Lecture 18
Differentiation

David Semeraro

University of Illinois at Urbana-Champaign

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Motivation, Simulating Newtonian Particles

http://www.youtube.com/watch?v=TaCmedX7ycs

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- Newton's law: $\mathbf{f} = d(m\mathbf{v})/dt$

$$\mathbf{p}_i = [x_i, y_i, z_i], \quad \mathbf{v}_i[x_i', y_i', z_i']$$

$$\frac{d\mathbf{p}}{dt} = \mathbf{p}_i' = \mathbf{v}_i$$

$$\mathbf{v}_i' = \frac{1}{m_i}\mathbf{f}_i(t)$$

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- Spring Force (Hooke's Law) with damping:

$$\mathbf{f} = -(k_s + k_d\mathbf{d}' \cdot \mathbf{d})\mathbf{d}$$

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- Spring Force (Hooke's Law) with damping:

$$\mathbf{f} = -(k_s + k_d\mathbf{d}' \cdot \mathbf{d})\mathbf{d}$$

- We need to numerically differentiate

Outline

Previous

- Given data y_i at node x_i for $i = 0, \ldots, n$, find a polynomial $p(x)$ that approximates the function.
- That is, approximate a function $f(x)$ with some function (polynomial) $g(x)$

Goals

- Now, try to approximate the derivative of $f'(x)$
- Begin with Taylor series
- Establish accuracy estimates

Problem Statement

Differentiation

- Given $f(x+h)$, $f(x)$ and $f(x-h)$, i.e. f evaluated at evenly spaced points
- Approximate $f'(x)$

Strategy

- Use Taylor Series

$$
\begin{aligned}
f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2}f''(\xi), & \text{for } \xi \in [x, x+h] \\
f(x) &= f(x) \\
f(x-h) &= f(x) - hf'(x) + \frac{h^2}{2}f''(\xi), & \text{for } \xi \in [x-h, x]
\end{aligned}
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\end{aligned}
$$

- Don't worry about ξ, some unknown point in the interval
- Manipulate, add and subtract the above Taylor Series, so that $f'(x)$ is isolated on one side of the equals sign and an approximation to $f'(x)$ is on the other side

First attempt: Taylor

- Taylor series:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(\xi)$$

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$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(\xi)$$

- Thus

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

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- Thus

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

- Called a forward difference because of the “forward” looking evaluation of f at $f(x+h)$

First attempt: Taylor

Forward Difference

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

with

$$error = -\frac{h}{2} f''(\xi) = \mathcal{O}(h)$$

Numerical Test, `diff_fwd.py`

- Consider

$$f(x) = \sin(\pi x) \text{ on } [-1, 1]$$

- Approximate $f'(x) = \pi \cos(\pi x)$ with

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

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- Numerically estimate p for

$$err = |f'_{exact}(x) - f'_{approx}(x)| = ch^p$$

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- Consider two h values, h_k and h_j, giving

$$err_k = c\,(h_k)^p$$
$$err_j = c\,(h_j)^p$$

Numerical Test, `diff_fwd.py`

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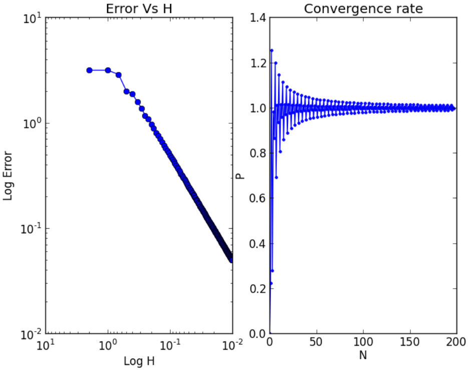
- So

$$p = \frac{\log(err_k/err_j)}{\log(h_k/h_j)}$$

diff_fwd.py



Error Vs H
Log Error
Log H
10^1
10^0
10^{-1}
10^{-2}
Convergence rate
P
N
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
0
50
100
150
200

Visualizing the Differencing

- `http://www.cse.illinois.edu/iem/integration/fda/`
- Choose “1st order forward” and “1st order backward” to experiment with forward and backward differencing

Can we do better?

Forward Difference

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

with

$$error = -\frac{h}{2} f''(\xi) = \mathcal{O}(h)$$

Backward Difference

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

with

$$error = \frac{h}{2} f''(\xi) = \mathcal{O}(h)$$

Can we do better?

- Look at the Forward AND Backward Taylor series together

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f''''(\xi_+)$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f''''(\xi_-)$$

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- Subtract them:

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{h^3}{3}f'''(x) + \mathcal{O}(h^4)$$

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Central Difference

Central Difference

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + \frac{h^2}{6} f'''(x) + \mathcal{O}(h^3)$$

with

$$error = -\frac{h^2}{6} f'''(\xi) = \mathcal{O}(h^2)$$

More Accurate

- Forward and backward differences are $\mathcal{O}(h)$
- Central difference is $\mathcal{O}(h^2)$

Numerical Test, `diff_central.py`

- Consider

$$f(x) = \sin(\pi x) \text{ on } [-1, 1]$$

- Approximate $f'(x) = \pi \cos(\pi x)$ with

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

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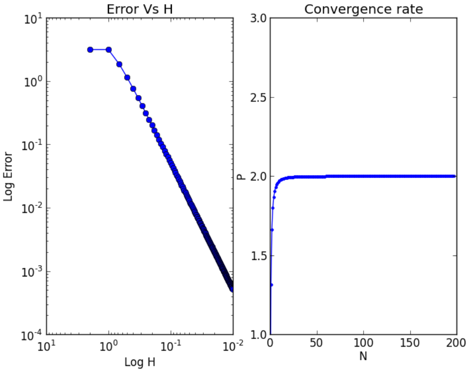
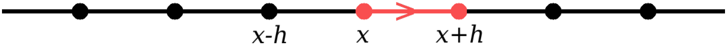
diff_central.py



What's with the Names?

- Forward difference looks forward

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



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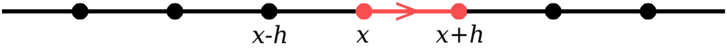
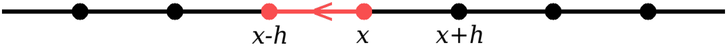


- Backward difference looks backward

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



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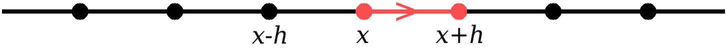

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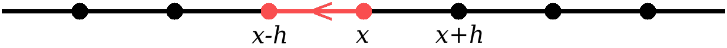
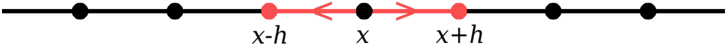


- Central difference centers the subtraction around x

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



Visualizing the Differencing

- `http://www.cse.illinois.edu/iem/integration/fda/`
- Choose “2nd order centered” to experiment with central differencing

Even Smarter?

- Take a look at the central difference:

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

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- We know that

$$\begin{aligned} f'(x) &= \frac{f(x+h) - f(x-h)}{2h} + c_2 h^2 + c_4 h^4 + c_6 h^6 + \dots \\ &= \phi(h) + c_2 h^2 + c_4 h^4 + c_6 h^6 + \dots \\ \phi(h) &= f'(x) - c_2 h^2 - c_4 h^4 - c_6 h^6 - \dots \end{aligned}$$

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- We expect the error to be reduced by 1/4 when h is cut in half.
- Utilize this!

$$\begin{aligned} \phi(h) &= f'(x) - c_2h^2 - c_4h^4 - c_6h^6 - \dots \\ \phi(h/2) &= f'(x) - c_2(h/2)^2 - c_4(h/2)^4 - c_6(h/2)^6 - \dots \end{aligned}$$

Richardson Extrapolation

- Utilize this!

$$\phi(h) = f'(x) - c_2 h^2 - c_4 h^4 - c_6 h^6 - \dots$$
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- Combine these to eliminate the "c_2" term:

$$\phi(h) - 4\phi(h/2) = -3f'(x) - (3/4)c_4h^4 - (15/16)c_6h^6 - \dots$$

Richardson Extrapolation

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- Dividing by -3

$$\phi(h/2) + (1/3)(\phi(h/2) - \phi(h)) = f'(x) + (1/4)c_4h^4 + (5/16)c_6h^6 - \dots$$

Richardson Extrapolation

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- Giving us

Fourth Order Richardson Extrapolation

$$f'(x) = \phi(h/2) + (1/3)(\phi(h/2) - \phi(h)) + \mathcal{O}(h^4)$$

where $\phi(h)$ is the central difference approximation.

Numerical Test, `diff_richard.py`

- Consider
$$f(x) = \sin(\pi x) \text{ on } [-1, 1]$$
- Approximate $f'(x) = \pi\cos(\pi x)$ with
$$f'(x) = \phi(h/2) + (1/3)(\phi(h/2) - \phi(h)) + \mathcal{O}(h^4)$$

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- Consider

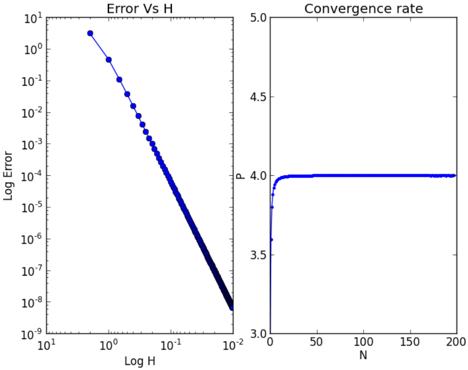
$$f(x) = \sin(\pi x) \text{ on } [-1, 1]$$

- Approximate $f'(x) = \pi\cos(\pi x)$ with

$$f'(x) = \phi(h/2) + (1/3)(\phi(h/2) - \phi(h)) + \mathcal{O}(h^4)$$

- Numerically estimate p as before

diff_central.py



And better?

- We can extend the Richardson extrapolation idea to any order.
- Idea: use $\psi(h) = \phi(h/2) + (1/3)(\phi(h/2) - \phi(h))$ to annihilate the fourth order error term:

And better?

- We can extend the Richardson extrapolation idea to any order.
- Idea: use $\psi(h) = \phi(h/2) + (1/3)(\phi(h/2) - \phi(h))$ to annihilate the fourth order error term:
- Giving us

Sixth Order Richardson Extrapolation

$$f'(x) = \psi(h/2) + (1/15)(\psi(h/2) - \psi(h)) + \mathcal{O}(h^6)$$

where $\psi(h)$ is the fourth order Richardson extrapolation.

Recap

Numerical Differentiation

- Approximate the derivative of $f'(x)$
  - Forward difference, $\mathcal{O}(h)$ error
  - Backward difference, $\mathcal{O}(h)$ error
  - Central difference, $\mathcal{O}(h^2)$ error
  - Richardson extrapolation, $\mathcal{O}(h^4)$ and better error
- Used Taylor series for deriving each method
- Established accuracy estimates using Taylor series