Chapter 4 Numerical Differentiation and Integration

4.1 Numerical Differentiation

1) Forward-difference and backward-difference formulas

By definition

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0+h) - f(x_0)}{h}$$

This gives an obvious way to approximate the derivative

$$f'(x_0) \approx \frac{f(x_0+h) - f(x_0)}{h}$$

for small values of h.

Def: If $h > 0$, then

$$f'(x_0) = \frac{f(x_0+h) - f(x_0)}{h}$$

is called a <u>forward-difference formula</u>

In general, the smaller h the better the approximation

Ex. For the function $f(x) = e^x \sin x$, $x_0 = 1.9$ compute approximations of $f'(x_0)$ using forward-differences starting with $h = 0.05$ and halfing on the next step.

Solution:

$$f'(x) = e^x \sin x + e^x \cos x$$

$$f'(1.9) = 4.165382579 \quad \text{(exact value)}$$

$$f(1.9) = 6.326862497$$

h	$f(x_0+h)$	$f'(x_0)$-appr.	Error	Ratio of error
0.05	6.5293676	4.05010	−0.11528	
0.05/2	6.429601513	4.10955	−0.05583	2.06
0.05/4	6.378586496	4.13795	−0.02743	2.04
0.05/8	6.352811	4.151842	−0.01354	2.03
0.05/16	6.339858	4.15872	−0.00666	2.03
0.05/32	6.333366	4.16256	−0.00282	2.36
0.05/64	6.3301154	4.16372	−0.001667	1.69
0.05/128	6.328489	4.16385	−0.00153	1.09

Notice that each successive error is about ½ of the previous error untill step $h = 0.05/64$. When h is too small the round off errors start playing a significant role. It doesn't make sence to decrease the step any further since the errors don't drop. Higher accuracy can be achieved only with double precision

If the step is negative, let's write it as $-h$, with $h>0$. Then the formula becomes

$$f'(x_0) \approx \frac{f(x_0)-f(x_0-h)}{h}$$

Def: This is called a <u>backward-difference formula</u>.

To estimate the errors from approximati[on] with forward-difference and backward difference formulas consider expansion in Taylor series.

$$f(x_0+h) = f(x_0)+f'(x_0)h + \frac{f''(\xi)}{2!}h^2$$

for some $\xi \in (x_0, x_0+h)$

Solving above for $f'(x_0)$ we get

$$f'(x_0) = \frac{f(x_0+h)-f(x_0)}{h} - \frac{h}{2}f''(\xi)$$

If $|f''(\xi)| \le M$ for all ξ in $[x_0, x_0+h]$ then the error of the approximation

$$|E| \le \frac{M}{2}h = O(h)$$

Thus, the error of the approximation is $O(h)$

Ex #112/176

Let $f(x)=\sin x$. Use the forward-difference and backward-difference formulas to complete the table. Compute the actual errors and error bounds using the error formulas

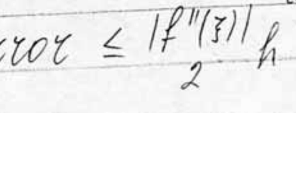
x	$f(x)$	FD $f'(x)$	BD $f'(x)$	FD Actual Error	BD Actual Error	Error bound
0.5	0.4794	0.852	—	0.02558256	—	
0.6	0.5646	0.796	0.852	0.0293356	-0.026664	
0.7	0.6442	—	0.796	—	-0.0311578	

$$\text{Error} = \frac{f''(\xi)}{2} h$$

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

$$|f''(\xi)| = |\sin \xi| \underset{\xi\in[0.5,0.6]}{\le} |\sin 0.6| = 0.564642$$

$$|f''(\xi)| = |\sin \xi| \underset{\xi\in[0.6,0.7]}{\le} |\sin 0.7| = 0.64422$$



$$\text{Error} \le \frac{|f''(\xi)|}{2} h \underset{[0.5,0.6]}{\le} \frac{0.564642}{2} \cdot 0.1 = 0.028232$$

$$\text{Error} \le \frac{|f''(\xi)|}{2} h \le \frac{0.64422}{2} \cdot 0.1 = 0.03221$$

2) Three and five point formulas and their errors.

One of the main methods of approximating the derivatives consists in constructing the approximation polynomials and differentiating this polynomial instead.

Suppose we are using 3 equally spaced points

$$x_0, \ x_0+h, \ x_0+2h$$

Writing Lagrange polynomial of degree 2 and differentiating it leads to the following formula

(1) $$f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)\right] + \frac{h^2}{3} f'''(\xi_1)$$

where $\xi_1 \in (x_0, x_0+2h)$.

We approximate

$$f'(x_0) \approx \frac{1}{2h}\left[-3f(x_0)+4f(x_0+h)-f(x_0+2h)\right]$$

Clearly, if we have to approximate

the derivative on the points

$$a = x_1 \quad x_2 \quad x_3 \quad \cdots \quad x_{n-2} \quad x_{n-1} \quad x_n = b$$

we can take for x_0 each of the points $x_1, x_2, \ldots, x_{n-2}$, but we cannot use this formula to approximate

$$f'(x_{n-1}) \text{ and } f'(x_n)$$

For this purpose another three-point formula is used, which is obtained by differentiating the Lagrange polynomial of degree 2 interpolating on the points

$$x_0 - 2h, \; x_0 - h, \; x_0$$

$$(2) \quad f'(x_0) = \frac{1}{2h}\left[f(x_0 - 2h) - 4f(x_0 - h) + 3f(x_0)\right] + \frac{h^2}{3} f'''(\xi_2)$$

where $\xi_2 \in (x_0 - 2h, x_0)$.

We approximate the derivative using

$$f'(x_0) \approx \frac{1}{2h}\left[f(x_0 - 2h) - 4f(x_0 - h) + 3f(x_0)\right]$$

This formula can be used with x_0 being $x_3, x_4, \dots, x_{n-1}, x_n$ but it cannot be used to compute

$$f'(x_1) \text{ and } f'(x_2).$$

The error of applying these 2 formulas is

$$Error = \frac{h^2}{3} f'''(\xi)$$

for ξ in (x_0, x_0+2h) in formula (1)
ξ in (x_0-2h, x_0) in formula (2).

If

$$|f'''(\xi)| \le M \quad \text{for } \xi \text{ in the corresponding interval}$$

then

$$|Error| \le \frac{M}{2} h^2$$

Thus, the error is $O(h^2)$

If we use the Lagrange polynomial to interpolate the points

$$x_0-h \quad x_0 \quad x_0+h$$

and then differentiate it we get the following symmetric three-point formula

(3) $$f'(x_0) = \frac{1}{2h}\left[-f(x_0-h) + f(x_0+h)\right] - \frac{h^2}{6} f'''(\xi_0)$$

where $\xi_0 \in (x_0-h, x_0+h)$.

Def: The formula
$$f'(x_0) \approx \frac{f(x_0+h) - f(x_0-h)}{2h}$$
is called centered-difference formula

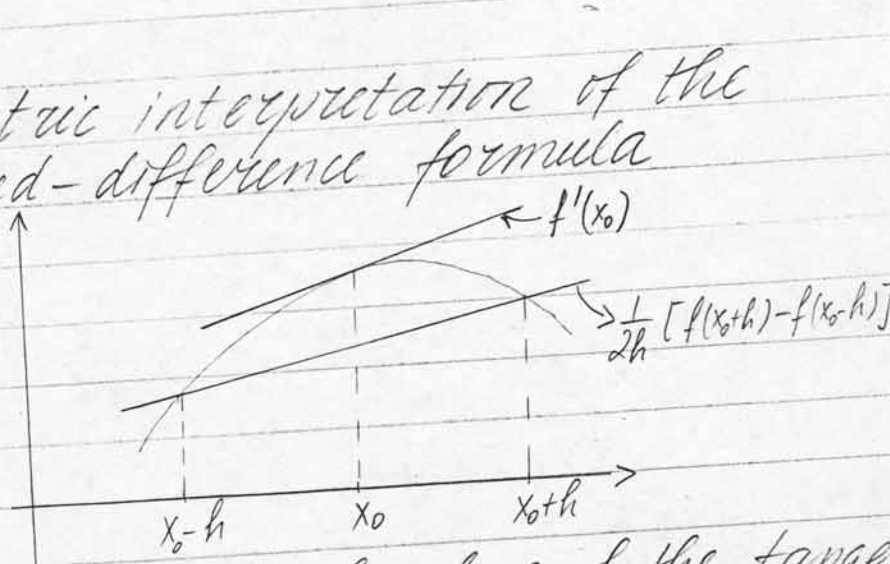
Clearly, this formula can be used to approximate the derivative at all interior points but not the endpoint. Thus, with this formula we cannot compute
$$f'(x_1) \text{ and } f'(x_n)$$
but we can take x_0 to be $x_2, \ldots, x_{n-1}$

The error of applying this formula is
$$\text{Error} = \frac{h^2}{6} f'''(\xi_0)$$
where $\xi_0 \in (x_0-h, x_0+h)$. This error is approximately half the error in formulas (1) and (2).

If $|f'''(\xi)| \leq M$ for all $\xi \in (x_0-h, x_0+h)$
then
$$|Error| \leq \frac{M}{6} h^2$$
Thus, the error is again $O(h^2)$.

<u>Remark:</u> All three-point formulas give approximation $O(h^2)$. Compare them with the forward-difference and backward-difference which approximate within $O(h)$. Also, the centered-difference formula gives 2 times smaller error then the other 2 three-point formulas.

Geometric interpretation of the centered-difference formula



We approximate the slope of the tangent line at $(x_0, f(x_0))$ with the slope of the secant through the points $(x_0-h, f(x_0-h))$ and $(x_0+h, f(x_0+h))$.

Ex. For the function $f(x) = e^x \sin x$ use the central-difference formula to approximate $f'(x_0)$ for $x_0 = 1.9$. Use steps h starting with 0.05 and halfing on the next computation

h	$f(x_0-h)$ $f(x_0+h)$	$f'(x_0)$-appr.	Error	Ratio of Errors
0.05	6.1135368 6.529367612	4.15831	−0.00708	
0.05/2	6.2214208 6.42960151	4.16361	−0.00177	4.00
0.05/4	6.274463 6.3785865	4.16494	−0.000442	4.00
0.05/8	6.30074511 6.35281101	4.16527	−0.000111	3.98
0.05/16	6.31382465 6.33985812	4.165355	−0.000027	4.11

We can see that the central difference is far more accurate than the forward or backward difference. Decreasing the size of h 2 times decreases the error 4 times. The balance between the error of the method and the round off error is reached for a larger $h = 0.05/16$

Ex. 3|4[b]/176

(a) Use the most accurate three-point formula to determine the missing entries in the table

(b) The data are taken from the function

$$f(x) = x\ln x$$

Compute the actual error and find the error bounds using the error formulas

x	$f(x)$	$f'(x)$	Actual error	Error bound
8.1	16.94410	3.09205	$1.85938*10^{-4}$	$2.032211*10^{-4}$
8.3	17.56492	3.11615	$1.055148*10^{-4}$	$1.01611*10^{-4}$
8.5	18.19056	3.139975	$9.11635*10^{-5}$	$9.677264*10^{-5}$
8.7	18.82091	3.163525	$2.01974*10^{-4}$	$1.935453*10^{-4}$

For $f'(8.1)$ we use formula (1)

$$f'(8.1) \approx \frac{1}{2\cdot(0.2)}\left[-3f(8.1)+4f(8.3)-f(8.5)\right] =$$

$$= \frac{1}{0.4}\left[-50.8323+70.25968-18.19056\right] =$$

$$= \frac{1}{0.4}\,1.23682 = 3.09205$$

For $f'(8.3)$ and $f'(8.5)$ we use centered difference formula

$$f'(8.3) \approx \frac{1}{2(0.2)}\left[-f(8.1)+f(8.5)\right] = \frac{1}{0.4}\left[18.19056-16.944\right.$$

$$= 3.11615$$

$$f'(8.5) \approx \frac{1}{2\cdot(0.2)}\left[-f(8.3)+f(8.7)\right] = \frac{1}{0.4}\left[18.82091-17.56492\right] = 3.1399$$

To estimate $f'(8.7)$ we use formula (2):

$$f'(8.7) \approx \frac{1}{2\cdot(0.2)}\left[f(8.3) - 4f(8.5) + 3\cdot f(8.7)\right] =$$

$$= \frac{1}{0.4}\left[17.56492 - 72.76224 + 56.46273\right]$$

$$= \frac{1}{0.4}\, 1.26541 = 3.163525$$

(b) $f(x) = x\ln x$ $\qquad f''(x) = \frac{1}{x}$ $\qquad h = 0.2$

$f'(x) = \ln x + 1$ $\qquad f'''(x) = -\frac{1}{x^2}$

$\text{Error}_1 = \frac{h^2}{3} f'''(\xi)$ $\quad \xi$ in $(8.1, 8.5)$ or ξ in $(8.3, 8.7)$

$\text{Error}_2 = \frac{h^2}{6} f'''(\xi)$ $\quad \xi$ in $(8.1, 8.5)$ or ξ in $(8.3, 8.7)$

$|f'''(x)| = \frac{1}{x^2}$ - decreasing

$$\underset{x \text{ in } (8.1,\, 8.5)}{|f'''(x)| \le} \frac{1}{(8.1)^2} = 0.015241579$$

$$\underset{x \text{ in } (8.3,\, 8.7)}{|f'''(x)| \le} \frac{1}{(8.3)^2} = 0.0145158949$$

1) EB for $f'(8.1) = \frac{0.015241579 * (0.2)^2}{3} = 2.03221 * 10^{-4}$

2) EB for $f'(8.3) = \frac{0.015241579 * (0.2)^2}{6} = 1.01611 * 10^{-4}$

3) EB for $f'(8.5) = \frac{0.0145158949 * (0.2)^2}{6} = 9.677264 * 10^{-}$

4) EB for $f'(8.7) = \frac{0.0145158949 * (0.2)^2}{3} = 1.9354527 * 10$

Note: The error bounds for $f'(8.3)$ and $f'(8.7)$ are slightly lower than the actual error. I believe that is because of round off error.

3) Approximating higher order derivatives

Suppose we want to approximate $f''(x$

$$f(x_0+h) = f(x_0) + f'(x_0)h + \frac{h^2}{2!}f''(x_0) + \frac{h^3}{3!}f'''(x_0) + \frac{h^4}{4!}f^{I}$$

where ξ_1 in (x_0, x_0+h)

$$f(x_0-h) = f(x_0) - f'(x_0)h + \frac{h^2}{2!}f''(x_0) - \frac{h^3}{3!}f'''(x_0) + \frac{h^4}{4!}f^{IV}(\xi_2)$$

where ξ_2 in (x_0-h, x_0)

Add these 2 equations

$$f(x_0+h)-f(x_0-h) = 2f(x_0) + f''(x_0)h^2$$
$$+ \frac{h^4}{24}\left[f^{IV}(\xi_1) + f^{IV}(\xi_2)\right]$$

Note: we have

$$f^{IV}(\xi) = \frac{1}{2}\left[f^{IV}(\xi_1) + f^{IV}(\xi_2)\right]$$

Thus

(4) $$f''(x_0) = \frac{f(x_0-h) - 2f(x_0) + f(x_0+h)}{h^2} - \frac{h^2}{24} f^{IV}(\xi)$$

where ξ in (x_0-h, x_0+h)