5]$	$f[y_4, y_5] = f'(x_1)$	$f[y_3, y_4, y_5] = \frac{1}{2} f''(x_1)$	$f[y_2, y_3, y_4, y_5]$

3rd and higher order divided differences are computed “as usual” in this case.

On the next slide we see four examples of 2nd order osculating polynomials.

