Differentiation

Forward, Backward, and Centered Difference Schemes

Ashley Gannon

Fall 2020



Deriving the Forward and Backward Difference Schemes



If we expand the Taylor series forward, we have that

■ The zero-order Taylor-series approximation is

$$f(x_{i+1}) \cong f(x_i)$$



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■ The first-order Taylor-series approximation is

$$f(x_{i+1}) \cong f(x_i) + \frac{h}{1!}f'(x_i)$$



4/41

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■ The first-order Taylor-series approximation is

$$f(x_{i+1}) \cong f(x_i) + \frac{h}{1!}f'(x_i)$$

■ The second-order Taylor series approximation is

$$f(x_{i+1}) \cong f(x_i) + \frac{h}{1!}f'(x_i) + \frac{h^2}{2!}f''(x_i)$$



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The second-order Taylor series approximation is

$$f(x_{i+1}) \cong f(x_i) + \frac{h}{1!}f'(x_i) + \frac{h^2}{2!}f''(x_i)$$

■ If we continue this trend, the n^{th} -order Taylor series approximate can be written as

$$f(x_{i+1}) \cong f(x_i) + \frac{h}{1!}f'(x_i) + \frac{h^2}{2!}f''(x_i) + \frac{h^3}{3!}f^{(3)}(x_i) + \dots + \frac{h^n}{n!}f^{(n)}(x_i)$$



Approximating Derivatives - Forward finite difference

Taylor series can be used to approximate derivatives. If we wish to approximate the first derivative, we rearrange the first-order Taylor series approximation

$$f(x_{i+1}) \cong f(x_i) + \frac{h}{1!}f'(x_i),$$

to solve for the derivative, $f'(x_i)$

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



7/41

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to solve for the derivative, $f'(x_i)$

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

If we have equispaced data, we can think of x_{i+1} as being the x located distance h away from x_i . We can rewrite out formula as

$$f'(x) = \frac{f(x+h) - f(x)}{h}$$



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If we have equispaced data, we can think of x_{i+1} as being the x located distance h away from x_i . We can rewrite out formula as

$$f'(x) = \frac{f(x+h) - f(x)}{h}$$

This is the *forward difference* scheme and it's approximation is O(h) accurate.



If we expand the Taylor series backward, we have that

■ The zero-order Taylor-series approximation is

$$f(x_{i-1}) \cong f(x_i)$$



If we expand the Taylor series backward, we have that

■ The zero-order Taylor-series approximation is

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■ The first-order Taylor-series approximation is

$$f(x_{i-1}) \cong f(x_i) - \frac{h}{1!}f'(x_i)$$



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$$f(x_{i-1}) \cong f(x_i) - \frac{h}{1!}f'(x_i)$$

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$$f(x_{i-1}) \cong f(x_i) - \frac{h}{1!}f'(x_i) + \frac{h^2}{2!}f''(x_i)$$



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The second-order Taylor series approximation is

$$f(x_{i-1}) \cong f(x_i) - \frac{h}{1!}f'(x_i) + \frac{h^2}{2!}f''(x_i)$$

■ The third-order Taylor series approximate can be written as

$$f(x_{i-1}) \cong f(x_i) - \frac{h}{1!}f'(x_i) + \frac{h^2}{2!}f''(x_i) - \frac{h^3}{3!}f^{(3)}(x_i) + \dots$$



Ashley Gannon Lecture 25 Fall 2020 13 / 41

Approximating Derivatives - Backward difference

If we again wish to approximate the first derivative, we rearrange the first-order Taylor series approximation

$$f(x_{i-1}) \cong f(x_i) - \frac{h}{1!}f'(x_i),$$

to solve for the derivative, $f'(x_i)$

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



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

If we have equispaced data, we can think of x_{i+1} as being the x located distance h away from x_i . We can rewrite out formula as

$$f'(x) = \frac{f(x) - f(x - h)}{h}$$



15 / 41

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If we have equispaced data, we can think of x_{i+1} as being the x located distance h away from x_i . We can rewrite out formula as

$$f'(x) = \frac{f(x) - f(x - h)}{h}$$

This is the *backward difference* scheme and it's approximation is O(h) accurate.



16 / 41

Use forward and backward difference approximations to estimate the first derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at x = 0.5, using a step size h = 0.5. Note that the derivative of this function is

$$f'(x) = -0.4x^3 - 0.45x^2 - x - 0.25,$$
 $f'(0.5) = -0.9125$



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Let's start with the forward difference scheme.

We have

$$x = 0.5,$$
 $f(x) = 0.925$
 $x + h = 1,$ $f(x + h) = 0.2$



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Plugging this into our forward difference scheme.

$$f'(x) = \frac{f(x+h) - f(x)}{h}$$

we have

$$f'(0.5) \approx \frac{0.2 - 0.925}{0.5}$$

$$\approx -1.45$$



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Plugging this into our forward difference scheme,

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we have

$$f'(0.5) \approx \frac{0.2 - 0.925}{0.5}$$

 ≈ -1.45

20 / 41

The percent relative error is 58.9%.

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 $f'(0.5) = -0.9125$

Now, applying the backward difference scheme.

We have

$$x = 0.5,$$
 $f(x) = 0.925$
 $x - h = 0,$ $f(x - h) = 1.2$



21/41

Use forward and backward difference approximations to estimate the first derivative of

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Now, applying the backward difference scheme.

We have

$$x = 0.5,$$
 $f(x) = 0.925$
 $x - h = 0,$ $f(x - h) = 1.2$

Plugging this into our backward difference scheme,

$$f'(x) = \frac{f(x) - f(x - h)}{h}$$

we have

$$f'(0.5) \approx \frac{0.925 - 1.2}{0.5}$$
$$\approx -0.55$$



22 / 41

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Plugging this into our backward difference scheme,

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we have

$$f'(0.5) \approx \frac{0.925 - 1.2}{0.5}$$

 ≈ -0.55

23 / 41

The percent relative error is 39.7%.

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Use forward and backward difference approximations to estimate the first derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at x = 0.5, using a step size h = 0.25. Note that the derivative of this function is

$$f'(x) = -0.4x^3 - 0.45x^2 - x - 0.25,$$
 $f'(0.5) = -0.9125$

Starting again with the forward difference scheme.

We have

$$x = 0.5,$$
 $f(x) = 0.925$
 $x + h = 0.75,$ $f(x + h) = 0.63632813$



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Use forward and backward difference approximations to estimate the first derivative of

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Starting again with the forward difference scheme.

We have

$$x = 0.5,$$
 $f(x) = 0.925$
 $x + h = 0.75,$ $f(x + h) = 0.63632813$

Plugging this into our forward difference scheme,

$$f'(x) = \frac{f(x+h) - f(x)}{h}$$

we have

$$f'(0.5) \approx \frac{0.63632813 - 0.925}{0.5}$$
$$\approx -1.155$$



Use forward and backward difference approximations to estimate the first derivative of

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at x = 0.5, using a step size h = 0.25. Note that the derivative of this function is

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Starting again with the forward difference scheme.

We have

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 $f(x) = 0.925$
 $x + h = 0.75,$ $f(x + h) = 0.63632813$

Plugging this into our forward difference scheme,

$$f'(x) = \frac{f(x+h) - f(x)}{h}$$

we have

$$f'(0.5) \approx \frac{0.63632813 - 0.925}{0.5}$$
$$\approx -1.155$$

The percent relative error is 26.5%. Roughly half of what it was when h = 0.5!



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Use forward and backward difference approximations to estimate the first derivative of

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 $f'(0.5) = -0.9125$

Now, applying the backward difference scheme.

We have

$$x = 0.5,$$
 $f(x) = 0.925$
 $x - h = 0.25,$ $f(x - h) = 1.10351563$



Use forward and backward difference approximations to estimate the first derivative of

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Now, applying the backward difference scheme.

We have

$$x = 0.5,$$
 $f(x) = 0.925$
 $x - h = 0.25,$ $f(x - h) = 1.10351563$

Plugging this into our backward difference scheme,

$$f'(x) = \frac{f(x) - f(x - h)}{h}$$

we have

$$f'(0.5) \approx \frac{0.925 - 1.10351563}{0.5}$$
$$\approx -0.714$$



Use forward and backward difference approximations to estimate the first derivative of

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at x = 0.5, using a step size h = 0.5. Note that the derivative of this function is

$$f'(x) = -0.4x^3 - 0.45x^2 - x - 0.25,$$
 $f'(0.5) = -0.9125$

Now, applying the backward difference scheme.

We have

$$x = 0.5,$$
 $f(x) = 0.925$
 $x - h = 0.25,$ $f(x - h) = 1.10351563$

Plugging this into our backward difference scheme,

$$f'(x) = \frac{f(x) - f(x - h)}{h}$$

we have

$$f'(0.5) \approx \frac{0.925 - 1.10351563}{0.5}$$
$$\approx -0.714$$

The percent relative error is 21.1%, roughly half of the error when h = 0.5.



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Example Forward and Backward difference summary

Since both the forward and backward schemes are $\mathcal{O}(h)$ accurate, when we halve h, we expect to halve the error - which is what we observed in this example.



Deriving the Centered Difference Scheme



Approximating Derivatives - Centered Difference

There's a third way to approximate the first derivative using Taylor series.

If we subtract the third-order backward Taylor series expansion

$$f(x_{i-1}) = f(x_i) - \frac{h}{1!}f'(x_i) + \frac{h^2}{2!}f''(x_i) - \frac{h^3}{3!}f^{(3)}(x_i)$$

from the third-order forward Taylor series expansion

$$f(x_{i+1}) = f(x_i) + \frac{h}{1!}f'(x_i) + \frac{h^2}{2!}f''(x_i) + \frac{h^3}{3!}f^{(3)}(x_i)$$



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Approximating Derivatives - Centered Difference

We have

$$f(x_{i+1}) - f(x_{i-1}) = f(x_i) + \frac{h}{1!}f'(x_i) + \frac{h^2}{2!}f''(x_i) + \frac{h^3}{3!}f^{(3)}(x_i)$$

$$-\left(f(x_i) - \frac{h}{1!}f'(x_i) + \frac{h^2}{2!}f''(x_i) - \frac{h^3}{3!}f^{(3)}(x_i)\right)$$

$$f(x_{i+1}) - f(x_{i-1}) = 2hf'(x_i) + \frac{2h^3}{3!}f^{(3)}(x_i)$$

Rearranging for $f'(x_i)$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} - \frac{h^2}{6}f^{(3)}(x_i)$$

which can be re-written as

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \mathcal{O}(h^2)$$

This is the *centered difference* scheme and has an accuracy of $\mathcal{O}(h^2)$.



Example Centered difference: h = 0.5

Deriving the Forward and Backward Difference Schemes

Use a centered difference approximation to estimate the first derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at x = 0.5, using a step size h = 0.5. Note that the derivative of this function is

$$f'(x) = -0.4x^3 - 0.45x^2 - x - 0.25,$$
 $f'(0.5) = -0.9125$

Now, applying the centered difference scheme.

We have

$$x + h = 1,$$
 $f(x + h) = 0.2$

$$x - h = 0,$$
 $f(x - h) = 1.2$



Ashley Gannon Lecture 25 Fall 2020 34 / 41 Deriving the Forward and Backward Difference Schemes

Use a centered difference approximation to estimate the first derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at x = 0.5, using a step size h = 0.5. Note that the derivative of this function is

$$f'(x) = -0.4x^3 - 0.45x^2 - x - 0.25,$$
 $f'(0.5) = -0.9125$

Now, applying the centered difference scheme.

We have

$$x + h = 1,$$
 $f(x + h) = 0.2$
 $x - h = 0.$ $f(x - h) = 1.2$

Plugging this into our centered difference scheme,

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h}$$

we have

$$f'(0.5) \approx \frac{0.2 - 1.2}{1}$$



Deriving the Forward and Backward Difference Schemes

Use a centered difference approximation to estimate the first derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at x = 0.5, using a step size h = 0.5. Note that the derivative of this function is

$$f'(x) = -0.4x^3 - 0.45x^2 - x - 0.25,$$
 $f'(0.5) = -0.9125$

Now, applying the centered difference scheme.

We have

$$x + h = 1,$$
 $f(x + h) = 0.2$
 $x - h = 0,$ $f(x - h) = 1.2$

Plugging this into our centered difference scheme,

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h}$$

we have

$$f'(0.5) \approx \frac{0.2 - 1.2}{1}$$
$$\approx -1$$

36 / 41

The percent relative error is 9.6%.

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Example Centered difference: h = 0.25

Use a centered difference approximation to estimate the first derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at x = 0.5, using a step size h = 0.25. Note that the derivative of this function is

$$f'(x) = -0.4x^3 - 0.45x^2 - x - 0.25,$$
 $f'(0.5) = -0.9125$

Now, applying the centered difference scheme.

We have

$$x + h = 0.75$$
, $f(x + h) = 0.63632813$
 $x - h = 0.25$, $f(x - h) = 1.10351563$

Plugging this into our centered difference scheme,

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h}$$

we have

$$f'(0.5) \approx \frac{0.63632813 - 1.10351563}{0.5}$$
$$\approx -0.934$$

37/41

Fall 2020

The percent relative error is 2.4%, a quarter of what is was when h=0.5.

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Lecture 25

Example centered difference summary

Since the centered difference scheme is $\mathcal{O}(h^2)$ accurate, when we halve h, we expect to quarter the error - which is what we observed in this example.

$$\left(\frac{h}{2}\right)^2 = \frac{h^2}{4}$$



Programming Finite Difference Methods



Let's code them!

We'll write 3 routines

```
forwardDifference(double x, double h)
   return (f(x + h) - f(x)) / h
```

backwardDifference(double x, double h)
return
$$(f(x) - f(x - h)) / h$$



centeredDifference(double x, double h) return
$$(f(x + h) - f(x - h)) / (2 * h)$$

And test it on the example

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$



40 / 41

Sign-off Activity

Add these functions to your library using the following syntax:

```
forwardDifference(double x, double h, double (*f)(double x)
backwardDifference(double x, double h, double (*f)(double x))
centeredDifference(double x, double h, double (*f)(double x))
```

