Conference 4

Numerical Differentiation: Optimal Step Size

Numerical Integration: Trapezoid Rule

Numerical Differentiation: Optimal Step Size

In class, the optimal step size h for the centered difference approximation of $f'(x_0)$ with $\mathcal{O}(h^2)$ error was derived. Write a matlab program and create a graph that shows this theoretically optimal h matches with the computations for the function $f(x) = x^2 \ln(x)$ at $x_0 = 2$.

Optimal h?

Earlier, for $M = \max_{a \le x \le b} \{|f^{(3)}(x)|\}$

$$f'(x_0) = \frac{f(x_0+h) - f(x_0-h)}{2h} - \frac{h^2 M}{6}$$

Taylor Series

Optimal h that: minimize derivative error

Error = Polynomial Error + Computational Error

Absolute Error $\le \frac{h^2 M}{6} + \frac{2\varepsilon}{2h}$ $\quad \varepsilon \approx 10^{-16}$

Derivation: Choose or find "best" h to minimize Error

Minimize: $\frac{h^2 M}{6} + \frac{2\varepsilon}{2h} = \frac{h^2 M}{6} + \frac{\varepsilon}{h}$

$$\frac{\partial}{\partial h}\left(\frac{h^2 M}{6} + \frac{\varepsilon}{h}\right) = \frac{hM}{3} + \frac{-\varepsilon}{h^2} = 0 \qquad h \neq 0$$

$$\frac{h^3 M}{3} = \varepsilon \Rightarrow h = \left(\frac{3\varepsilon}{M}\right)^{1/3}$$

optimal h!

See Code

Numerical Differentiation: Optimal Step Size

a. Derive the five-point midpoint approximation of $f'(x_0)$.

Five-Point Midpoint Formula

- $$f'(x_0) = \frac{1}{12h}[f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)] + \frac{h^4}{30}f^{(5)}(\xi), \tag{4.6}$$

where ξ lies between $x_0 - 2h$ and $x_0 + 2h$.

$$f(x) = f(x_0) + f'(x_0)(x-x_0) + \frac{f''(x_0)}{2}(x-x_0)^2 + \frac{f'''(x_0)}{3!}(x-x_0)^3 + \frac{f^{(4)}(x_0)}{4!}(x-x_0)^4 + \frac{f^{(5)}(\xi)}{5!}(x-x_0)^5$$

with ξ btwn x_0 and x

$x = x_0 + h \quad (h > 0)$

(1) $f(x_0+h) = f(x_0) + hf'(x_0) + \frac{h^2}{2}f''(x_0) + \frac{h^3}{3!}f'''(x_0) + \frac{h^4}{4!}f^{(4)}(x_0) + \frac{h^5}{5!}f^{(5)}(c_1)$

with $x_0 < c_1 < x_0 + h$

$x = x_0 - h$

(2) $f(x_0-h) = f(x_0) - hf'(x_0) + \frac{h^2}{2}f''(x_0) - \frac{h^3}{3!}f'''(x_0) + \frac{h^4}{4!}f^{(4)}(x_0) - \frac{h^5}{5!}f^{(5)}(c_2)$

with $x_0 - h < c_2 < x_0$

$x = x_0 + 2h$

(3) $f(x_0+2h) = f(x_0) + 2hf'(x_0) + \frac{4h^2}{2}f''(x_0) + \frac{8h^3}{3!}f'''(x_0) + \frac{16h^4}{4!}f^{(4)}(x_0) + \frac{32h^5}{5!}f^{(5)}(c_3)$

with $x_0 < c_3 < x_0 + 2h$

$x = x_0 - 2h$

(4) $f(x_0+2h) = f(x_0) - 2hf'(x_0) + \frac{4h^2}{2}f''(x_0) - \frac{8h^3}{3!}f'''(x_0) + \frac{16h^4}{4!}f^{(4)}(x_0) - \frac{32h}{5!}f^{(5)}(c_4)$

with $x_0 - 2h < c_4 < x_0$

Subtract (1) - (2) := (5)

$f(x_0+h) - f(x_0-h) = 2hf'(x_0) + \frac{2h^3}{3!}f'''(x_0) + \frac{h^5}{5!}\left[f^{(5)}(c_1) + f^{(5)}(c_2)\right]$

Subtract (3) − (4) := (6)

$$f(x_0+2h) - f(x_0-2h) = 4hf'(x_0) + \frac{16h^3}{3!}f'''(x_0) + \frac{32h^5}{5!}\left[f^{(5)}(c_3) + f^{(5)}(c_4)\right]$$

To eliminate $f'''(x_0)$, 8(Eqn 5) − Eqn 6

$$8f(x_0+h) - 8f(x_0-h) - f(x_0+2h) + f(x_0-2h) =$$
$$12hf'(x_0) + \frac{h^5}{5!}\left[8f^{(5)}(c_1) + 8f^{(5)}(c_2) - 32f^{(5)}(c_3) - 32f^{(5)}(c_4)\right]$$

$$\rightarrow f'(x_0) = \frac{f(x_0-2h) + 8f(x_0+h) - 8f(x_0-h) + f(x_0+2h)}{12h}$$
$$+ \frac{1}{12h}\frac{h^5}{5!}\left[-8f^{(5)}(c_1) - 8f^{(5)}(c_2) + 32f^{(5)}(c_3) + 32f^{(5)}(c_4)\right]$$

$\underline{\text{IVT}}$: Given $g(a) \le y \le g(b)$, there is a $c \in (a,b)$ s.t. $g(c) = y$.
[or $g(b) \le y \le g(a)$]
In particular, $g(a) \le \frac{g(a)+g(b)}{2} \le g(b)$ (or reverse)
so there is a $c \in (a,b)$ s.t. $2g(c) = g(a) + g(b)$.

$$8f^{(5)}(c_1) + 8f^{(5)}(c_2) = 16f^{(5)}(c^*), \quad x_0 - h < c^* < x_0 + h$$
$$32f^{(5)}(c_3) + 32f^{(5)}(c_4) = 64f^{(5)}(c^+), \quad x_0 - 2h < c^+ < x_0 + 2h$$

So,

$$-8f^{(5)}(c_1) - 8f^{(5)}(c_2) + 32f^{(5)}(c_3) + 32f^{(5)}(c_4) = -16f^{(5)}(c^*) + 64f^{(5)}(c^+)$$

$$\therefore f'(x_0) = \frac{f(x_0-2h) + 8f(x_0+h) - 8f(x_0-h) + f(x_0+2h)}{12h} + \frac{h^4}{12\cdot 5!}\left[-16f^{(5)}(c^*) + 64f^{(5)}(c^+)\right]$$

This is as far as you need to go. The IVT cannot be used here, however it turns out there does indeed exist a $c \in (x_0-2h, x_0+2h)$ s.t. $-16f^{(5)}(c^*) + 64f^{(5)}(c^+) = -16f^{(5)}(c) + 64f^{(5)}(c) = 48f^{(5)}(c)$.

Then $\frac{h^4}{12\cdot 5!}48f^{(5)}(c) = \frac{h^4 f^{(5)}(c)}{30}$ like the formula. (see pg 190)

b. Find the optimal h that minimizes both the computational and truncation (Taylor) error in the five-point midpoint approximation of $f'(x_0)$.

Five-Point Midpoint Formula

- $$f'(x_0) = \frac{1}{12h}[f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)] + \frac{h^4}{30}f^{(5)}(\xi), \tag{4.6}$$

where ξ lies between $x_0 - 2h$ and $x_0 + 2h$.

Suppose all round off error terms bdd by ε and $|f^{(5)}(\xi)| \le M$.

Error: $|E|$ = Computation Error + Truncation Error

$$= \frac{\varepsilon + 8\varepsilon + 8\varepsilon + \varepsilon}{12h} + \frac{h^4 M}{30}$$

$$= \frac{18\varepsilon}{12h} + \frac{h^4 M}{30}$$

$$= \frac{3\varepsilon}{2h} + \frac{h^4 M}{30}$$

Set $0 = \frac{\partial |E|}{\partial h} = \frac{-3\varepsilon}{2h^2} + \frac{4h^3 M}{30}$

$$\rightarrow \boxed{h^* = \sqrt[5]{\frac{45\varepsilon}{4M}}}$$

$$\left.\frac{\partial^2 |E|}{\partial h^2}\right|_{h^*} = \frac{3\varepsilon}{h^3} + \frac{12h^2}{30}M > 0$$

So h^* is a minimum.

c. For the function $f(x) = x^2 \ln(x)$ evaluated at the point $x_0 = 2$, show that this theoretically optimal h actually matches with the computations.

See code

Numerical Integration: Trapezoid Rule

a. Evaluate using the trapezoid rule with $x_0 = -1/4$, $x_1 = 1/4$.

$$\int_{-1/4}^{1/4} \cos^2(x)\, dx\ .$$

b. What is the actual error of the approximation in part a?

c. What is the theoretical upper bound on the error of the approximation in part a?

$n = 1$: Trapezoidal rule

$$\int_{x_0}^{x_1} f(x)\,dx = \frac{h}{2}[f(x_0) + f(x_1)] - \frac{h^3}{12} f''(\xi), \quad \text{where} \quad x_0 < \xi < x_1$$

$$h = x_1 - x_0 = 1/2$$

$$\int_{-1/4}^{1/4} \cos^2 x\, dx \approx \frac{1/2}{2}\left[\cos^2\left(-\tfrac{1}{4}\right) + \cos^2\left(\tfrac{1}{4}\right)\right]$$

$$= 0.469395640472593$$

b. $$\int_{-1/4}^{1/4} \cos^2 x\, dx = \int_{-1/4}^{1/4} \left(\tfrac{1}{2} + \tfrac{1}{2}\cos 2x\right) dx$$

$$= \frac{x}{2} + \frac{1}{4}\sin 2x \Big|_{-1/4}^{1/4}$$

$$= 0.489712769302102$$

$$\text{Error} = |\,0.489712769302102 - 0.469395640472593\,| = 0.020317128829508$$

c. Maximize $\left|\frac{h^3}{12} f''(\xi)\right|$

$$f'(x) = -2\cos x \sin x$$

$$f''(x) = -2\cos^2 x + 2\sin^2 x < 0 \quad \text{for } -1/4 \le x \le 1/4$$

Set $0 = f'''(x) = 8\cos x \sin x \rightarrow x = 0$

$f^{(4)}(x) = -8\sin^2 x + 8\cos^2 x$, $f^{(4)}(0) = 8 > 0$ ($x=0$ is a min)

Since $f''(x)$ is negative on $[-1/4, 1/4]$ and has a min. at $x=0$

$$\left|\frac{h^3}{12} f''(\xi)\right| \le \left|\frac{h^3}{12} f''(0)\right| = \frac{(1/2)^3}{12}|f''(0)| = 1/48$$

Numerical Integration: Trapezoid Rule

Assuming that the interval $[a, b]$ is divided evenly by the points $a = x_0 < x_1 < ... < x_N = b$ with step size h, develop a composite trapezoid rule for approximating $\int_a^b f(x)\,dx$.

$$\int_a^b f(x)\,dx \approx \sum_{j=0}^{N-1} \frac{h}{2}\left(f(x_j) + f(x_{j+1})\right)$$

$$= \frac{h}{2}\left[\left(f(x_0)+f(x_1)\right) + \left(f(x_1)+f(x_2)\right) + \ldots + \left(f(x_{N-1})+f(x_N)\right)\right]$$

$$= \frac{h}{2}\left[f(x_0) + 2f(x_1) + \ldots + 2f(x_{N-1}) + f(x_N)\right]$$

$$= \frac{h}{2}\left[f(x_0) + f(x_N) + 2\sum_{j=1}^{N-1} f(x_j)\right]$$

This form only uses the intermediate terms once instead of twice like the original equation.