# Numerical Analysis and Computing

## Lecture Notes #5 — Interpolation and Polynomial Approximation

## Divided Differences, and Hermite Interpolatory Polynomials

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# Outline

## 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.

## 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 $a_0, a_1, \ldots, a_n$; $x_0$

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

1. Set $y = a_n$, $z = a_n$
2. For $j = (n-1), (n-2), \ldots, 1$
   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

# Representing Polynomials

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

$$\begin{aligned} P_n(x) \quad = \quad & a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + \cdots \\ & \cdots + a_n(x - x_0)(x - x_1) \cdots (x - x_{n-1}) \end{aligned}$$

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

$$\begin{aligned} P_n(x) \quad = \quad & a_0 + (x - x_0)\left(a_1 + (x - x_1)\left(a_2 + \cdots\right.\right. \\ & \left.\left.\cdots + (x - x_{n-2})\left(a_{n-1} + a_n(x - x_{n-1})\right)\right)\right), \end{aligned}$$

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

## Finding the Constants $\{a_0, a_1, \ldots, a_n\}$ "Just Algebra"

Given the relation

$$\begin{aligned} P_n(x) \quad = \quad & a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + \cdots \\ & \cdots + a_n(x - x_0)(x - x_1)\cdots(x - x_{n-1}) \end{aligned}$$

at $\mathbf{x_0}$: $\quad a_0 = P_n(x_0) = f(x_0)$.

at $\mathbf{x_1}$: $\quad f(x_0) + a_1(x_1 - x_0) = P_n(x_1) = f(x_1)$

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

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

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**:

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

$k$**th Divided Difference**:

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

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

We had

at $\mathbf{x_0}$: $\quad a_0 = P_n(x_0) = f(x_0).$

at $\mathbf{x_1}$: $\quad f(x_0) + a_1(x_1 - x_0) = P_n(x_1) = f(x_1)$

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

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

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

$$\mathbf{a_k = f[x_0, x_1, \ldots, x_k]}.$$

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

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

# Newton's Interpolatory Divided Difference Formula

Hence, we can write

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

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

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. |
|---|---|---|---|
| $x_0$ | $f[x_0]$ | | |
| | | $f[x_0,x_1] = \frac{f[x_1]-f[x_0]}{x_1-x_0}$ | |
| $x_1$ | $f[x_1]$ | | $f[x_0,x_1,x_2] = \frac{f[x_1,x_2]-f[x_0,x_1]}{x_2-x_0}$ |
| | | $f[x_1,x_2] = \frac{f[x_2]-f[x_1]}{x_2-x_1}$ | |
| $x_2$ | $f[x_2]$ | | $f[x_1,x_2,x_3] = \frac{f[x_2,x_3]-f[x_1,x_2]}{x_3-x_1}$ |
| | | $f[x_2,x_3] = \frac{f[x_3]-f[x_2]}{x_3-x_2}$ | |
| $x_3$ | $f[x_3]$ | | $f[x_2,x_3,x_4] = \frac{f[x_3,x_4]-f[x_2,x_3]}{x_4-x_2}$ |
| | | $f[x_3,x_4] = \frac{f[x_4]-f[x_3]}{x_4-x_3}$ | |
| $x_4$ | $f[x_4]$ | | $f[x_3,x_4,x_5] = \frac{f[x_4,x_5]-f[x_3,x_4]}{x_5-x_3}$ |
| | | $f[x_4,x_5] = \frac{f[x_5]-f[x_4]}{x_5-x_4}$ | |
| $x_5$ | $f[x_5]$ | | |

**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 $n^{th}$ divided difference is in some sense an approximation to the $n^{th}$ derivative of $f$.*

## Newton vs. Taylor...

Using Newton's Divided Differences...

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

Using Taylor expansion

$$\begin{aligned} P_n^T(x) \;=\; & f(x_0) + f'(x_0)(x-x_0) + \\ & \frac{1}{2!} f''(x_0)(x-x_0)^2 + \\ & \frac{1}{3!} f'''(x_0)(x-x_0)^3 + \cdots \end{aligned}$$

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

# Simplification: Equally Spaced Points

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

$$h = x_{i+1} - x_i, \;\; i = 0, \ldots, n-1,$$

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

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

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

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

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:

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

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

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

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

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

# Notation, Notation, Notation... Backward Formulas

If we reorder $\{x_0, x_1, \ldots, x_n\} \to \{x_n, \ldots, x_1, x_0\}$, 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:

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

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

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

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. |
|---|---|---|---|
| $x_0$ | $f[x_0]$ | | |
| | | $\mathbf{f[x_0, x_1] = \frac{f[x_1]-f[x_0]}{x_1-x_0}}$ | |
| $x_1$ | $f[x_1]$ | | $\mathbf{f[x_0, x_1, x_2] = \frac{f[x_1,x_2]-f[x_0,x_1]}{x_2-x_0}}$ |
| | | $f[x_1, x_2] = \frac{f[x_2]-f[x_1]}{x_2-x_1}$ | |
| $x_2$ | $f[x_2]$ | | $f[x_1, x_2, x_3] = \frac{f[x_2,x_3]-f[x_1,x_2]}{x_3-x_1}$ |
| | | $f[x_2, x_3] = \frac{f[x_3]-f[x_2]}{x_3-x_2}$ | |
| $x_3$ | $f[x_3]$ | | $f[x_2, x_3, x_4] = \frac{f[x_3,x_4]-f[x_2,x_3]}{x_4-x_2}$ |
| | | $f[x_3, x_4] = \frac{f[x_4]-f[x_3]}{x_4-x_3}$ | |
| $x_4$ | $f[x_4]$ | | $\mathbf{f[x_3, x_4, x_5] = \frac{f[x_4,x_5]-f[x_3,x_4]}{x_5-x_3}}$ |
| | | $\mathbf{f[x_4, x_5] = \frac{f[x_5]-f[x_4]}{x_5-x_4}}$ | |
| $x_5$ | $f[x_5]$ | | |

**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. |
|---|---|---|---|---|---|
| $x_{-2}$ | $f[x_{-2}]$ | | | | |
| | | $f[x_{-2}, x_{-1}]$ | | | |
| $x_{-1}$ | $f[x_{-1}]$ | | $f[x_{-2}, x_{-1}, x_0]$ | | |
| | | $\mathbf{f[x_{-1}, x_0]}$ | | $\mathbf{f[x_{-2}, x_{-1}, x_0, x_1]}$ | |
| $x_0$ | $\mathbf{f[x_0]}$ | | $\mathbf{f[x_{-1}, x_0, x_1]}$ | | $\mathbf{f[x_{-2}, x_{-1}, x_0, x_1, x_2]}$ |
| | | $\mathbf{f[x_0, x_1]}$ | | $\mathbf{f[x_{-1}, x_0, x_1, x_2]}$ | |
| $x_1$ | $f[x_1]$ | | $f[x_0, x_1, x_2]$ | | $f[x_{-1}, x_0, x_1, x_2, x_3]$ |
| | | $f[x_1, x_2]$ | | $f[x_0, x_1, x_2, x_3]$ | |
| $x_2$ | $f[x_2]$ | | $f[x_1, x_2, x_3]$ | | |
| | | $f[x_2, x_3]$ | | | |
| $x_3$ | $f[x_3]$ | | | | |

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 $x_0$:

$$\begin{aligned}
P_n(x) \quad = \quad & P_{2m+1}(x) = f[x_0] + sh\,\frac{f[x_{-1},x_0]+f[x_0,x_1]}{2} \\
& + s^2h^2\; f[x_{-1},x_0,x_1] \\
& + s(s^2-1)h^3\;\frac{f[x_{-2},x_{-1},x_0,x_1]+f[x_{-1},x_0,x_1,x_2]}{2} \\
& + s^2(s^2-1)h^4\; f[x_{-2},x_{-1},x_0,x_1,x_2] \\
& + \;\ldots \\
& + s^2(s^2-1)\cdots(s^2-(m-1)^2)h^{2m}\; f[x_{-m},\ldots,x_m] \\
& + s(s^2-1)\cdots(s^2-m^2)h^{2m+1} \\
& \cdot\frac{f[x_{-m-1},\ldots,x_m]+f[x_{-m},\ldots,x_{m+1}]}{2}
\end{aligned}$$

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

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

## Newton's Forward Divided Difference Formula

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

## 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

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

## 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 $\{x_0, x_1, \ldots, x_n\} \in [a, b]$, and non-negative integers $\{m_0, m_1, \ldots, m_n\}$.

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

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

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

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**.

## Hermite Interpolatory Polynomials — The Existence Statement

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

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

where

$$H_{n,j}(x) = \left[1 - 2(x - x_j) L'_{n,j}(x_j)\right] L^2_{n,j}(x)$$
$$\hat{H}_{n,j}(x) = (x - x_j) L^2_{n,j}(x),$$

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 $\xi(x) \in [a,b]$

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

## That's Hardly Obvious — Proof Needed!



**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).

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

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

Thus, $\mathbf{H_{2n+1}(x_j) = f(x_j)}$.

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

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...

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

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

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

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

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

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

## 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

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

it can be written explicitly as

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

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 $\epsilon \to 0$ (formally), and identify:

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

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. |
|---|---|---|---|---|
| $y_0 = x_0$ | $f[y_0]$ | | | |
| | | $f[y_0, y_1] = f'(y_0)$ | | |
| $y_1 = x_0$ | $f[y_1]$ | | $f[y_0, y_1, y_2]$ | |
| | | $f[y_1, y_2]$ | | $f[y_0, y_1, y_2, y_3]$ |
| $y_2 = x_1$ | $f[y_2]$ | | $f[y_1, y_2, y_3]$ | |
| | | $f[y_2, y_3] = f'(y_2)$ | | $f[y_1, y_2, y_3, y_4]$ |
| $y_3 = x_1$ | $f[y_3]$ | | $f[y_2, y_3, y_4]$ | |
| | | $f[y_3, y_4]$ | | $f[y_2, y_3, y_4, y_5]$ |
| $y_4 = x_2$ | $f[y_4]$ | | $f[y_3, y_4, y_5]$ | |
| | | $f[y_4, y_5] = f'(y_4)$ | | $f[y_3, y_4, y_5, y_6]$ |
| $y_5 = x_2$ | $f[y_5]$ | | $f[y_4, y_5, y_6]$ | |
| | | $f[y_5, y_6]$ | | $f[y_4, y_5, y_6, y_7]$ |
| $y_6 = x_3$ | $f[y_6]$ | | $f[y_5, y_6, y_7]$ | |
| | | $f[y_6, y_7] = f'(y_6)$ | | $f[y_5, y_6, y_7, y_8]$ |
| $y_7 = x_3$ | $f[y_7]$ | | $f[y_6, y_7, y_8]$ | |
| | | $f[y_7, y_8]$ | | $f[y_6, y_7, y_8, y_9]$ |
| $y_8 = x_4$ | $f[y_8]$ | | $f[y_7, y_8, y_9]$ | |
| | | $f[y_8, y_9] = f'(y_8)$ | | |
| $y_9 = x_4$ | $f[y_9]$ | | | |

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

Old notation

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

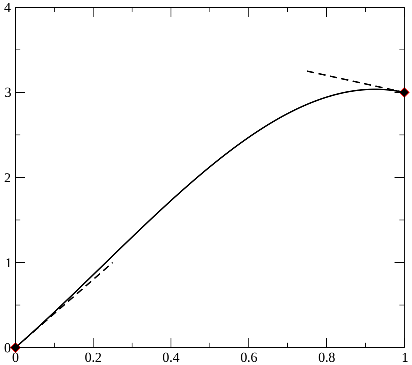
Divided difference notation

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

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 $(x_i, f(x_i), f'(x_i))$, $i = 0, \ldots, n$.

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

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

## Higher Order Osculating Polynomials



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 $f(x_k)$.

## Higher Order Osculating Polynomials



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.

## Higher Order Osculating Polynomials

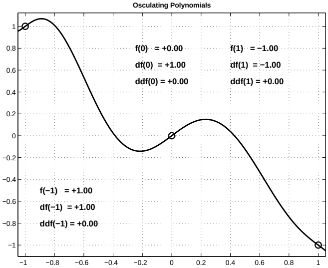


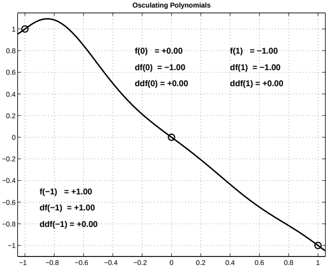
| y | f(x) | 1st Div. Diff. | 2nd Div. Diff. | 3rd Div. Diff. |
|---|---|---|---|---|
| $y_0 = x_0$ | $f[y_0]$ | | | |
| | | $f[y_0, y_1] = f'(x_0)$ | | |
| $y_1 = x_0$ | $f[y_1]$ | | $f[y_0, y_1, y_2] = \frac{1}{2} f''(x_0)$ | |
| | | $f[y_1, y_2] = f'(x_0)$ | | $f[y_0, y_1, y_2, y_3]$ |
| $y_2 = x_0$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

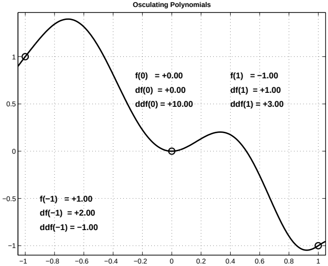
3rd and higher order divided differences are computed "as usual" in this case.

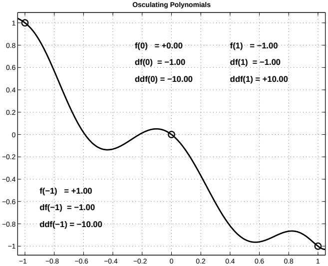
On the next slide we see four examples of 2nd order osculating polynomials.

# Examples...


Osculating Polynomials
f(0) = +0.00
df(0) = +1.00
ddf(0) = +0.00
f(1) = −1.00
df(1) = −1.00
ddf(1) = +0.00
f(−1) = +1.00
df(−1) = +1.00
ddf(−1) = +0.00


Osculating Polynomials
f(0) = +0.00
df(0) = −1.00
ddf(0) = +0.00
f(1) = −1.00
df(1) = −1.00
ddf(1) = +0.00
f(−1) = +1.00
df(−1) = +1.00
ddf(−1) = +0.00


Osculating Polynomials
f(0) = +0.00
df(0) = +0.00
ddf(0) = +10.00
f(1) = −1.00
df(1) = +1.00
ddf(1) = +3.00
f(−1) = +1.00
df(−1) = +2.00
ddf(−1) = −1.00


Osculating Polynomials
f(0) = +0.00
df(0) = −1.00
ddf(0) = −10.00
f(1) = −1.00
df(1) = −1.00
ddf(1) = +10.00
f(−1) = +1.00
df(−1) = −1.00
ddf(−1) = −10.00