Lecture 21

Numeric Differentiation

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Nov. 12, 2024

Outline

The next topic is numerical differentiation:

- Wrap up linear algebra
- Try to approximate the derivative of $f'(x)$
- Begin with Taylor series
- Establish accuracy estimates

End of Linear Algebra

I just wanted to stick with a theme.

- Least-squares and normal equations: Chapter 4
- Power Method and SVD: Chapter 12

Now back to Chapter 5

And now for something completely different.

Taylor Approximation Recall

Infinite Taylor Series Expansion (exact)

$$f(x) = f(c) + (x-c)f'(c) + \frac{(x-c)^2}{2!}f''(c) + \cdots + \frac{(x-c)^n}{n!}f^{(n)}(c) + \ldots$$

Finite Taylor Series Approximation

$$f(x) \approx f(c) + (x-c)f'(c) + \frac{(x-c)^2}{2!}f''(c) + \cdots + \frac{(x-c)^n}{n!}f^{(n)}(x),$$

Finite Taylor Series Expansion (exact)

$$f(x) = f(c) + (x-c)f'(c) + \cdots + \frac{(x-c)^n}{n!}f^{(n)}(x) + \frac{(x-c)^{n+1}}{(n+1)!}f^{(n+1)}(\xi),$$

but we don't know ξ (it has to be somewhere between x and c) and it could be different for every x.

Confusing notation!

$$f(x) = f(c) + f'(c)(x-c) + f''(c)(x-c)^2/2 + f'''(c)(x-c)^3/3! + \dots$$

c is the "center" of the Taylor Series, x is "some other point".

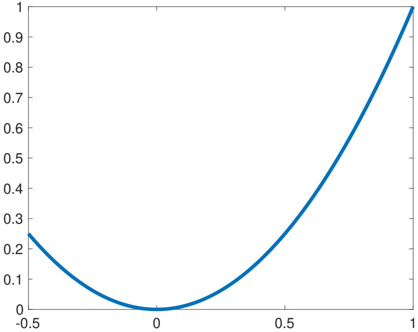
We change labels, now x is the "center" and the "other point" is $x+h$.

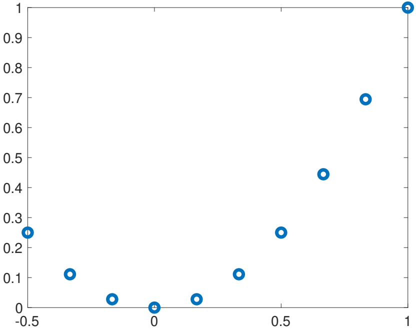
$$f(x+h) = f(x) + f'(x)h + f''(x)h^2/2 + f'''(x)h^3/3! + \dots$$

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

$$
\begin{aligned}
f(x+h) &= f(x) + hf'(x) + \frac{h^2}{2} f''(\xi_1), && \text{for } \xi_1 \in [x, x+h] \\
f(x) &= f(x) \\
f(x-h) &= f(x) - hf'(x) + \frac{h^2}{2} f''(\xi_2), && \text{for } \xi_2 \in [x-h, x]
\end{aligned}
$$

(Known) (Possibly Useful?)

Strategy

- Use Taylor Series

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(Known) (Possibly Useful?)

- Don't worry about ξ, some unknown point in the interval

Strategy

- Use Taylor Series

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(Known) (Possibly Useful?)

- Don't worry about ξ, some unknown point in the interval
- Manipulate, add, and then 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

Notes

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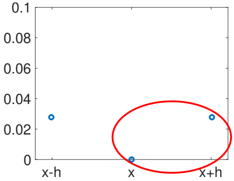
- Called a forward difference because of the “forward” looking evaluation of f at $f(x+h)$



First attempt: Taylor

Forward Difference

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

with truncation error of

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

To cut our error in half, we need to cut h in half. To decrease our error by a factor of 10, decrease h by a factor of 10 ...

Notes

Numerical Test, `diff_fwd.m`, `diff_fwd_plot.m`

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

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

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- Next, we run the code and observe p (`diff_fwd.m` and `diff_fwd_plot.m`)

Can we do better?

Forward Difference

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

with truncation error of

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Backward Difference

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

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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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More Accurate

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

Numerical Test, `diff_central.m`

- Consider

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

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What's with the Names?

- Forward difference looks forward

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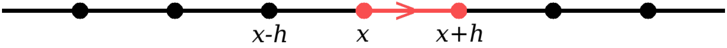

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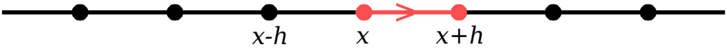

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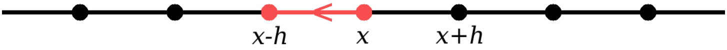

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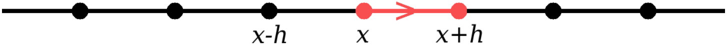

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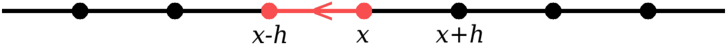
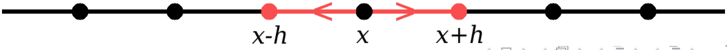


- Central difference centers the subtraction around x

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



Even More Accurate?

In general, if we want an approximation of order $\mathcal{O}(h^k)$, we write down a Taylor series at $k+1$ points, and then add/subtract them cleverly to eliminate all error terms up to order k.

But can we do this systematically so that we don't need to redo a ton of work?

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!

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

Richardson Extrapolation

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

$$\phi(h) - 4\phi(h/2) = -3f'(x) - (3/4)c_4 h^4 - (15/16)c_6 h^6 - \dots$$

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- Dividing by -3

$$\phi(h/2) + (1/3)(\phi(h/2) - \phi(h)) = f'(x) + (1/4)c_4 h^4 + (5/48)c_6 h^6 - \dots$$

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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.

Notes

Numerical Test, `diff_richard.m`

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

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- Next, we run the example code and observe the p value
- By decreasing h to 0.001 and smaller, we actually run out of numerical precision for computing the derivative!

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:

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- 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