Lecture 24

Numerical Differentiation

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ISC3313 Fall 2021

Introduction

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$$v(t) = \sqrt{\frac{gm}{c_d}} tanh \left(\sqrt{\frac{gc_d}{m}} t \right)$$

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At the beginning of the integration unit, we used calculus to integrate this equation to determine the vertical distance y the jumper has fallen after a time t.

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Now suppose that you were given the reverse problem. That is, you were asked to determine velocity based on the jumper's position as a function of time. Because it is the inverse of integration, differentiation could be used to make the determination:

$$v(t) = \frac{dz(t)}{dt} = \sqrt{\frac{gm}{c_d}} tanh\left(\sqrt{\frac{gc_d}{m}}t\right)$$

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Beyond velocity, you might also be asked to compute the jumper's acceleration. To do this, we could either take the first derivative of velocity, or the second derivative of displacement:

$$a(t) = \frac{dv(t)}{dt} = \frac{d^2y(t)}{dt^2} = gsech^2\left(\sqrt{\frac{gc_d}{m}}t\right)$$

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- Because engineers and scientists must continuously deal with systems and processes that change, calculus is an essential tool of our profession. Standing at the heart of calculus is the mathematical concept of differentiation.
- Mathematically, the derivative, which serves as the fundamental vehicle for differentiation, represents the rate of change of a dependent variable with respect to an independent variable.

Differentiation

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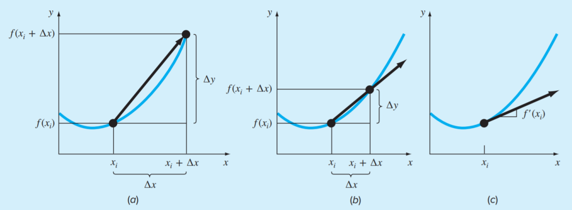

- As depicted in figure (a) above, the mathematical definition of the derivative begins with a difference approximation:

$$\frac{\Delta y}{\Delta x} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

where y and $f(x)$ are alternative representatives for the dependent variable and x is the independent variable.

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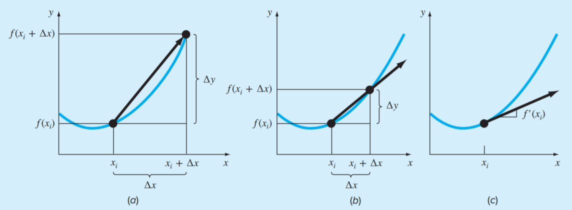

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- If Δx is allowed to approach 0, demonstrated in figures (a) to (c), the difference becomes the derivative

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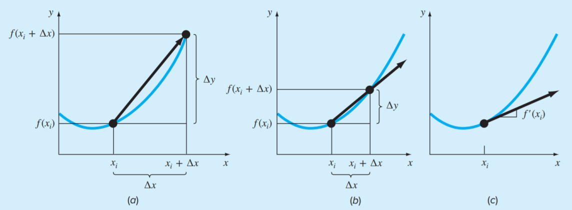

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$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

- The derivative is the slope of the tangent line to to curve at x_i

Taylor Series

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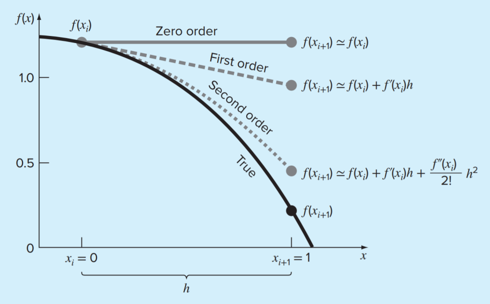
- In essence, the Taylor theorem states that any smooth function can be approximated as a polynomial.
- The Taylor series then provides a means to express this idea mathematically in a form that can be used to generate practical results.



Deriving the Forward and Backward Difference Schemes

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If we expand the Taylor series forward, we have that

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

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

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

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

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

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

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The percent relative error is 58.9%.

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Now, applying the backward difference scheme.

We have

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we have

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The percent relative error is 39.7%.

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

we have

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we have

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

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Now, applying the backward difference scheme.

We have

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

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Plugging this into our backward difference scheme,

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

we have

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

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Now, applying the backward difference scheme.

We have

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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

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

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

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

Plugging this into our centered difference scheme,

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

we have

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

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

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

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))
```