## ECE 204 Numerical methods

## Approximating derivatives using interpolating polyhomials

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## Introduction

- In this topic, we will
- Find different formulas for approximating the derivative and second derivative
- Use information on both sides of the point, and then only information to the left of the point
- See that these formulas depend on the step size
- Note that the $\mathrm{O}\left(h^{2}\right)$ formulas converge more quickly as $h$ is made smaller
- Discuss the differences between the formulas


## Review

- In the previous topic, we discussed estimating the value of a function by interpolating sampled points
- We will now estimate the derivative and second derivative at the point $x_{k}$ or $t_{k}$
- In the first case, we have access to $f\left(x_{k-1}\right), f\left(x_{k+1}\right)$, etc.
- In the second, we only have access to $y\left(t_{k-1}\right), y\left(t_{k-2}\right), \ldots$
- To compare methods, we will use a consistent step size $h$
- Thus, $t_{k}=t_{0}+k h$


## Forward divided difference

- In calculus, you learned that the derivative is the slope at a point
- Suppose we have the points

$$
\left(x_{k}, f\left(x_{k}\right)\right),\left(x_{k+1}, f\left(x_{k+1}\right)\right)
$$

- The slope of the line interpolating these two points should be close to the slope of $f$ at $x_{k}$
- The slope of this line is

$$
\frac{f\left(x_{k+1}\right)-f\left(x_{k}\right)}{x_{k+1}-x_{k}}
$$

$$
f\left(x_{k+1}\right)
$$



## Forward divided difference

- Now, given this slope:

$$
\frac{f\left(x_{k+1}\right)-f\left(x_{k}\right)}{x_{k+1}-x_{k}}
$$

- Note that $x_{k}+h=x_{k+1}$ and that $x_{k+1}-x_{k}=h$
- Thus, this formula is equivalent to

$$
\frac{f\left(x_{k}+h\right)-f\left(x_{k}\right)}{h}
$$

- We are periodically sampling, so we cannot reduce $h$, so what is the error of this approximation? $f\left(x_{k}\right)$



## Forward divided difference

- The only formulas we know that describe the error are Taylor series:

$$
\begin{aligned}
& f\left(x_{k}+h\right)=f\left(x_{k}\right)+f^{(1)}\left(x_{k}\right) h+\frac{1}{2} f^{(2)}(\xi) h^{2} \\
& f^{(1)}\left(x_{k}\right) h=f\left(x_{k}+h\right)-f\left(x_{k}\right)-\frac{1}{2} f^{(2)}(\xi) h^{2} \\
& f^{(1)}\left(x_{k}\right)=\frac{f\left(x_{k}+h\right)-f\left(x_{k}\right)}{h}-\frac{1}{2} f^{(2)}(\xi) h \\
&=\frac{f\left(x_{k}\right)}{x_{k-2}} x_{k-1} \quad x_{k} \\
&\left.x_{k+1}\right)
\end{aligned}
$$

## Forward divided difference

- Therefore,

$$
f^{(1)}\left(x_{k}\right) \approx \frac{f\left(x_{k}+h\right)-f\left(x_{k}\right)}{h}
$$

and the error is $-\frac{1}{2} f^{(2)}(\xi) h$ for some $x_{k}<\xi<x_{k+1}$


## Forward divided difference

- Note that to reduce the error, we must increase our sampling rate
- Doubling the sampling rate reduces $h$ by half and thus reduces the error by approximately half
- Halving the sampling rate doubles $h$ and thus increases the error by a factor of two



## Forward divided difference

- Suppose we want to approximate the derivative of $\sin (x)$ at $x=1$

| $n$ | $h=2^{-n}$ | Approximation | Error | $\frac{1}{2} \sin (1) h$ | Ratio |
| :--- | :--- | ---: | :--- | :--- | :--- |
| 1 | 0.5 | 0.312048003592316 | 0.2283 | 0.2104 |  |
| 2 | 0.25 | 0.430054538190759 | 0.1102 | 0.1052 | 0.4830 |
| 3 | 0.125 | 0.486372874329589 | 0.05393 | 0.05259 | 0.4892 |
| 4 | 0.0625 | 0.513663205746793 | 0.02664 | 0.02630 | 0.4940 |
| 5 | 0.03125 | 0.527067456146781 | 0.01323 | 0.01315 | 0.4968 |
| 6 | 0.015625 | 0.533706462857715 | 0.006596 | 0.006574 | 0.4984 |
| 7 | 0.0078125 | 0.537009830329723 | 0.003292 | 0.003287 | 0.4992 |
| 8 | 0.00390625 | 0.538657435881987 | 0.001645 | 0.001643 | 0.4996 |
| 9 | 0.001953125 | 0.539480213605884 | 0.0008221 | 0.0008217 | 0.4998 |
| 10 | 0.0009765625 | 0.539891345517731 | 0.0004110 | 0.0004109 | 0.4999 |

## Centered divided difference

- Can we do better?
- Let us find an interpolating quadratic passing through the three points

$$
\left(x_{k-1}, f\left(x_{k-1}\right)\right),\left(x_{k}, f\left(x_{k}\right)\right) \text { and }\left(x_{k+1}, f\left(x_{k+1}\right)\right)
$$

- Finding this interpolating polynomial is more difficult, so we will shift but not scale
- The derivative will change if we scale



## Centered divided difference

- Shifting to $x=0$, we subtract $x_{k}$ from each $x$-value
- Thus, we will interpolate

$$
\left(-h, f\left(x_{k-1}\right)\right),\left(0, f\left(x_{k}\right)\right) \text { and }\left(h, f\left(x_{k+1}\right)\right)
$$

- Thus, we will:
- Find the interpolating polynomial
- Differentiate it
- Evaluate the derivative at $x=0$

$$
f\left(x_{k+1}\right)
$$

$$
\left(\begin{array}{lrr}
h^{2} & -h & 1 \\
0 & 0 & 1 \\
h^{2} & h & 1
\end{array}\right)\left(\begin{array}{l}
a_{2} \\
a_{1} \\
a_{0}
\end{array}\right)=\left(\begin{array}{c}
f\left(x_{k-1}\right) \\
f\left(x_{k}\right) \\
f\left(x_{k+1}\right)
\end{array}\right) \xrightarrow{\substack{1 \\
-2 h \\
-h}} \begin{array}{lllll} 
& f\left(x_{k-1}\right) & f\left(x_{k}\right) \\
\hline
\end{array}
$$

## Centered divided difference

- Thus, we find:

$$
\frac{f\left(x_{k+1}\right)-2 f\left(x_{k}\right)+f\left(x_{k-1}\right)}{2 h^{2}} x^{2}+\frac{f\left(x_{k+1}\right)-f\left(x_{k-1}\right)}{2 h} x+f\left(x_{k}\right)
$$

- Differentiating this with respect to $x$, we get

$$
2 \frac{f\left(x_{k+1}\right)-2 f\left(x_{k}\right)+f\left(x_{k-1}\right)}{2 h^{2}} x+\frac{f\left(x_{k+1}\right)-f\left(x_{k-1}\right)}{2 h}
$$

- Evaluating this at $x=0$, we get

$$
\begin{aligned}
& \frac{f\left(x_{k+1}\right)-f\left(x_{k-1}\right)}{2 h} \\
& f\left(x_{k-1}\right) \quad f\left(x_{k}\right) \\
& \begin{array}{ccccc}
-1 & \mid & \mid & \mid & \mid \\
-2 h & -h & 0 & h & 2 h
\end{array}
\end{aligned}
$$

## Centered divided difference

- Now we have an alternate formula:

$$
\frac{f\left(x_{k+1}\right)-f\left(x_{k-1}\right)}{2 h}
$$

- Note that this is also equal to

$$
\frac{f\left(x_{k}+h\right)-f\left(x_{k}-h\right)}{2 h}
$$

- Question: What is the error?



## Centered divided difference

- Here is the Taylor series:

$$
f\left(x_{k}+h\right)=f\left(x_{k}\right)+f^{(1)}\left(x_{k}\right) h+\frac{1}{2} f^{(2)}\left(x_{k}\right) h^{2}+\frac{1}{6} f^{(3)}(\xi) h^{3}
$$

- Suppose we substitute $h$ with $-h$ in this Taylor series:

$$
f\left(x_{k}+(-h)\right)=f\left(x_{k}\right)+f^{(1)}\left(x_{k}\right)(-h)+\frac{1}{2} f^{(2)}\left(x_{k}\right)(-h)^{2}+\frac{1}{6} f^{(3)}(\xi)(-h)^{3}
$$

- Now, $(-h)^{2}=h^{2}$ but $(-h)^{3}=-h^{3}$

$$
\begin{aligned}
& f\left(x_{k}-h\right)=f\left(x_{k}\right)+f^{(1)}\left(x_{k}\right)(-h)+\frac{1}{2} f^{(2)}\left(x_{k}\right) h^{2}+\frac{1}{6} f^{(3)}(\xi)\left(-h^{3}\right) \\
& f\left(x_{k}-h\right)=f\left(x_{k}\right)-f^{(1)}\left(x_{k}\right) h+\frac{1}{2} f^{(2)}\left(x_{k}\right) h^{2}-\frac{1}{6} f^{(3)}(\xi) h^{3}
\end{aligned}
$$

- For this, $x_{k}-h<\xi<x_{k}$


## Centered divided difference

- In this expression, we have two piece

$$
\frac{f\left(x_{k}+h\right)-f\left(x_{k}-h\right)}{2 h}
$$

- Let's write the two Taylor series:

$$
\begin{aligned}
& f\left(x_{k}+h\right)=f^{\prime}\left(x_{k}\right)+f^{(1)}\left(x_{k}\right) h+\frac{1}{2} f^{(2)}\left(x_{k}\right) h^{2}+\frac{1}{6} f^{(3)}\left(\xi_{+}\right) h^{3} \\
& \begin{aligned}
& f\left(x_{k}-h\right)=f^{\prime}\left(x_{k}\right)-f^{(1)}\left(x_{k}\right) h+\frac{1}{2} f^{(2)}\left(x_{k}\right) h^{2}-\frac{1}{6} f^{(3)}\left(\xi_{-}\right) h^{3} \\
& f\left(x_{k}+h\right)-f\left(x_{k}-h\right)=2 f^{(1)}\left(x_{k}\right) h+\frac{1}{6} f^{(3)}\left(\xi_{+}\right) h^{3}+\frac{1}{6} f^{(3)}\left(\xi_{-}\right) h^{3} \\
&=2 f^{(1)}\left(x_{k}\right) h+\frac{1}{3}\left(\frac{1}{2} f^{(3)}\left(\xi_{+}\right)+\frac{1}{2} f^{(3)}\left(\xi_{-}\right)\right) h^{3} \\
&=2 f^{(1)}\left(x_{k}\right) h+\frac{1}{3} f^{(3)}(\xi) h^{3} \\
& x_{k}-h<\xi<x_{k}+h
\end{aligned}
\end{aligned}
$$

## Centered divided difference

- Next, we isolate the derivate:

$$
\frac{f\left(x_{k}+h\right)-f\left(x_{k}-h\right)}{2 h}
$$

$$
\begin{aligned}
f\left(x_{k}+h\right)-f\left(x_{k}-h\right) & =2 f^{(1)}\left(x_{k}\right) h+\frac{1}{3} f^{(3)}(\xi) h^{3} \\
f^{(1)}\left(x_{k}\right) & =\frac{f\left(x_{k}+h\right)-f\left(x_{k}-h\right)}{2 h}-\frac{1}{6} f^{(3)}(\xi) h^{2}
\end{aligned}
$$

- This formula is $\mathrm{O}\left(h^{2}\right)$

$$
x_{k}-h<\xi<x_{k}+h
$$

- Double the sampling rate (halve $h$ ),
the error drops by a factor of four
- We can get a better approximation with a larger $h$
- Less impact from subtractive cancellation


## Centered divided difference

- Suppose we want to approximate the derivative of $\sin (x)$ at $x=1$

| $n$ | $h=2^{-n}$ | Approximation | Error | $\frac{1}{6} \cos (1) h^{2}$ | Ratio |
| :--- | :--- | :---: | :--- | :--- | :--- |
|  |  |  | 0.5 | 0.5180694479998514 | 0.02223 |
| 1 | 0.5 | 0.5346917186645042 | 0.005611 | 0.02251 |  |
| 2 | 0.25 | 0.5388963674522724 | 0.001406 | 0.001407 | 0.2524 |
| 3 | 0.125 | 0.5399506152510245 | 0.0003517 | 0.0003518 | 0.2506 |
| 4 | 0.0625 | 0.5402143703335476 | 0.00008794 | 0.00008794 | 0.2501 |
| 5 | 0.03125 | 0.5402803211794023 | 0.00002198 | 0.00002198 | 0.2500 |
| 6 | 0.015625 | 0.5402968096456391 | 0.000005496 | 0.000005496 | 0.2500 |
| 7 | 0.0078125 | 0.5403009318093694 | 0.000001374 | 0.000001374 | 0.2500 |
| 8 | 0.00390625 | 0.050 |  |  |  |
| 9 | 0.001953125 | 0.5403019623532543 | 0.0000003435 | 0.0000003435 | 0.2500 |
| 10 | 0.0009765625 | 0.5403022199893712 | 0.00000008588 | 0.00000008588 | 0.2500 |
|  |  | 0.540302305868140 |  |  |  |

Previous $\mathrm{O}(h)$ formula when $h=2^{-10}$ :

$$
0.539891345517731
$$

## Backward divided difference

- The forward divided-difference formula came from calculus
- The centered divided-difference formula assumes information on both sides
- What if these come from sensor readings in time?

$$
\begin{aligned}
& y\left(t_{k}-h\right)=y\left(t_{k}\right)-y^{(1)}\left(t_{k}\right) h+\frac{1}{2} y^{(2)}(\tau) h^{2} \\
& y^{(1)}\left(t_{k}\right)=\frac{y\left(t_{k}\right)-y\left(t_{k}-h\right)}{h}+\frac{1}{2} y^{(2)}(\tau) h
\end{aligned}
$$

## Backward divided difference

- One issue, is that this approximation is only $\mathrm{O}(h)$
- Can we do better?
- How about interpolating the last three points?
- Let us find an interpolating quadratic passing through the three points

$$
\left(t_{k-2}, y\left(t_{k-2}\right)\right),\left(t_{k-1}, y\left(t_{k-1}\right)\right) \text { and }\left(t_{k}, y\left(t_{k}\right)\right)
$$

- As before, we will shift to zero to solve this



## Backward divided difference

- Shifting to $t=0$, we subtract $t_{k}$ from each $t$-value
- Thus, we will interpolate

$$
\left(-2 h, y\left(t_{k-2}\right)\right),\left(-h, y\left(t_{k-1}\right)\right) \text { and }\left(0, y\left(t_{k}\right)\right)
$$

- Thus, we will:
- Find the interpolating polynomial
- Differentiate it
- Evaluate the derivative at $t=0$


## Backward divided difference

- Thus, we find:

$$
\frac{y\left(t_{k}\right)-2 y\left(t_{k-1}\right)+y\left(t_{k-2}\right)}{2 h^{2}} t^{2}+\frac{3 y\left(t_{k}\right)-4 y\left(t_{k-1}\right)+y\left(t_{k-2}\right)}{2 h} t+y\left(t_{k}\right)
$$

- Differentiating this with respect to $t$, we get

$$
2 \frac{y\left(t_{k}\right)-2 y\left(t_{k-1}\right)+y\left(t_{k-2}\right)}{2 h^{2}} t+\frac{3 y\left(t_{k}\right)-4 y\left(t_{k-1}\right)+y\left(t_{k-2}\right)}{2 h}
$$

- Evaluating this at $t=0$, we get

$$
\frac{3 y\left(t_{k}\right)-4 y\left(t_{k-1}\right)+y\left(t_{k-2}\right)}{2 h}
$$



## Backward divided difference

- Now we have an alternate formula:

$$
\frac{3 y\left(t_{k}\right)-4 y\left(t_{k-1}\right)+y\left(t_{k-2}\right)}{2 h}
$$

- Note that this is also equal to

$$
\frac{3 y\left(t_{k}\right)-4 y\left(t_{k}-h\right)+y\left(t_{k}-2 h\right)}{2 h}
$$

- Question: What is the error?



## Backward divided difference

- Suppose we substitute $h$ with $-2 h$ in the Taylor series:

$$
\begin{gathered}
y\left(t_{k}+(-2 h)\right)=y\left(t_{k}\right)+y^{(1)}\left(t_{k}\right)(-2 h)+\frac{1}{2} y^{(2)}\left(t_{k}\right)(-2 h)^{2}+\frac{1}{6} y^{(3)}(\tau)(-2 h)^{3} \\
- \text { Now, }(-2 h)^{2}=4 h^{2} \operatorname{but}(-2 h)^{3}=-8 h^{3} \\
y\left(t_{k}-2 h\right)=y\left(t_{k}\right)+y^{(1)}\left(t_{k}\right)(-2 h)+\frac{1}{2} y^{(2)}\left(t_{k}\right)\left(4 h^{2}\right)+\frac{1}{6} y^{(3)}(\tau)\left(-8 h^{3}\right) \\
y\left(t_{k}-2 h\right)=y\left(t_{k}\right)-2 y^{(1)}\left(t_{k}\right) h+2 y^{(2)}\left(t_{k}\right) h^{2}-\frac{4}{3} y^{(3)}(\tau) h^{3}
\end{gathered}
$$

- For this, $t_{k}-2 h<\tau<t_{k}$


## Backward divided difference

- In this expression, we have both $-h$ and $-2 h$ :

$$
\frac{3 y\left(t_{k}\right)-4 y\left(t_{k}-h\right)+y\left(t_{k}-2 h\right)}{2 h}
$$

- Let's write the two Taylor series:

$$
\begin{aligned}
y\left(t_{k}-h\right) & =y\left(t_{k}\right)-y^{(1)}\left(t_{k}\right) h+\frac{1}{2} y^{(2)}\left(t_{k}\right) h^{2}-\frac{1}{6} y^{(3)}\left(\tau_{-1}\right) h^{3} \\
y\left(t_{k}-2 h\right) & =y\left(t_{k}\right)-2 y^{(1)}\left(t_{k}\right) h+2 y^{(2)}\left(t_{k}\right) h^{2}-\frac{4}{3} y^{(3)}\left(\tau_{-2}\right) h^{3} \\
-4 y\left(t_{k}-h\right)+y\left(t_{k}-2 h\right) & =-3 y\left(t_{k}\right)+2 y^{(1)}\left(t_{k}\right) h+\frac{2}{3} y^{(3)}\left(\tau_{-1}\right) h^{3}-\frac{4}{3} y^{(3)}\left(\tau_{-2}\right) h^{3} \\
& =-3 y\left(t_{k}\right)+2 y^{(1)}\left(t_{k}\right) h-\frac{2}{3}\left(2 y^{(3)}\left(\tau_{-2}\right)-y^{(3)}\left(\tau_{-1}\right)\right) h^{3}
\end{aligned}
$$

## Backward divided difference

- Now, generally, analyzing the error is a little more difficult:

$$
-\frac{2}{3}\left(2 y^{(3)}\left(\tau_{-2}\right)-y^{(3)}\left(\tau_{-1}\right)\right) h^{3} \neq-\frac{2}{3} y^{(3)}(\tau) h^{3}
$$

as while we have a weighted average, it is no longer a convex combination

- We can, however, make the following statement:

$$
-\frac{2}{3}\left(2 y^{(3)}\left(\tau_{-2}\right)-y^{(3)}\left(\tau_{-1}\right)\right) h^{3}=-\frac{2}{3} y^{(3)}\left(t_{k}\right) h^{3}+O\left(h^{4}\right)
$$

## Backward divided difference

- Thus, we isolate the derivative to get:

$$
\begin{aligned}
-4 y\left(t_{k}-h\right)+y\left(t_{k}-2 h\right) & =-3 y\left(t_{k}\right)+2 y^{(1)}\left(t_{k}\right) h-\frac{2}{3} y^{(3)}\left(t_{k}\right) h^{3}+O\left(h^{4}\right) \\
y^{(1)}\left(t_{k}\right) & =\frac{3 y\left(t_{k}\right)-4 y\left(t_{k}-h\right)+y\left(t_{k}-2 h\right)}{2 h}+\frac{1}{3} y^{(3)}\left(t_{k}\right) h^{2}+O\left(h^{3}\right)
\end{aligned}
$$

- This formula is $\mathrm{O}\left(h^{2}\right)$


## Backward divided difference

- Suppose we want to approximate the derivative of $\sin (x)$ at $x=1$

| $n$ | $h=2^{-n}$ |  |  |  |  | Approximation |
| ---: | :--- | :---: | :--- | :--- | :--- | :--- |
|  | Error | $-\frac{1}{3} \cos (1) h^{2}$ | Ratio |  |  |  |
| 1 | 0.5 | 0.6067108000068773 | -0.06641 | -0.04503 |  |  |
| 2 | 0.25 | 0.5545669058691116 | -0.01426 | -0.01126 | 0.2148 |  |
| 3 | 0.125 | 0.5435108220116605 | -0.003209 | -0.002814 | 0.2249 |  |
| 4 | 0.0625 | 0.5410561889355545 | -0.0007539 | -0.0007035 | 0.2350 |  |
| 5 | 0.03125 | 0.5404845442853681 | -0.0001822 | -0.0001759 | 0.2417 |  |
| 6 | 0.015625 | 0.5403470744818577 | -0.00004477 | -0.00004397 | 0.2457 |  |
| 7 | 0.0078125 | 0.5403133984220077 | -0.00001109 | -0.00001099 | 0.2478 |  |
| 8 | 0.00390625 | 0.5403050665119196 | -0.000002761 | -0.000002748 | 0.2489 |  |
| 9 | 0.001953325 | 0.5403029444644402 | -0.0000006886 | -0.0000006870 | 0.2494 |  |
| 10 | 0.0009765625 | 0.5403024778212853 | -0.0000001720 | -0.0000001718 | 0.2497 |  |
|  |  | 0.540302305868140 |  |  |  |  |

## Comparison

- Let us compare these two formulas:

$$
\begin{aligned}
f^{(1)}\left(x_{k}\right) & =\frac{f\left(x_{k}+h\right)-f\left(x_{k}-h\right)}{2 h}-\frac{1}{6} f^{(3)}(\xi) h^{2} \\
y^{(1)}\left(t_{k}\right) & =\frac{3 y\left(t_{k}\right)-4 y\left(t_{k}-h\right)+y\left(t_{k}-2 h\right)}{2 h}+\frac{1}{3} y^{(3)}\left(t_{k}\right) h^{2}+O\left(h^{3}\right)
\end{aligned}
$$

- The centered divided difference formula has half the errors
- It uses information closer to the point at which we're estimating


## Approximating the $2^{\text {nd }}$ derivative

- We will now approximate the second derivative using similar techniques:
- Find interpolating quadratic polynomials
- Differentiate twice
- Evaluate at a point


## Centered divided difference

- Recall how we found the interpolating cubic

$$
\frac{f\left(x_{k+1}\right)-2 f\left(x_{k}\right)+f\left(x_{k-1}\right)}{2 h^{2}} x^{2}+\frac{f\left(x_{k+1}\right)-f\left(x_{k-1}\right)}{2 h} x+f\left(x_{k}\right)
$$

- Differentiating this twice with respect to $x$, we get

$$
\frac{f\left(x_{k+1}\right)-2 f\left(x_{k}\right)+f\left(x_{k-1}\right)}{h^{2}}
$$

- You will note this is already a constant



## Centered divided difference

- Now we have a formula for the second derivative:

$$
\frac{f\left(x_{k+1}\right)-2 f\left(x_{k}\right)+f\left(x_{k-1}\right)}{h^{2}}
$$

- Note that this is also equal to

$$
\frac{f\left(x_{k}+h\right)-2 f\left(x_{k}\right)+f\left(x_{k}-h\right)}{h^{2}}
$$

- Question: What is the error?



## Centered divided difference

- Once again, this is the formula with $+h$ and $-h$ :

$$
\frac{f\left(x_{k}+h\right)-2 f\left(x_{k}\right)+f\left(x_{k}-h\right)}{h^{2}}
$$

- Let's write the two Taylor series:

$$
\begin{aligned}
& f\left(x_{k}+h\right)=f\left(x_{k}\right)+f^{(1)}\left(x_{k}\right) h+\frac{1}{2} f^{(2)}\left(x_{k}\right) h^{2}+\frac{1}{6} f^{(2)}\left(x_{k}\right) h^{3}+\frac{1}{24} f^{(4)}\left(\xi_{+}\right) h^{4} \\
& f\left(x_{k}-h\right)=f\left(x_{k}\right)-f^{(1)}\left(x_{k}\right) h+\frac{1}{2} f^{(2)}\left(x_{k}\right) h^{2}-\frac{1}{6} f^{(3)}\left(x_{k}\right) h^{3}+\frac{1}{24} f^{(4)}\left(\xi_{-}\right) h^{4} \\
& f\left(x_{k}+h\right)+f\left(x_{k}-h\right)=2 f\left(x_{k}\right)+f^{(2)}\left(x_{k}\right) h^{2}+\frac{1}{24} f^{(4)}\left(\xi_{+}\right) h^{4}+\frac{1}{24} f^{(4)}\left(\xi_{-}\right) h^{4} \\
& = \\
& =2 f\left(x_{k}\right)+f^{(2)}\left(x_{k}\right) h^{2}+\frac{1}{12}\left(\frac{1}{2} f^{(4)}\left(\xi_{+}\right)+\frac{1}{2} f^{(4)}\left(\xi_{-}\right)\right) h^{4} \\
& =
\end{aligned}
$$

## Centered divided difference

- Thus, we isolate the second derivate to get:

$$
\begin{aligned}
& f\left(x_{k}+h\right)+f\left(x_{k}-h\right)=2 f\left(x_{k}\right)+f^{(2)}(x) h^{2}+\frac{1}{12} f^{(4)}(\xi) h^{4} \\
& \qquad f^{(2)}(x)=\frac{f\left(x_{k}+h\right)-2 f\left(x_{k}\right)+f\left(x_{k}-h\right)}{h^{2}}-\frac{1}{12} f^{(4)}(\xi) h^{2} \\
& \quad x_{k}-h<\xi<x_{k}+h
\end{aligned}
$$

## Centered divided difference

- Let's approximate the second derivative of $\sin (x)$ at $x=1$

| $n$ | $h=2^{-n}$ | Approximation | Error | $-\frac{1}{24} \sin (1) h^{2}$ | Ratio |
| ---: | :--- | :--- | :--- | :--- | :--- |
| 1 | 0.5 | -0.8240857776301422 | -0.01739 | -0.01753 |  |
| 2 | 0.25 | -0.8370974437899648 | -0.004374 | -0.004383 | 0.2516 |
| 3 | 0.125 | -0.8403758899629281 | -0.001095 | -0.001096 | 0.2504 |
| 4 | 0.0625 | -0.8411971041354036 | -0.0002739 | -0.0002739 | 0.2501 |
| 5 | 0.03125 | -0.8414025079530347 | -0.00006848 | -0.00006848 | 0.2500 |
| 6 | 0.015625 | -0.8414538651759358 | -0.00001712 | -0.00001712 | 0.2500 |
| 7 | 0.0078125 | -0.8414667048746196 | -0.000004280 | -0.000004270 | 0.2500 |
| 8 | 0.00390625 | -0.8414699148197542 | -0.000001070 | -0.000001070 | 0.2500 |
| 9 | 0.001953125 | -0.8414707173069473 | -0.0000002675 | -0.0000002675 | 0.2500 |
| 10 | 0.0009765625 | -0.8414709179196507 | -0.00000006689 | -0.00000006687 | 0.2500 |

## Backward divided difference

- Recall how we found the interpolating cubic

$$
\frac{y\left(t_{k}\right)-2 y\left(t_{k-1}\right)+y\left(t_{k-2}\right)}{2 h^{2}} t^{2}+\frac{3 y\left(t_{k}\right)-4 y\left(t_{k-1}\right)+y\left(t_{k-2}\right)}{2 h} t+y\left(t_{k}\right)
$$

- Differentiating this twice with respect to $t$, we get

$$
\frac{y\left(t_{k}\right)-2 y\left(t_{k-1}\right)+y\left(t_{k-2}\right)}{h^{2}}
$$

- As before, this is a constant



## Backward divided difference

- Now we have an alternate formula:

$$
\frac{y\left(t_{k}\right)-2 y\left(t_{k-1}\right)+y\left(t_{k-2}\right)}{h^{2}}
$$

- Note that this is also equal to

$$
\frac{y\left(t_{k}\right)-2 y\left(t_{k}-h\right)+y\left(t_{k}-2 h\right)}{h^{2}}
$$

- Question: What is the error?


## Backward divided difference

- In this expression, we have $-h$ and $-2 h$ :

$$
\frac{y\left(t_{k}\right)-2 y\left(t_{k}-h\right)+y\left(t_{k}-2 h\right)}{h^{2}}
$$

- Let's write the two Taylor series:

$$
\begin{aligned}
& y\left(t_{k}-h\right)=y\left(t_{k}\right)-y^{(1)}\left(t_{k}\right) h+\frac{1}{2} y^{(2)}\left(t_{k}\right) h^{2}-\frac{1}{6} y^{(3)}\left(\tau_{-1}\right) h^{3} \\
& y\left(t_{k}-2 h\right)=y\left(t_{k}\right)-2 y^{(1)}\left(t_{k}\right) h+2 y^{(2)}\left(t_{k}\right) h^{2}-\frac{4}{3} y^{(3)}\left(\tau_{-2}\right) h^{3} \\
& -2 y\left(t_{k}-h\right)+y\left(t_{k}-2 h\right)=-y\left(t_{k}\right)+y^{(2)}\left(t_{k}\right) h^{2}+\frac{1}{3} y^{(3)}\left(\tau_{-1}\right) h^{3}-\frac{4}{3} y^{(3)}\left(\tau_{-2}\right) h^{3} \\
& =-y\left(t_{k}\right)+y^{(2)}\left(t_{k}\right) h^{2}-\left(\frac{4}{3} y^{(3)}\left(\tau_{-2}\right)-\frac{1}{3} y^{(3)}\left(\tau_{-1}\right)\right) h^{3} \\
& =-y\left(t_{k}\right)+y^{(2)}\left(t_{k}\right) h^{2}-y^{(3)}\left(t_{k}\right) h^{3}+O\left(h^{4}\right)
\end{aligned}
$$

## Backward divided difference

- Thus, we isolate the derivate to get:

$$
\begin{aligned}
&-2 y\left(t_{k}-h\right)+y\left(t_{k}-2 h\right)=-y\left(t_{k}\right)+y^{(2)}\left(t_{k}\right) h^{2}-y^{(3)}\left(t_{k}\right) h^{3}+O\left(h^{4}\right) \\
& y^{(2)}\left(t_{k}\right)=\frac{y\left(t_{k}\right)-2 y\left(t_{k}-h\right)+y\left(t_{k}-2 h\right)}{h^{2}}+y^{(3)}\left(t_{k}\right) h+O\left(h^{2}\right)
\end{aligned}
$$

- This formula only $\mathrm{O}(h)$


## Backward divided difference

- Let's approximate the second derivative of $\sin (x)$ at $x=1$

| $n$ | $h=2^{-n}$ | Approximation | Error | $-\cos (1) h$ | Ratio |
| :--- | :--- | :--- | :--- | :--- | :--- |
| 1 | 0.5 | -0.469520369602038 | -0.3720 | -0.2701 |  |
| 2 | 0.25 | -0.678095946153100 | -0.1634 | -0.1351 | 0.4392 |
| 3 | 0.125 | -0.7665446170127055 | -0.07493 | -0.06754 | 0.4586 |
| 4 | 0.0625 | -0.8058187462303863 | -0.03565 | -0.03377 | 0.4758 |
| 5 | 0.03125 | -0.8241113750362956 | -0.01736 | -0.01688 | 0.4869 |
| 6 | 0.015625 | -0.8329094424607320 | -0.008562 | -0.008442 | 0.4932 |
| 7 | 0.0078125 | -0.8372199781206291 | -0.004251 | -0.004221 | 0.4965 |
| 8 | 0.00390625 | -0.8393529470995418 | -0.002118 | -0.002111 | 0.4982 |
| 9 | 0.001953125 | -0.8404138353944290 | -0.001057 | -0.001055 | 0.4991 |
| 10 | 0.0009765625 | -0.8409428779268637 | -0.0005281 | -0.0005276 | 0.4996 |

## Backward divided difference

- If you want a backward divided-difference formula for approximating the second derivative that is $\mathrm{O}\left(h^{2}\right)$, you must resort to interpolating four points
- Again, the weighted average is not a convex combination, so we must assume the $4^{\text {th }}$ derivative is approximately smooth

$$
y^{(2)}\left(t_{k}\right)=\frac{2 y\left(t_{k}\right)-5 y\left(t_{k}-h\right)+4 y\left(t_{k}-2 h\right)-y\left(t_{k}-3 h\right)}{h^{2}}+\frac{11}{12} y^{(4)}\left(t_{k}\right) h^{2}+O\left(h^{3}\right)
$$

## Backward divided difference

- Let's approximate the second derivative of $\sin (x)$ at $x=1$

| $n$ | $h=2^{-n}$ | Approximation | Error | $\frac{11}{12} \sin (1) h^{2}$ | Ratio |
| :---: | :--- | :--- | :--- | :--- | :--- | :--- |
| 1 | 0.5 | -0.9390407392040760 | 0.09757 | 0.1928 |  |
| 2 | 0.25 | -0.8792581654174150 | 0.03779 | 0.04821 | 0.3873 |
| 3 | 0.125 | -0.8523375623339433 | 0.01087 | 0.01205 | 0.2876 |
| 4 | 0.0625 | -0.8443438090947666 | 0.002873 | 0.003013 | 0.2644 |
| 5 | 0.03125 | -0.8422072387249955 | 0.0007363 | 0.0007533 | 0.2563 |
| 6 | 0.015625 | -0.8416572080732294 | 0.0001862 | 0.0001883 | 0.2529 |
| 7 | 0.0078125 | -0.8415178044597269 | 0.00004682 | 0.00004708 | 0.2514 |
| 8 | 0.00390625 | -0.8414827223168686 | 0.00001174 | 0.00001177 | 0.2507 |
| 9 | 0.001953125 | -0.8414739231229760 | 0.000002938 | 0.000002942 | 0.2503 |
| 10 | 0.0009765625 | -0.8414717204868793 | 0.0000007357 | 0.0000007356 | 0.2504 |

## Summary of $\mathrm{O}\left(h^{2}\right)$ approximations

- Comparing these:

$$
\begin{aligned}
& f^{(1)}\left(x_{k}\right)=\frac{f\left(x_{k}+h\right)-f\left(x_{k}-h\right)}{2 h}-\frac{1}{6} f^{(3)}(\xi) h^{2} \\
& y^{(1)}\left(t_{k}\right)=\frac{3 y\left(t_{k}\right)-4 y\left(t_{k}-h\right)+y\left(t_{k}-2 h\right)}{2 h}+\frac{1}{3} y^{(3)}\left(t_{k}\right) h^{2}+O\left(h^{3}\right) \\
& f^{(2)}(x)=\frac{f\left(x_{k}+h\right)-2 f\left(x_{k}\right)+f\left(x_{k}-h\right)}{h^{2}}-\frac{1}{12} f^{(4)}(\xi) h^{2} \\
& y^{(2)}\left(t_{k}\right)=\frac{2 y\left(t_{k}\right)-5 y\left(t_{k}-h\right)+4 y\left(t_{k}-2 h\right)-y\left(t_{k}-3 h\right)}{h^{2}}+\frac{11}{12} y^{(4)}\left(t_{k}\right) h^{2}+O\left(h^{3}\right)
\end{aligned}
$$

## Summary

- Following this topic, you now
- Are aware of numerous approximations of the derivative and second derivative
- Understand that the error should likely be $\mathrm{O}\left(h^{2}\right)$ to be reasonable
- Have seen $\mathrm{O}\left(h^{2}\right)$ approximations that are both centered and backward
- Have observed how these formulas actually work by looking at examples


## References

[1] https://en.wikipedia.org/wiki/Taylor_series

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## Colophon

These slides were prepared using the Cambria typeface. Mathematical equations use Times New Roman, and source code is presented using Consolas. Mathematical equations are prepared in MathType by Design Science, Inc.
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