Differentiation

Forward, Backward, and Centered Difference Schemes

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Fall 2020

Deriving the Forward and Backward Difference Schemes

Taylor Series

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

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

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, $f'(x_i)$

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

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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

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

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

This is the *forward difference* scheme and it's approximation is $\mathcal{O}(h)$ accurate.

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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

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

Approximating Derivatives - Backward difference

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

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

This is the *backward difference* scheme and it's approximation is $\mathcal{O}(h)$ accurate.

Example Forward and Backward difference: $h = 0.5$

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

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

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Let's start with the forward difference scheme.

We have

$$\begin{aligned} x = 0.5, &\qquad f(x) = 0.925 \\ x + h = 1, &\qquad f(x+h) = 0.2 \end{aligned}$$

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Plugging this into our forward difference scheme,

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

we have

$$\begin{aligned} f'(0.5) &\approx \frac{0.2 - 0.925}{0.5} \\ &\approx -1.45 \end{aligned}$$

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The percent relative error is 58.9%.

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Now, applying the backward difference scheme.

We have

$$\begin{aligned} x &= 0.5, & f(x) &= 0.925 \\ x - h &= 0, & f(x-h) &= 1.2 \end{aligned}$$

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Now, applying the backward difference scheme.

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$$\begin{aligned} x &= 0.5, & f(x) &= 0.925 \\ x - h &= 0, & f(x-h) &= 1.2 \end{aligned}$$

Plugging this into our backward difference scheme,

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

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$$\begin{aligned} f'(0.5) &\approx \frac{0.925 - 1.2}{0.5} \\ &\approx -0.55 \end{aligned}$$

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The percent relative error is 39.7%.

Example Forward and Backward difference: $h = 0.25$

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Starting again with the forward difference scheme.

We have

$$\begin{aligned} x &= 0.5, & f(x) &= 0.925 \\ x + h &= 0.75, & f(x+h) &= 0.63632813 \end{aligned}$$

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Plugging this into our forward difference scheme,

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

we have

$$\begin{aligned} f'(0.5) &\approx \frac{0.63632813 - 0.925}{0.5} \\ &\approx -1.155 \end{aligned}$$

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

we have

$$\begin{aligned} f'(0.5) &\approx \frac{0.63632813 - 0.925}{0.5} \\ &\approx -1.155 \end{aligned}$$

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

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

Now, applying the backward difference scheme.

We have

$$\begin{aligned} x &= 0.5, & f(x) &= 0.925 \\ x - h &= 0.25, & f(x-h) &= 1.10351563 \end{aligned}$$

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Now, applying the backward difference scheme.

We have

$$\begin{aligned} x &= 0.5, & f(x) &= 0.925 \\ x - h &= 0.25, & f(x-h) &= 1.10351563 \end{aligned}$$

Plugging this into our backward difference scheme,

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

we have

$$\begin{aligned} f'(0.5) &\approx \frac{0.925 - 1.10351563}{0.5} \\ &\approx -0.714 \end{aligned}$$

Example Forward and Backward difference: $h = 0.25$

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

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Now, applying the backward difference scheme.

We have

$$\begin{aligned} x &= 0.5, & f(x) &= 0.925 \\ x - h &= 0.25, & f(x-h) &= 1.10351563 \end{aligned}$$

Plugging this into our backward difference scheme,

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

we have

$$\begin{aligned} f'(0.5) &\approx \frac{0.925 - 1.10351563}{0.5} \\ &\approx -0.714 \end{aligned}$$

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

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

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

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: $h = 0.5$

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

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

Now, applying the centered difference scheme.

We have

$$\begin{aligned} x + h &= 1, \qquad & f(x+h) &= 0.2 \\ x - h &= 0, \qquad & f(x-h) &= 1.2 \end{aligned}$$

Example Centered difference: $h = 0.5$

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

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

Now, applying the centered difference scheme.

We have

$$\begin{aligned} x + h &= 1, & f(x+h) &= 0.2 \\ x - h &= 0, & f(x-h) &= 1.2 \end{aligned}$$

Plugging this into our centered difference scheme,

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

we have

$$\begin{aligned} f'(0.5) &\approx \frac{0.2 - 1.2}{1} \\ &\approx -1 \end{aligned}$$

Example Centered difference: $h = 0.5$

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

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

Now, applying the centered difference scheme.

We have

$$\begin{aligned} x + h &= 1, \qquad & f(x+h) &= 0.2 \\ x - h &= 0, \qquad & f(x-h) &= 1.2 \end{aligned}$$

Plugging this into our centered difference scheme,

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

we have

$$\begin{aligned} f'(0.5) &\approx \frac{0.2 - 1.2}{1} \\ &\approx -1 \end{aligned}$$

The percent relative error is 9.6%.

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

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

Now, applying the centered difference scheme.

We have

$$\begin{aligned} x + h &= 0.75, \qquad & f(x+h) &= 0.63632813 \\ x - h &= 0.25, \qquad & f(x-h) &= 1.10351563 \end{aligned}$$

Plugging this into our centered difference scheme,

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

we have

$$\begin{aligned} f'(0.5) &\approx \frac{0.63632813 - 1.10351563}{0.5} \\ &\approx -0.934 \end{aligned}$$

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

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

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

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))
```