Numerical differentiation

Problem formulation

Let the function $y = f(x)$ be defined in the interval $[a,b]$ and have derivatives of a given order. If there is a known table with the values $y_i = f(x_i)$ of the function in points (nodes) $x_0, x_1, x_2, ..., x_n \in [a,b]$ the methods of numerical differentiation allow the finding of the approximated value of the derivative $y'(x) = f'(x)$ in the given point x, the value of the second derivative etc. Particularly important for numerical differentiation of some functions is the **possible instability** of the problem, i.e. small errors in the input data leading to big errors in the result and sometimes even to the so called "error explosion". Such is the case when derivatives grow significantly which is noticeable by the big differences in the finite differences. In the last example such a type of function is illustrated and it is shown how to solve the instability problem.

Further down we will only consider the case of equally distanced nodes in the given interval $[a,b]$ for which $x_{i+1} = x_i + h$ where h is the step between the nodes. The table will be of the following type:

x_i	x_0	x_1	...	x_i	...	x_n
y_i	y_0	y_1	...	y_i	...	y_n

I) The formula for numerical differentiation based on Newton's interpolation polynomial for forward interpolation:

(1) $$y'(t) \approx \frac{1}{h}\left(\Delta y_0 + \frac{2t-1}{2!}\Delta^2 y_0 + \frac{3t^2-6t+2}{3!}\Delta^3 y_0 + \frac{4t^3-18t^2+22t-6}{4!}\Delta^4 y_0 + ... \right),$$

(2) $$y''(t) \approx \frac{1}{h^2}\left(\Delta^2 y_0 + (t-1)\Delta^3 y_0 + \frac{6t^2-18t+11}{12}\Delta^4 y_0 + ... \right),$$

Here $t = \frac{x-x_0}{h}$ and $\Delta^k y_0$ is the finite difference from *k*-th order in point x_0.

In particular for $x = x_0$ we have $t = 0$ from where we get

(3) $$y'_0 \approx \frac{1}{h}\left(\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0 - \frac{1}{4}\Delta^4 y_0 + ... \right),$$

(4) $$y_0'' \approx \frac{1}{h^2}\left(\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12}\Delta^4 y_0 + \ldots\right).$$

II) The formula for numerical differentiation base on Newton's interpolation polynomial for backward interpolation:

(5) $$t = \frac{x - x_n}{h},\quad y'(t) \approx \frac{1}{h}\left(\Delta y_{n-1} + \frac{2t+1}{2!}\Delta^2 y_{n-2} + \frac{3t^2+6t+2}{3!}\Delta^3 y_{n-3} + \ldots\right)$$

(6) $$y''(t) \approx \frac{1}{h^2}\left(\Delta^2 y_{n-2} + (t+1)\Delta^3 y_{n-3} + \frac{6t^2+18t+11}{12}\Delta^4 y_{n-4} + \ldots\right)$$

In particular for $x = x_n$ we have $t = 0$ from where we get

(7) $$y_n' \approx \frac{1}{h}\left(\Delta y_{n-1} + \frac{1}{2}\Delta^2 y_{n-2} + \frac{1}{3}\Delta^3 y_{n-3} + \frac{1}{4}\Delta^4 y_{n-4} + \ldots\right)$$

(8) $$y_n'' \approx \frac{1}{h^2}\left(\Delta^2 y_{n-2} + \Delta^3 y_{n-3} + \frac{11}{12}\Delta^4 y_{n-4} + \ldots\right).$$

Note. Formulas (1) - (8) give an opportunity for effective calculation of the derivatives because they offer posterior error evaluation. The latter means that the addition of every other summand to the right side of the formulas leads to particularization of the sought value. That is why calculations are terminated when the summand to be added has an absolute value smaller than the accuracy of the data (the so called irreversible error).

III) Formulas for numerical differentiation using point stencils on uniform mesh:

(9)

№	Point stencil	Formula for numerical differentiation	Local absolute error
1.	x_i, x_{i+1}	$y_i' \approx \frac{y_{i+1} - y_i}{h}$	$\frac{h}{2!}M_2 = O(h)$, $M_2 = \max\limits_{x_i \le \xi \le x_{i+1}} \lvert f''(\xi)\rvert$
2.	x_{i-1}, x_i	$y_i' \approx \frac{y_i - y_{i-1}}{h}$	$\frac{h}{2!}M_2 = O(h)$, $M_2 = \max\limits_{x_{i-1} \le \xi \le x_i} \lvert f''(\xi)\rvert$
3.	x_i, x_{i+1}, x_{i+2}	$y_i' \approx \frac{-3y_i + 4y_{i+1} - y_{i+2}}{2h}$	$\frac{2h^2}{3}M_3 = O(h^2)$, $M_3 = \max\limits_{x_{i-1} \le \xi \le x_i+1} \lvert f'''(\xi)\rvert$
4.	x_{i-2}, x_{i-1}, x_i	$y_i' \approx \frac{y_{i-2} - 4y_{i-1} + 3y_i}{2h}$	$\frac{2h^2}{3}M_3 = O(h^2)$, $M_3 = \max\limits_{x_{i-1} \le \xi \le x_i+1} \lvert f'''(\xi)\rvert$
5.	x_{i-1}, x_i, x_{i+1}	$y_i' \approx \frac{y_{i+1} - y_{i-1}}{2h}$	$\frac{h^2}{3}M_3 = O(h^2)$, $M_3 = \max\limits_{x_{i-1} \le \xi \le x_i+1} \lvert f'''(\xi)\rvert$
6.	x_{i-1}, x_i, x_{i+1}	$y_i'' \approx \frac{y_{i-1} - 2y_i + y_{i+1}}{h^2}$	$\frac{h^2}{12}M_4 = O(h^2)$, $M_4 = \max\limits_{x_{i-1} \le \xi \le x_i+1} \lvert f^{IV}(\xi)\rvert$

Example 1. The values of the function $y = f(x) = \ln(x^2)$ in the interval $[2,3]$ are given in the first two columns of table 1. Calculate the approximated values of the first derivatives in nodes $x_0 = 2$, $x_1 = 2{,}1$, $\xi = 2{,}04$, $x_{10} = 3$.

Solution:

We calculate consecutively the finite differences Δy_i, $\Delta^2 y_i$, ... which we enter into table 1. For the step h by x we have $h = x_{i+1} - x_i = 0{,}1$.

Table 1

i	x_i	y_i	Δy_i	$\Delta^2 y_i$	$\Delta^3 y_i$	$\Delta^4 y_i$	$\Delta^5 y_i$
0	2,0	1,38629	0,09758	-0,00454	0,00040	-0,00005	0,00001
1	2,1	1,48387	0,09304	-0,00414	0,00035	-0,00004	0,00000
2	2,2	1,57691	0,08890	-0,00378	0,00031	-0,00004	0,00001
3	2,3	1,66582	0,08512	-0,00348	0,00027	-0,00003	0,00000
4	2,4	1,75094	0,08164	-0,00320	0,00024	-0,00003	0,00001
5	2,5	1,83258	0,07844	-0,00296	0,00022	-0,00002	0,00000
6	2,6	1,91102	0,07548	-0,00275	0,00019	-0,00002	
7	2,7	1,98650	0,07274	-0,00255	0,00017		
8	2,8	2,05924	0,07018	-0,00238			
9	2,9	2,12942	0,06780				
10	3,0	2,19722					

When $x_0 = 2$ by substitution in formula (3) we get

$$y'_0 \approx \frac{1}{0{,}1}\left(0{,}09758 - \frac{1}{2}(-0{,}00454) + \frac{1}{3}0{,}00040 - \frac{1}{4}(-0{,}00005) + \ldots\right) \approx 0{,}99998 .$$

Here it is obvious that the member containing $\Delta^5 y_i$ (and those following it) is very small and can be disregarded. The exact value in this example is known, it is $y'(x) = (\ln(x^2))' = \frac{2x}{x^2} = \frac{2}{x}$, i.e. $f'(2) = \frac{2}{2} = 1$. Consequently the resulting approximated value $y'_0 \approx 0{,}99998$ has an absolute error of 0,00002.

Analogically for the other point $x_1 = 2{,}1$ using the same formula but by utilizing the second row of the table we find that:

$$y'_1 \approx \frac{1}{0{,}1}\left(0{,}09304 - \frac{1}{2}(-0{,}00414) + \frac{1}{3}0{,}00035 - \frac{1}{4}(-0{,}00004) + \ldots\right) \approx 0{,}95236 .$$

Let us now take the point $\xi = 2{,}04$. It is located in the beginning of the interval close to $x_0 = 2$ and it is most natural to utilize the general formula (1). We calculate the deviation from the beginning $t = (\xi - x_0)/h = (2{,}04 - 2)/0{,}1 = 0{,}4$. Then

$$y'(\xi) = y'(t) = y'(0,4) \approx \frac{1}{0,1}\left(0,09758 + \frac{2.0,4-1}{2}(-0,00454) + \ldots\right) \approx 0,98040 .$$

For the first derivative in point $x_{10} = 3$ we utilize formula (7):

$$y'_{10} \approx \frac{1}{0,1}\left(0,06780 + \frac{1}{2}(-0,00238) + \frac{1}{3}0,00017 + \frac{1}{4}(-0,00002) + \ldots\right) \approx 0,66667 .$$

Note. The exact values of the derivative $y'(x) = \ln(x^2)' = \frac{2}{x}$ in the given nodes with an accuracy of five digits are respectively: $y'(2,1) = 0,95238$, $y'(3) = 0,66667$, $y'(2,04) = 0,98039$.

Example 2. With the help of the data from table 1 calculate the approximated value of the second derivative in point $x_0 = 2$.

Solution:

From formula (4) we have:

$$y''_0 \approx \frac{1}{0,01}\left(-0,00454 - 0,00040 + \frac{11}{12}(-0,00005) + \ldots\right) \approx 0,4986 .$$

Example 3. In the first two columns of table 2 are given the values of the function which have been found by way of experiment. Calculate the approximated values of the derivatives in points x_i.

Solution:

We have interval $[1;\ 1{,}4]$ and step $h = 0{,}05$. In the point $x_0 = 1$ we calculate the derivative using the formula for left three point stencil – (9.3) and in point $x_8 = 1{,}4$ using the formula for right three point stencil – (9.4). In the inner points of the interval it is convenient to utilize the central finite difference from formula (9.5). The results are given in the last column of the table. As the data has an accuracy $0{,}0001$ and $h = 0{,}05$ then the formulas used by us with a local error $O(h^2)$ in this case give an error around $0{,}0025$. This means that the last digit in the values of the derivative can be expected to be insignificant. As we don't know the exact formula of the function and consequently we cannot evaluate to what extent the theoretical error is real, the only indication for the reliability of the result being the gradual change of values for y_i', $i = 0,...,8$ if of course we presume the continuity of the derivative.

Table 2

i	x_i	y_i	Approximations for y_i'
0	1,00	-0,2475	-0,0353
1	1,05	-0,2490	-0,0229
2	1,10	-0,2498	-0,0104
3	1,15	-0,2500	0,0021
4	1,20	-0,2496	0,0146
5	1,25	-0,2485	0,0270
6	1,30	-0,2469	0,0394
7	1,35	-0,2446	0,0517
8	1,40	-0,2417	0,0639

Example 4. Calculate the approximated values of the derivative of the function $y = \cos(8x)$ in points $x_0 = 0$ and $x_1 = 0,1$.

Solution:

In this example we come across a case indicative of the instability of numerical differentiation. The function has infinitely many derivatives and there seems to be no problem. Let us choose, for example, the interval $[0;\ 0,5]$ and divide it into five sub-intervals with step $h = 0,1$. We calculate the table of the finite differences – table 3. We notice that the values of $\Delta^k y_i$ do not get smaller as with previous examples (compare!)

Table 3

x_i	$y_i = \cos(8x_i)$	Δy_i	$\Delta^2 y_i$	$\Delta^3 y_i$	$\Delta^4 y_i$
0,0	1,00000	-0,30329	-0,42261	0,44032	-0,01074
0,1	0,69671	-0,72591	0,01771	0,42958	-0,27132
0,2	-0,02920	-0,70819	0,44729	0,15826	
0,3	-0,73739	-0,26090	0,60555		
0,4	-0,99829	0,34465			
0,5	-0,65364				

Utilizing the first row of finite differences from table 3 and formula (3) for $x_0 = 0$ we get:

$$y_0' \approx \frac{1}{0,1}\left(-0,30329 - \frac{1}{2}(-0,42261) + \frac{1}{3}0,44032 - \frac{1}{4}(-0,01074)\right) \approx$$

$$\approx \frac{1}{0,1}(-0,30329+0,21131+0,14678+0,00269) \approx \frac{1}{0,1}0,05748 \approx 0,5748.$$

However, this result is **significantly different from the correct one.** Indeed the derivative $y'(x)=-8\sin(8x)$ for $x=0$ is $y'(0)=0$. This way the real error of the numerical differentiation $\varepsilon=|y'(0)-y_0'|=|0-0,5748|=0,5748 \approx 0,6$ is much bigger and obviously isn't due to the rounding off which is in the area of 10^{-5}.

The result in point $x_1=0,1$ is analogical. Using the given finite differences from the second row of table 3 and formula (3) we calculate:

$$y_1' \approx \frac{1}{0,1}\left(-0,72591-\frac{1}{2}0,01771+\frac{1}{3}0,42958-\frac{1}{4}(-0,27132)\right) \approx -5,23738.$$

The exact value is: $y'(0,1)=-5,73885$. The error in this case, too is very significant - 0,50147.

Note. For experimental data, for which we don't know the formula of the function, one criterion is the presence of big and non-decreasing values of the finite differences. To solve the problem and find satisfactory approximated values of the derivatives of instable problems we can **use a very small step *h*.** Try to use this suggestion by choosing h=0,0001 and calculating y_0'. There are some special methods for reducing the error, like for example, the Runge-Romberg method.

Example 5. Using the formulas for numerical differentiation with an error of $O(h^2)$ fill in the empty cells in the table:

x	0,1	0,2	0,3	0,4	0,5
y	-4		1	11	20
y'	35				
y''	X				X

Solution:

To calculate the value $y(0,2)$ we will use formula (9-3.) for $y'(0,1)$:

$$y_i' \approx \frac{-3y_i+4y_{i+1}-y_{i+2}}{2h} \Rightarrow y'(0,1) \approx \frac{-3y(0,1)+4y(0,2)-y(0,3)}{2h} \Rightarrow$$

$$y(0,2)=\frac{2hy'(0,1)+3y(0,1)+y(0,3)}{4}=\frac{2.0,1.35+3(-4)+1}{4}=-1.$$

Then once again using formulas (9) we find:

$$y'(0,2) = \frac{y(0,3) - y(0,1)}{2h} = \frac{1+4}{2.0,1} = 25; \quad y'(0,3) = \frac{y(0,4) - y(0,4)}{2h} = \frac{11+1}{2.0,1} = 60;$$

$$y'(0,4) = \frac{y(0,5) - y(0,3)}{2h} = \frac{20-1}{2.0,1} = 95; \quad y'(0,5) = \frac{y(0,3) - 4y(0,4) + y(0,5)}{2h} = \frac{1-44+60}{2.0,1} = 85;$$

For the second derivatives we have respectively:

$$y''(0,2) = \frac{y(0,3) - 2y(0,2) + y(0,1)}{h^2} = \frac{1-2(-1)-4}{0,01} = -100;$$

$$y''(0,3) = \frac{y(0,4) - 2y(0,3) + y(0,2)}{h^2} = \frac{11-2.1+(-1)}{0,01} = 800;$$

$$y''(0,4) = \frac{y(0,5) - 2y(0,4) + y(0,3)}{h^2} = \frac{20-2.11+1}{0,01} = -100.$$

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