10-31-17, Mon

$\boxed{\approx}$

Section 7.1: Numerical differention

The formulas before are good for solving DE's.
The formulas can lead to serious errors when applied to data (function values).

Example: Approximate $f''(x)$

(1) $f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) + \frac{h^4}{4!} f^{(4)}(\xi)$

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

(1)+(2) yields

$$f(x+h) + f(x-h) = 2f(x) + h^2 f''(x) + \frac{h^4}{12} f^{(4)}(\xi)$$

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{h^2}{12} f^{(4)}(\xi).$$

Now let

$$f(x) = \underbrace{\tilde{f}(x)}_{\text{floating point number for } f(x)} + \varepsilon \quad \leftarrow \text{roundoff error}$$

$$f(x) - \tilde{f}(x) = \varepsilon.$$

So the error in the approximation is

$$(*) \quad \underset{(\text{true})}{f''(x)} - \underbrace{\frac{f(x+h) - 2f(x) + f(x-h)}{h^2}}_{\text{approximate}} + \underbrace{\frac{\varepsilon_2 - 2\varepsilon_1 + \varepsilon_0}{h^2}}_{\text{roundoff error}}.$$

where ε_2 is the roundoff for $f(x+h)$, ε_1 is the roundoff for $f(x)$, and ε_0 is the roundoff for $f(x-h)$.

Then,

$$(\ast) = \underbrace{-\frac{h^2}{12} f^{(4)}(\xi)}_{\text{local truncation error}} + \underbrace{\frac{\varepsilon_2 - 2\varepsilon_1 + \varepsilon_0}{h^2}}_{\text{roundoff error}}.$$

We could also say

$$\left\| f''(x) - \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} \right\| \le \frac{h^2}{12} f^{(4)}(\xi) + \underbrace{\frac{4E}{h^2}}$$

where $|\varepsilon_i| \le E$, $i = 0, 1, 2$.

Too small h gives worse error.

As h decreases, this bound initially gets better, but eventually as h gets small, roundoff dominates and the derivative approximation gets worse.

Example: Let $f(x) = -\cos x$. Compute $f''(0)$. Compute $f''(0)$ using the above approximation.

h	Error $f''(0) - \tilde{f}''(0)$
0.5	2.07 E-2
0.25	5.2 E-3
0.125	1.3 E-3
0.0625	3.25 E-4
0.0325	8.45 E-5
0.015625	2.56 E-6
0.0078125	-7.94 E-5
0.00390625	-7.94 E-5
0.001953125	-1.39 E-3

So there is some optimal value of h that minizes the error.

Q: How to find formulas for numeric differentiation in a systematic way?

A: Method of undeterminded coeffecients.

Example:

① $f''(x) = Af(x+h) + Bf(x) + Cf(x-h)$.

Suppose we want a formula for the second derivative with these 3 points.

Goal: Find A, B, C.

Replace $f(x+h)$ and $f(x-h)$ by their Taylor series.

$$Af(x+h) + Bf(x) + Cf(x-h) =$$

$$A\left[f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(\xi)\right] +$$

$$Bf(x) +$$

$$C\left[f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(\xi)\right] =$$

$$= (A+B+C)(f(x)) + h(A-C)f'(x) + \frac{h^2}{2}(A+C)f''(x) +$$

$$+ \frac{h^3}{3!}(A-C)f'''(x) + \frac{h^4}{4!}f^{(4)}(\xi)(A+C)f^{(4)}(\xi).$$

Thus for this to equal $f''(x)$, we need

$$\begin{cases} A+B+C=0, \\ h(A-C)=0 \\ \frac{h^2}{2}(A+C)=1 \end{cases}$$

$A - C = 0 \Rightarrow A = C$

$A + C = \frac{2}{h^2}$

$2A = \frac{2}{h^2} \Rightarrow A = C = \frac{1}{h^2}$

$B = -\frac{2}{h^2}$.

Therefore,

$$f''(x) \approx \frac{1}{h^2} f(x+h) - \frac{2}{h^2} f(x) + \frac{1}{h^2} f(x-h)$$
$$= \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}.$$

Error formula also falls out. So

$$-\frac{h^4}{24}(A+C) f^{(4)}(\xi) = \frac{-h^4}{24} \cdot \frac{2}{h^2} f^{(4)}(\xi) =$$

$$= -\frac{h^2}{12} f^{(4)}(\xi).$$

<u>Richardson extrapolation:</u>

Richardson extrapolation is a way to get more accurate formulas from these truncated taylor series.

① $f(x+h) = f(x) + h f'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) + \dots$

② $f(x-h) = f(x) - h f'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f'''(x) + \dots$

Then ① − ② gives

$$f(x+h) - f(x-h) = 2h f'(x) + 2\frac{h^3}{3!} f'''(x) + \dots$$

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f'''(x) - \frac{h^4}{5!} f^{(5)}(x) - \frac{h^6}{7!} f^{(7)}(x) + \dots$$

Rewrite this as

① $\underset{f'(x)}{\underset{\downarrow}{L}} = \underset{\substack{\text{derivative} \\ \text{approximation}}}{\underset{\downarrow}{\varphi(h)}} + \underbrace{a_2 h^2 + a_4 h^4 + a_6 h^6 + \dots}_{\text{error}}$

If we replace h by $\frac{h}{2}$ in ① we get

$$L = \varphi\left(\frac{h}{2}\right) + a_2\left(\frac{h}{2}\right)^2 + a_4\left(\frac{h}{2}\right)^4 + a_6\left(\frac{h}{2}\right)^6 + \dots$$

$$② \quad L = \varphi\left(\frac{h}{2}\right) + \frac{h^2}{4}a_2 + a_4\frac{h^4}{16} + a_6\frac{h^6}{32} + \dots$$

Thus, $4 \cdot ② - ①$ gives

$$4L = 4\varphi\left(\frac{h}{2}\right) + a_2h^2 + a_4\frac{h^4}{4} + a_6\frac{h^6}{16} + \dots$$

$$- \quad L = \varphi(h) + a_2h^2 + a_4h^4 + a_6h^6 + \dots$$

$$3L = \varphi\left(\frac{h}{2}\right) - \varphi(h) - \frac{3}{4}a_4h^4 - \frac{15}{16}a_6h^6 + \dots$$

$$L = 3\varphi\left(\frac{h}{2}\right) - 3\varphi(h) - \frac{1}{4}a_4h^4 - \frac{5}{16}a_6h^6 + \dots$$

So the approximation

$$L = 3\varphi\left(\frac{h}{2}\right) - 3\varphi(h)$$

has error $\mathcal{O}(h^4)$. We can repeat this process to reduce the error further.

Section 7.2: Numerical integration (Quadrature)
(Based on polynomial interpolation)

Goal: To find numerical methods for evaluating definite integrals of the form

$$I(f) = \int_a^b f(x)\,dx$$

with $[a,b]$ finite interval. Many integral cannot be evaluated explicitly and with others it is faster to evaluate them numerically.

Example: (pdf for normal distribution)

$$\int_0^2 e^{-x^2}\,dx$$

$$\int_{-\infty}^{0} e^{-x^2}\,dx = \text{erf}.$$

Idea: Replace integrand by something easy to evaluate which we hope has an antiderivative close to the true function. That is, if

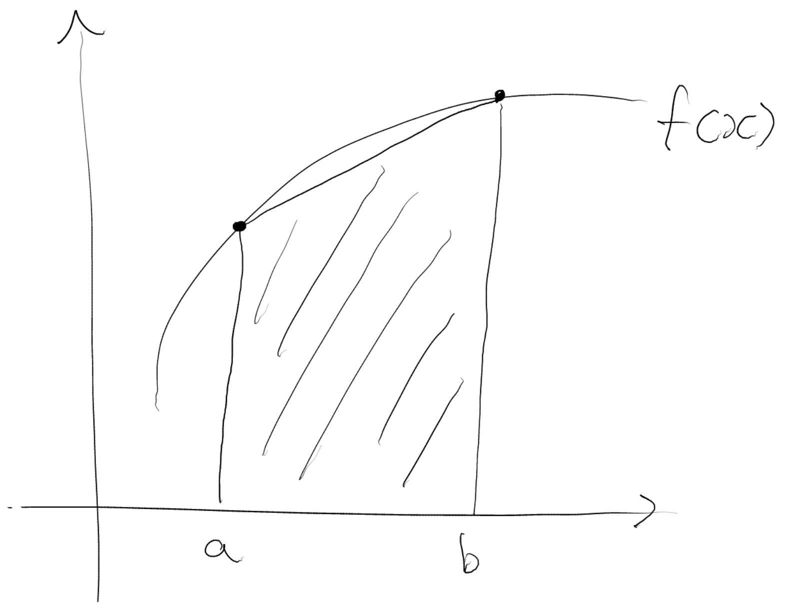
Hope: $f \approx g$ the $\int_a^b f(x)dx \approx \int_a^b g(x)\,dx$.

Note: Numerical integration is a smoothing operation, so this is reasonable whereas differentiation makes things rougher.

Good candidates are polynomials.

Ex: Trapezoid rule

Idea: Approximate $f(x)$ by a straight line that joins $(a, f(a))$ and $(b, f(b))$.



$$\int_a^b f(x)\,dx \simeq \text{area of trapezoid.}$$

Recall the linear Lagrange interpolating polynomial between 2 points is

$$p(x) = \frac{b-x}{b-a} f(a) + \frac{x-a}{b-a} f(b)$$

$$p(x) = \frac{(b-x) f(a) + (x-a) f(b)}{b-a}.$$

Then

$$\int_a^b \frac{(b-x)f(a) + (x-a)f(b)}{b-a}\,dx = \frac{b-a}{2}\left(f(a)+f(b)\right).$$

Recall the error formula for polynomial interpolation.

$$f(x) - \sum_{j=0}^{n} f(x_j)\,\ell(x_j) = \frac{f^{(n+1)}(\xi)}{(n+1)!} \prod_{i=0}^{n} (x-x_i) \,.$$