Chapter 6:

Numerical differentiation.

Some functions its very hard to find the derivatives algebraicly, therefore we approximate the derivatives to solve ODE &/or PDE.

Thm: Centered difference formula of order $O(h^2)$

Assume that $f \in C^3[a,b]$ and that $x-h$, $\underline{x}$, $x+h$ are in $[a,b]$, then:

$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$. h is called step size

Furthermore: there exists a number $c = c(x) \in [a,b]$ such that:

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + E_{trun}(f,h).$$

where: $$E_{trun}(f,h) = \frac{-h^2 f^{(3)}(c)}{6} = O(h^2)$$

$E_{trun}(f,h)$ is called the truncation error.

Note: The order of the formula is the power of h in the error term. # of points different from x.

proof: start with second degree Taylor expansion

$$f(x) = P_2(x) + E_2(x) \quad \text{about } x.$$

then

$$f(x+h) = f(x) + h f'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(c_1)$$

$$f(x-h) = f(x) - h f'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f'''(c_2)$$

$$\Rightarrow \quad f(x+h) - f(x-h) = 2h f'(x) + \frac{h^3}{3!}\left(f'''(c_1) + f'''(c_2)\right)$$

$c_1 \in [x, x+h]$, $c_2 \in [x-h, x]$.

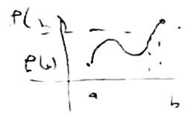
Using Intermediate value thm: (since $f^{(3)}(x)$) is continuous)

then exist $c \in (c_1, c_2)$ such that

$$f^{(3)}(c) = \frac{f^{(3)}(c_1) + f^{(3)}(c_2)}{2}$$

$$\Rightarrow \quad f(x+h) - f(x-h) = 2h f'(x) + \frac{h^3}{3!} \cdot 2 f^{(3)}(c)$$

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



Example:

x	2	3	4	5	6
y	-1	2	2	-2	4

find $f'(4)$ with $h=1$, $h=2$?

Note, with centered difference formula, we can't find $f'(2)$ or $f'(6)$.

If $h=1 \Rightarrow f'(4) = \dfrac{f(5)-f(3)}{2 \cdot 1} = \dfrac{-2-2}{2} = -2.$

If $h=2 \Rightarrow f'(4) = \dfrac{f(6)-f(2)}{2 \cdot 2} = \dfrac{4+1}{4} = \dfrac{5}{4}.$

Note: Suppose that $f^{(3)}(c)$ does not change too rapidly, then the truncation error goes to zero in the same manner as h^2.

When computer calculations are used, it's not desirable to choose h too small, therefore we go to use a formula with truncation error $O(h^4)$.

Example: Use Newton polynomial to derive centered difference formula of $O(h^2)$.

Sol: Let $x-h,\ x,\ x+h \in [a,b]$, then

$$P_2(x) = a_0 + a_1(x-x_0) + a_2(x-x_0)(x-x_1)$$

$$P_2'(x) = a_1 + a_2\left[(x-x_0) + (x-x_1)\right].$$

Now: $a_1 = f[x_0,x_1] = \dfrac{f(x_1)-f(x_0)}{x_1-x_0}$

$$a_1 = \frac{f(x)-f(x-h)}{h}$$

$$a_2 = f[x_0,x_1,x_2] = \frac{\dfrac{f(x+h)-f(x)}{x+h-x} - \dfrac{f(x)-f(x-h)}{x-(x-h)}}{x+h-(x-h)}$$

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

$$\Rightarrow P_2'(x) = \frac{f(x)-f(x-h)}{h} + \frac{f(x+h)-2f(x)+f(x-h)}{2h^2}(h+0)$$

$$\Rightarrow P_2'(x) = \frac{f(x+h)-f(x-h)}{2h}.$$

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Thm: Centered formula of order $O(h^4)$.

Assume that $f \in C^5[a,b]$ and $x-2h, x-h, x, x+h, x+2h$ are all in $[a,b]$, then:

$$f'(x) \approx \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h}.$$

Furthermore, $\exists\, c \in [a,b]$ such that:

$$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} + E_{trun}(f,h)$$

where $E_{trun}(f,h) = \dfrac{h^4 f^{(5)}(c)}{30} = O(h^4)$.

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proof: Start with the fourth degree taylor polynomial

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

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

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{2h^3}{3!} f^{(3)}(x) + 2\frac{h^5}{5!} f^{(5)}(c_*)$$ IVT again

Similarly:

$$f(x+2h) - f(x-2h) = 4hf'(x) + \frac{16h^3}{3!} f^{(3)}(x) + \frac{64}{5!} h^5 f^{(5)}(c_{**})$$ IVT

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Compute :

$$8\big(f(x+h)-f(x-h)\big)-\big(f(x+2h)-f(x-2h)\big)$$ we have

$$-f(x+2h)+8f(x+h)-8f(x-h)+f(x-2h)=$$

$$=12hf'(x)+\frac{h^5}{5!}\left(16f^{(5)}(c_*)-64f^{(5)}(c_{**})\right)\quad\cdots ①$$

Now, suppose that $f^{(5)}(x)$ has one sign and Its magnitude does not change rapidly, then we can find $c\in[x-2h,x+h]$ such that: (i-e) $f^{(5)}(c_*)\approx f^{(5)}(c_{**})$

$$16f^{(5)}(c_*)-64f^{(5)}(c_{**})=-48f^{(5)}(c)\quad\cdots ②$$

substitute ② in ①, we get :

$$-f(x+2h)+8f(x+h)-8f(x-h)+f(x-2h)=$$

$$=12hf'(x)+\frac{h^5}{5!}\cdot\left(-48f^{(5)}(c)\right).$$

$$\Rightarrow\quad f'(x)=\frac{-f(x+2h)+8f(x+h)-8f(x-h)+f(x-2h)}{12h}+\frac{h^4}{30}f^{(5)}(c)$$

Example:

x	0.1	0.2	0.3	0.4	0.5
y	13.25	18.53	21.25	24.30	27.12

We can find only $f'(0.3)$, with $h = 0.1$

$$f'(0.3) \cong \frac{-f(0.5) + 8f(0.4) - 8f(0.2) + f(0.1)}{12(0.1)}.$$

Example: Let $f(x) = \cos x$, find $f'(0.8)$, $h = 0.01$.

$$f'(0.8) \cong \frac{-f(0.82) + 8f(0.81) - 8f(0.79) + f(0.78)}{0.12}$$

$$f'(0.8) \approx -0.717356108.$$

while Exact: $f'(0.8) = -\sin(0.8) = -0.71735609\,1$

we have 7 significant digits.

& error $c(0.01)^4 = c(10^{-8})$.

error of order $O(h^4)$, c is a constant.

Error Analysis and optimum step size (h):

We need to study the effect of the computer's round-off error.

Assume computer is used to make numerical computations.

Let $f(x_0-h) = y_{-1} + e_{-1}$

$f(x_0+h) = y_1 + e_1$

where y_1, y_{-1} are Numerical values

e_1, e_{-1} are associated round-off errors.

Then: we have the following results:

Corrollary: Assume that f satisfies the hypothesis that

$f \in C^3[a,b]$ and $x-h, x, x+h \in [a,b]$. $f'(x) \approx \frac{f_1 - f_0}{2h}$

use the computational formula:

$$f'(x_0) \approx \frac{y_1 - y_{-1}}{2h}$$, then the error Analysis

is explained by:

$$f'(x_0) = \frac{y_1 - y_{-1}}{2h} + E_{tot}(f,h)$$

where $E_{tot}(f,h) = E_{round}(f,h) + E_{trun}(f,h)$

$$= \frac{e_1 - e_{-1}}{2h} + -\frac{h^2}{6} f^{(3)}(c).$$

Corollary: Assume that $f \in C^3[a,b]$,

$x-h$, x, $x+h \in [a,b]$ and that $|e_{-1}|$, $|e_1|$ both are less or equal ϵ, and $M = \max\limits_{a \le x \le b} |f^{(3)}(x)|$.

then

$$|E_{tot}(f,h)| \leqslant \frac{\epsilon}{h} + \frac{M h^2}{6} \qquad --- (*)$$

and the value of h that minimize $(*)$ is given by

$$h = \left(\frac{3\epsilon}{M}\right)^{\frac{1}{3}}$$

proof: Just substitute to get $(*)$, and to find the optimum h:

$$E' \leqslant \frac{-\epsilon}{h^2} + \frac{2hM}{6}.$$

$$\Rightarrow \quad \frac{-\epsilon}{h^2} + \frac{2hM}{6} = 0$$

solving for h, we get:

$$h = \left(\frac{3\epsilon}{M}\right)^{\frac{1}{3}}.$$

Corollary: Assume f satisfies the hypotheses that

$f \in C^5[a,b]$ & $x-2h, x-h, x, x+h, x+2h \in [a,b]$

Use computational formula:

$$f'(x) \approx \frac{-y_2 + 8y_1 - 8y_{-1} + y_{-2}}{12h}.$$

and the error:

$$f'(x) = \frac{-y_2 + 8y_1 - 8y_{-1} + y_{-2}}{12h} + E_{tot}(f,h)$$

when $E_{tot}(f,h) = E_{round}(f,h) + E_{trun}(f,h)$

$$E_{tot}(f,h) = \frac{-e_2 + 8e_1 - 8e_{-1} + e_{-2}}{12h} + \frac{h^4}{30} f^{(5)}(c)$$

Corollary: If $|e_k| \leq \epsilon$, $k = \{-1,-2,1,2\}$

and $M = \max_{a \leq x \leq b} |f^{(5)}(x)|$, then:

$$|E_{tot}(f,h)| \leq \frac{3\epsilon}{2h} + \frac{Mh^4}{30} \quad \dots (**)$$

and the value of h that minimize $(**)$ is given by:

$$h = \left(\frac{45\epsilon}{4M}\right)^{\frac{1}{5}}.$$

Notes:

If we have only one point, then.

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

& $$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2!} f^{(2)}(c).$$

therefore the order of the formula is 1

(i.e) $O(h)$.

therefore, we conclude that the order of formula depends on the number of given points different from x.

So, if we have 2 points rather than x, we have order 2, and so on..

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6.2 High order derivations:

Centered Numerical differentiation formulas: $O(h^2)$

$$f''(x) = \frac{f_1 - 2f_0 + f_{-1}}{h^2} + O(h^2)$$

where $$O(h^2) = -\frac{h^2}{12} f^{(4)}(c)$$

proof:

$$f(x+h) = f(x) + h f'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f^{(3)}(x) + \frac{h^4}{4!} f^{(4)}(\xi_1) + \cdots$$

$$f(x-h) = f(x) - h f'(x) + \frac{h^2}{2} f''(x) - \frac{h^3}{3!} f^{(3)}(x) + \frac{h^4}{4!} f^{(4)}(\xi_2) + \cdots$$

IVT

$$\Rightarrow \quad f(x+h) + f(x-h) = 2f(x) + h^2 f''(x) + 2\frac{h^4}{4!} f^{(4)}(x) + \cdots$$

Solve for $f''(x)$ and assume that the truncated error is at the forth derivative: $\frac{h^4}{4!}\left(f^{(4)}(c_1) + f^{(4)}(c_2)\right)$

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

for $c \in [x-h, x+h]$.

Note: This formula is centered formula for $f''(x)$.

Error Analysis:

$$f''(x) \approx \frac{f_1 - 2f_0 + f_{-1}}{h^2}$$

Let $f_k = y_k + e_k$, where e_k is the error in computing $f(x_k)$ Including noise and round-off error.

then:
$$f''(x) = \frac{y_1 - 2y_0 + y_{-1}}{h^2} + E_{tot}(f,h)$$

where
$$E_{tot}(f,h) = \frac{e_1 - 2e_0 + e_{-1}}{h^2} - \frac{h^2}{12} f^{(4)}(c)$$

Corollary: Assume $|f^{4}(x)| \leq M$ and $|e_k| \leq \epsilon$, $\forall k$

then
$$|E_{tot}(f,h)| \leq \frac{4\epsilon}{h^2} + \frac{Mh^2}{12} \quad \cdots (***)$$

and the value of h that minimize $(***)$ (optimum h) , when h is the step size.

$$-\frac{8\epsilon}{h^3} + \frac{Mh}{6} = 0 \iff h = \left(\frac{48\epsilon}{M}\right)^{\frac{1}{4}}.$$

Notes: (1) power of h is the order of the formula.

(2) number of points determine the order ($\#x$).

(3) we stop at $f^{(n+2)}(c)$, where n # of points. (without x) for $f''(x)$

Example: Let $f(x) = \cos x$. find $f''(0.8)$ with $h = 0.01$.

$$f''(0.8) \approx \frac{f(0.81) - 2f(0.8) + f(0.79)}{0.0001} \approx -0.69669000.$$

while $f''(0.8) = -\cos(0.8) = -0.696706709$

Then the error in the approximation is -0.000016709

To find the optimal step size:

$$M = \max_{a \le x \le b} |f^{(4)}(x)| \qquad 1$$

Use $\epsilon = 0.5 \times 10^{-9}$, then the optimal step size is

$$h = \left(\frac{48 \cdot (0.5 \times 10^{-9})}{1} \right)^{\frac{1}{4}} \cong 0.01244666.$$

therefore our choice $h = 0.01$ was close to the optimal step size.

Note: Like in $f'(x)$, we will get more accuracy in $f''(x)$ using a formula with order 4 $(O(h^4))$.

Centered Formula of order 4:

$$f''(x) = \frac{-f_2 + 16 f_1 - 30 f_0 + 16 f_{-1} - f_{-2}}{12 h^2} + E(f,h)$$

when $|E(f,h)| = \frac{16 \epsilon}{3 h^2} + \frac{h^4 f^{(6)}(c)}{90}$, $c \in [x-2h, x+2h]$

Assuming $M = \max |f^{(6)}(x)|$, then the optimal value for h is given by:

$$h = \left(\frac{240 \epsilon}{M}\right)^{\frac{1}{6}}$$

Example: Let $f(x) = \cos x$, find $f''(0.8)$, $h = 0.1$.

$$f''(0.8) = \frac{-f(1) + 16 f(0.9) - 30 f(0.8) + 16 f(0.7) - f(0.6)}{0.12}$$

$$\approx -0.696705958$$

Back ward and forward difference formulas of order h^2.

Forward: Find the optimum h

$$f'(x_0) \simeq \frac{-3f_0 + 4f_1 - f_2}{2h} \longrightarrow O(h^2) \quad \left(\text{two points after}\right)$$

The same error

Back ward:

$$f'(x_0) \simeq \frac{3f_0 - 4f_{-1} + f_{-2}}{2h} \longrightarrow O(h^2) \quad \left(\text{two points before}\right).$$

proof: (Back ward) start with second degree taylor expanssion.

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

$$f(x-2h) = f(x) - 2h f'(x) + \frac{4h^2}{2!} f''(x) - \frac{8h^3}{3!} f^{(3)}(c).$$

$$\Rightarrow \quad -4f_{-1} + f_{-2} = -3f_0 + 2h f'(x) - \frac{4h^3}{3!} f'''(c)$$

Solve it for $f'(x)$, we get.

$$f'(x) = \frac{3f_0 - 4f_{-1} + f_{-2}}{2h} + \frac{h^2}{3} f^{(3)}(c)$$

Corollary: If $|e_k| \leq \epsilon$, & $M = \max|f^{(4)}(x)|$

$$\Rightarrow \quad |E_{bt}(E,f)| \leq \frac{8\epsilon}{2h} + \frac{h^2}{3} M.$$

Example: Derive the following formula Using Lagrange Interpolating polynomial:

$$f'(x_0) = \frac{-3f_0 + 4f_1 - f_2}{2h} \qquad [\underline{\text{forward}}]$$

Let $x_0, \; x_0+h, \; x_0+2h \in [a,b]$.

$$P_2(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f_0 + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f_1 + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f_2$$

$$P_2(x) = \frac{f_0}{(-h)(-2h)}(x-x_1)(x-x_2) + \frac{f_1}{h(-h)}(x-x_0)(x-x_2) + \frac{f_2}{(2h)(h)}(x-x_0)(x-x_1)$$

$$P_2'(x) = \frac{f_0}{2h^2}\left[(x-x_1)+(x-x_2)\right] + \frac{f_1}{-h^2}\left[(x-x_0)+(x-x_2)\right]$$
$$+ \frac{f_2}{2h^2}\left[(x-x_0)+(x-x_1)\right]$$

$$P_2'(x_0) = \frac{f_0}{2h^2}\left[(-h)+(-2h)\right] + \frac{f_1}{-h^2}\left[-2h\right] + \frac{f_2}{2h^2}\left[-h\right]$$

$$= \frac{f_0}{2h^2}\left[-3h\right] + \frac{2f_1}{h} - \frac{f_2}{2h}$$

$$= \frac{-3f_0 + 4f_1 - f_2}{2h}$$

Example: Use Newton polynomial to derive backward formula of order $O(h^2)$

$$f'(x_0) = \frac{3f_0 - 4f_{-1} + f_{-2}}{2h}$$

Let $x_0 - 2h = t_0$, $x_0 - h = t_1$, $x_0 = t_2$

$$P_2(t) = a_0 + a_1(t - t_0) + a_2(t - t_0)(t - t_1)$$

$$P_2'(t) = a_1 + a_2[(t - t_0) + (t - t_1)]$$

$$P_2'(x_0) = a_1 + a_2[(x_0 - (x_0 - 2h)) + (x_0 - (x_0 - h))]$$

$$= a_1 + a_2[2h + h]$$

$$a_1 = \frac{f_1 - f_0}{h} \Rightarrow a_1 = \frac{f_{-1} - f_{-2}}{h}$$

$$a_2 = \frac{\frac{f_2 - f_1}{h} - \frac{f_1 - f_0}{h}}{2h} = \frac{f_2 - 2f_1 + f_0}{2h^2} = \frac{f_0 - 2f_{-1} + f_{-2}}{2h^2}$$

$$P_2'(x_0) = \frac{\overset{f_{-1}}{\cancel{f_1}} - \overset{f_{-2}}{\cancel{f_0}}}{h} + \left(\frac{\overset{f_0 - 2f_{-1} + f_{-2}}{\cancel{f_2} - 2f_1 + f_0}}{2h^2}\right)[3h]$$

$$= \frac{2f_{-1} - 2f_{-2} + 3f_0 - 6f_{-1} + 3f_{-2}}{2h}$$

$$= \frac{+3f_0 - 4f_1 + f_2}{2h}$$

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Note: If there is a loss in the given data or the partition are not equal, then we go back to chapter 4 (Lagrange & Newton).

Moreover, we can use Newton and Lagrange methods to prove the formulas.

Example: Use Newton polynomial to derive forward formula of order $o(h^2)$.

Sol: we need three points to find $P_2(x)$, say

or x_0, x_0+h, x_0+2h

~~$x-h, x, x+h$.~~ (to make it easier)

$x, x+h, x+2h$

$$P_2(x) = a_0 + a_1(x-x_0) + a_2(x-x_0)(x-x_1).$$

$$P_2'(x) = a_1 + a_2\big((x-x_0)+(x-x_1)\big)$$

where $a_1 = \dfrac{f_1 - f_0}{h}$, $a_2 = \dfrac{\frac{f_2-f_1}{h} - \frac{f_1-f_0}{h}}{2h}$

$$\Rightarrow a_2 = \frac{f_2 - 2f_1 + f_0}{2h^2}$$

$$\Rightarrow P_2'(x_0) = \frac{f_1 - f_0}{h} + \left(\frac{f_2 - 2f_1 + f_0}{2h^2}\right)[0 - h]$$

$$\Rightarrow P_2'(x_0) \cong \frac{-3f_0 + 4f_1 - f_2}{2h}$$

To find $E(f,h)$:

$$|E_2(x)| \leq \left|\frac{(x-x_0)(x-x_1)(x-x_2)\cdot M_3}{3!}\right|$$

$$|E_2'(x)| \leq \frac{[(x-x_0)(x-x_1)+(x-x_0)(x-x_2)+(x-x_1)(x-x_2)]M_3}{3!}$$

$$\Rightarrow \quad E_2'(x_0) \leq \frac{(-h)(-2h)\cdot M_3}{3!} = \frac{h^2}{3} M_3 .$$

Example: Let $f(x) = \cos x$, $h = 0.01$ find $f'(0.8)$.

Forward:

$$f'(0.8) \cong \frac{-3\cos(0.8) + 4\cos(0.81) - \cos(0.82)}{2(0.01)}$$

$$\cong -0.717380176$$

Backward:

$$f'(0.8) \cong \frac{3\cos(0.8) - 4\cos(0.79) + \cos(0.78)}{2(0.01)}$$

$$\cong -0.717379827$$

Use the nodes x_0, x_0+h and x_0+3h to approximate $f'(x_0+2h)$.

Sol: $P_2(x) = a_0 + a_1(x-x_0) + a_2(x-x_0)(x-x_1)$

$$P_2'(x) = a_1 + a_2\big((x-x_0) + (x-x_1)\big)$$

$x_0+2h - x_0$ $\qquad$ $x_0+2h - x_0 - h$

$$P_2'(x_0+2h) = a_1 + a_2[2h+h] = a_1 + 3h\,a_2$$

$$a_1 = \frac{f_1 - f_0}{x_1 - x_0} = \frac{f_1 - f_0}{h}$$

$$a_2 = \frac{\dfrac{f_3 - f_1}{x_3 - x_1} - \dfrac{f_1 - f_0}{x_1 - x_0}}{x_3 - x_0}$$

$x_0+3h - x_0$

$$= \left(\frac{f_3 - f_1}{2h} - \frac{f_1 - f_0}{h}\right)\Big/ 3h$$

$$\Rightarrow P_2'(x_0+2h) = \frac{f_1 - f_0}{h} + 3h\,\frac{\left[\dfrac{f_3 - f_1}{2h} - \dfrac{f_1 - f_0}{h}\right]}{3h}$$

$$= \frac{f_1 - f_0}{h} + \frac{f_3 - f_1}{2h} - \frac{f_1 - f_0}{h}$$

$$= \frac{-f_1 + f_3}{2h}.$$

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