Lecture 4: Numerical differentiation

Finite difference formulas

Suppose you are given a data set of N non-equispaced points at $x = x_i$ with values $f(x_i)$ as shown in Figure 1. Because the data are not equispaced in general, then $\Delta x_i \neq \Delta x_{i+1}$.

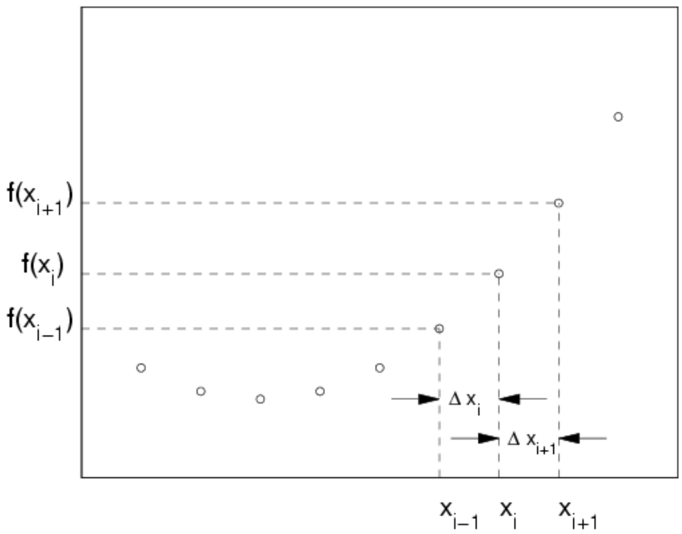

Figure 1: Data set of N points at $x = x_i$ with values $f(x_i)$

Let's say we wanted to compute the derivative $f'(x)$ at $x = x_i$. For simplicity of notation, we will refer to the value of $f(x)$ at $x = x_i$ as f_i. Because, in general, we do not know the form of $f(x)$ when dealing with disrete points, then we need to determine the derivatives of $f(x)$ at $x = x_i$ in terms of the known quantities f_i. Formulas for the derivatives of a data set can be derived using Taylor series.

The value of $f(x)$ at $x = x_{i+1}$ can be written in terms of the Taylor series expansion of f about $x = x_i$ as

$$f_{i+1} = f_i + \Delta x_{i+1} f_i' + \frac{\Delta x_{i+1}^2}{2} f_i'' + \frac{\Delta x_{i+1}^3}{6} f_i''' + \mathcal{O}\left(\Delta x_{i+1}^4\right) . \tag{1}$$

This can be rearranged to give us the value of the first derivative at $x = x_i$ as

$$f_i' = \frac{f_{i+1} - f_i}{\Delta x_{i+1}} - \frac{\Delta x_{i+1}}{2} f_i'' - \frac{\Delta x_{i+1}^2}{6} f_i''' + \mathcal{O}\left(\Delta x_{i+1}^3\right) . \tag{2}$$

If we assume that the value of f_i'' does not change significantly with changes in Δx_{i+1}, then this is the first order derivative of $f(x)$ at $x = x_i$, which is written as

$$f_i' = \frac{f_{i+1} - f_i}{\Delta x_{i+1}} + \mathcal{O}\left(\Delta x_{i+1}\right) . \tag{3}$$

This is known as a **forward difference**. The first order backward difference can be obtained by writing the Taylor series expansion about f_i to obtain f_{i-1} as

$$f_{i-1} = f_i - \Delta x_i f_i' + \frac{\Delta x_i^2}{2} f_i'' - \frac{\Delta x_i^3}{6} f_i''' + \mathcal{O}\left(\Delta x_i^4\right) , \tag{4}$$

which can be rearranged to yield the **backward difference** of $f(x)$ at x_i as

$$f_i' = \frac{f_i - f_{i-1}}{\Delta x_i} + \mathcal{O}\left(\Delta x_i\right) . \tag{5}$$

The first order forward and backward difference formulas are first order accurate approximations to the first derivative. This means that decreasing the grid spacing by a factor of two will only increase the accuracy of the approximation by a factor of two. We can increase the accuracy of the finite difference formula for the first derivative by using both of the Taylor series expansions about f_i,

$$\begin{aligned} f_{i+1} &= f_i + \Delta x_{i+1} f_i' + \frac{\Delta x_{i+1}^2}{2} f_i'' + \frac{\Delta x_{i+1}^3}{6} f_i''' + \mathcal{O}\left(\Delta x_{i+1}^4\right) & (6) \\ f_{i-1} &= f_i - \Delta x_i f_i' + \frac{\Delta x_i^2}{2} f_i'' - \frac{\Delta x_i^3}{6} f_i''' + \mathcal{O}\left(\Delta x_i^4\right) . & (7) \end{aligned}$$

Subtracting equation (7) from (6) yields

$$\begin{aligned} f_{i+1} - f_{i-1} &= \left(\Delta x_{i+1} + \Delta x_i\right) f_i' + \frac{\Delta x_{i+1}^2 - \Delta x_i^2}{2} f_i'' + \frac{\Delta x_{i+1}^3 + \Delta x_i^3}{6} f_i''' \\ &+ \mathcal{O}\left(\Delta x_{i+1}^4\right) + \mathcal{O}\left(\Delta x_i^4\right) \\ \frac{f_{i+1} - f_{i-1}}{\Delta x_{i+1} + \Delta x_i} &= f_i' + \frac{\Delta x_{i+1}^2 - \Delta x_i^2}{2\left(\Delta x_{i+1} + \Delta x_i\right)} f_i'' + \frac{\Delta x_{i+1}^3 + \Delta x_i^3}{6\left(\Delta x_{i+1} + \Delta x_i\right)} f_i''' \\ &+ \mathcal{O}\left(\frac{\Delta x_{i+1}^4}{\Delta x_{i+1} + \Delta x_i}\right) + \mathcal{O}\left(\frac{\Delta x_i^4}{\Delta x_{i+1} + \Delta x_i}\right) , \end{aligned} \tag{8}$$

which can be rearranged to yield

$$f_i' = \frac{f_{i+1} - f_{i-1}}{\Delta x_{i+1} + \Delta x_i} - \frac{\Delta x_{i+1}^2 - \Delta x_i^2}{2\left(\Delta x_{i+1} + \Delta x_i\right)} f_i'' + \mathcal{O}\left(\frac{\Delta x_{i+1}^3 + \Delta x_i^3}{6\left(\Delta x_{i+1} + \Delta x_i\right)}\right) \tag{9}$$

In most cases if the spacing of the grid points is not too eratic, such that $\Delta x_{i+1} \approx \Delta x_i$, equation (9) can be written as the **central difference** formula for the first derivative as

$$f_i' = \frac{f_{i+1} - f_{i-1}}{2\Delta x_i} + \mathcal{O}\left(\Delta x_i^2\right) . \tag{10}$$

What is meant by the "order of accuracy"?

Suppose we are given a data set of $N = 16$ points on an equispaced grid as shown in Figure 2, and we are asked to compute the first derivative f_i' at $i = 2, \ldots, N-1$ using the forward, backward, and central difference formulas (3), (5), and (10). If we refer to the approximation

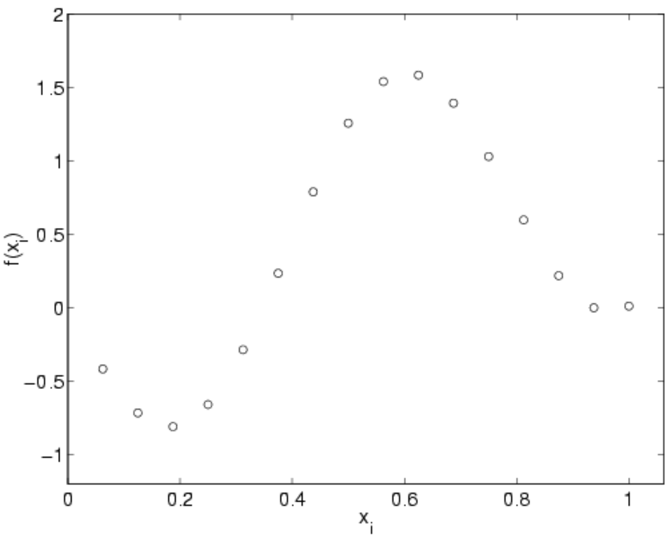

Figure 2: A data set consisting of $N = 16$ points.

of the first derivative as $\frac{\delta f}{\delta x}$, then these three formulas for the first derivative on an equispaced grid with $\Delta x_i = \Delta x$ can be approximated as

$$\begin{aligned}
\text{Forward difference} \quad \frac{\delta f}{\delta x} &= \frac{f_{i+1} - f_i}{\Delta x}\,, && (11)\\
\text{Backward difference} \quad \frac{\delta f}{\delta x} &= \frac{f_i - f_{i-1}}{\Delta x}\,, && (12)\\
\text{Central difference} \quad \frac{\delta f}{\delta x} &= \frac{f_{i+1} - f_{i-1}}{2\Delta x}\,. && (13)
\end{aligned}$$

These three approximations to the first derivative of the data shown in Figure 2 are shown in Figure 3. Now let's say we are given five more data sets, each of which defines the same function $f(x_i)$, but each one has twice as many grid points as the previous one to define the function, as shown in Figure 4. The most accurate approximations to the first derivatives will be those that use the most refined data with $N = 512$ data points. In order to quantify how much more accurate the solution gets as we add more data points, we can compare the derivative computed with each data set to the most resolved data set. To compare them, we can plot the difference in the derivative at $x = 0.5$ and call it the error, such that

$$\text{Error} = \left| \left.\frac{\delta f}{\delta x}\right)_n - \left.\frac{\delta f}{\delta x}\right)_{n=6} \right| \qquad (14)$$

where $n = 1, \ldots, 5$ is the data set and $n = 6$ corresponds to the most refined data set. The result is shown in Figure 5 on a log-log plot. For all three cases we can see that the error closely follows the form

$$\text{Error} = k\Delta x^n\,, \qquad (15)$$

where $k = 1.08$ and $n = 1$ for the forward and backward difference approximations, and $k = 8.64$ and $n = 2$ for the central difference approximation. When we plot the error of a numerical method and it follows the form of equation (15), then we say that the method is

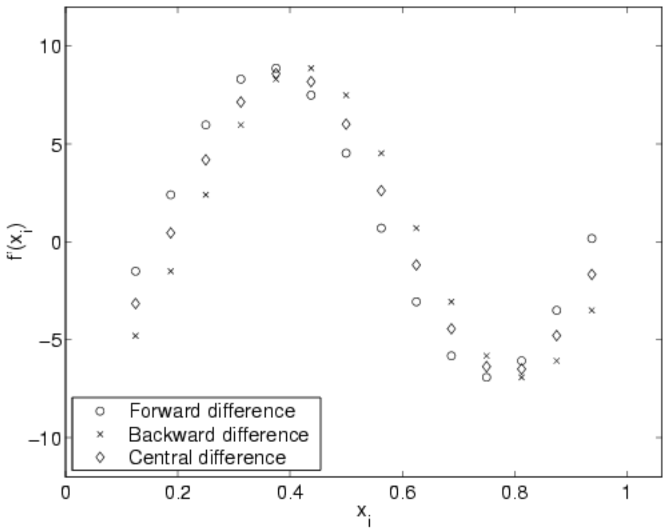

Figure 3: Approximation to the first derivative of the data shown in Figure 2 using three different approximations.

n_{th} order and that the error can be written as $\mathcal{O}(\Delta x^n)$. Because $n = 1$ for the forward and backward approximations, they are said to be **first order methods**, while since $n = 2$ for the central approximation, it is a **second order method**.

Taylor tables

The first order finite difference formulas in the previous sections were written in the form

$$\frac{df}{dx} = \frac{\delta f}{\delta x} + \text{Error}\,, \tag{16}$$

where $\frac{\delta f}{\delta x}$ is the approximate form of the first derivative $\frac{df}{dx}$ with some error that determines the order of accuracy of the approximation. In this section we define a general method of estimating derivatives of arbitrary order of accuracy. We will assume equispaced points, but the analysis can be extended to arbitrarily spaced points. The n_{th} derivative of a discrete function f_i at points $x = x_i$ can be written in the form

$$\left.\frac{d^n f}{dx^n}\right|_{x=x_i} = \frac{\delta^n f}{\delta x^n} + \mathcal{O}(\Delta x^m)\,, \tag{17}$$

where

$$\frac{\delta^n f}{\delta x^n} = \sum_{j=-N_l}^{j=+N_r} a_{j+N_l} f_{i+j}\,, \tag{18}$$

and m is the order of accuracy of the approximation, a_{j+N_l} are the coefficients of the approximation, and N_l and N_r define the width of the approximation stencil. For example, in the central difference approximation to the first derivative,

$$\begin{aligned} f_i' &= -\frac{1}{2\Delta x} f_{i-1} + 0 f_i + \frac{1}{2\Delta x} f_{i+1} + \mathcal{O}\left(\Delta x^2\right)\,, & (19)\\ &= a_0 f_{i-1} + a_1 f_i + a_2 f_{i+1} + \mathcal{O}\left(\Delta x^2\right)\,. & (20)\end{aligned}$$

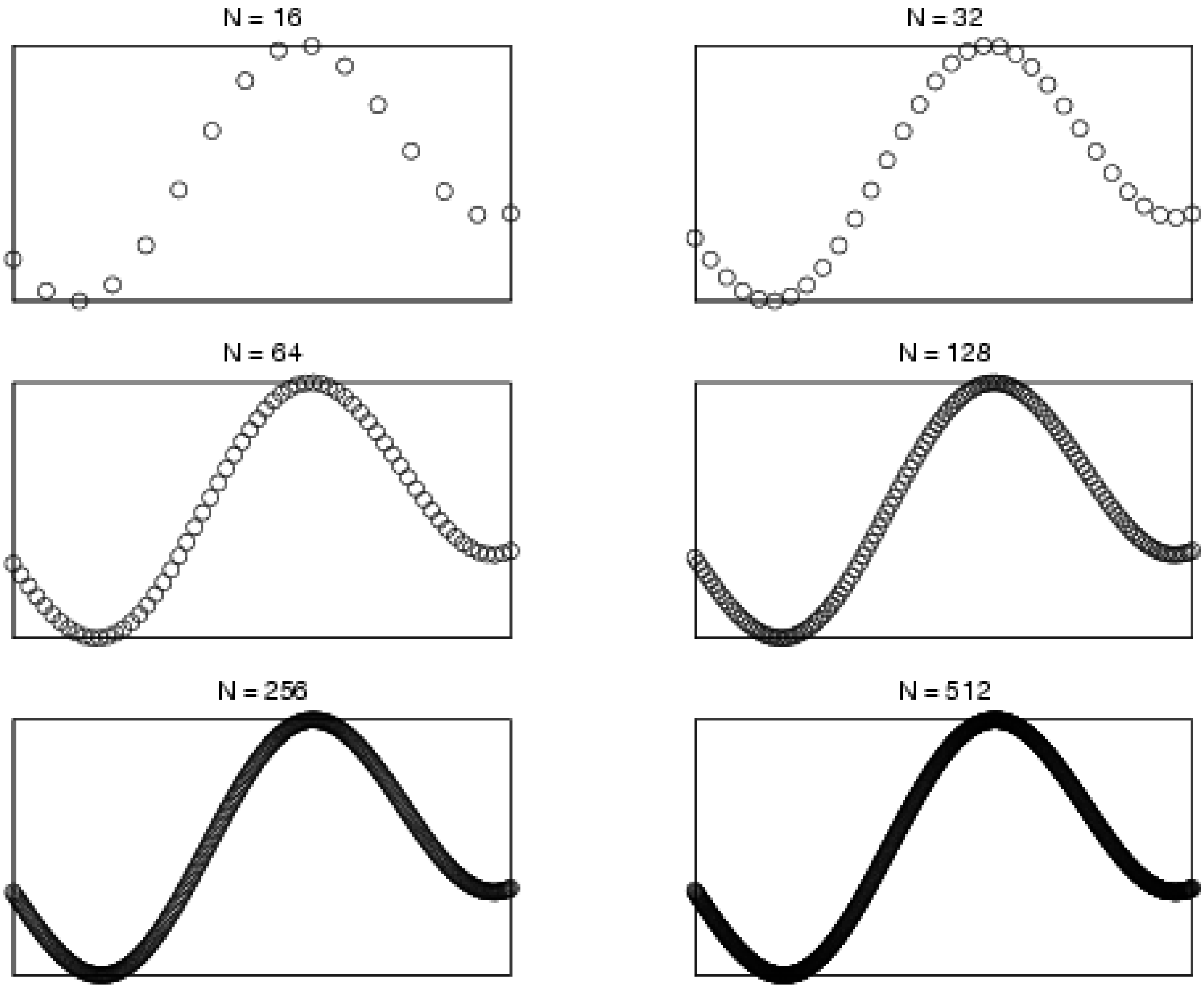

Figure 4: The original data set and 5 more, each with twice as many grid points as the previous one.

In this case, $N_l = 1$, $N_r = 1$, $a_0 = -1/2\Delta x$, $a_1 = 0$, and $a_2 = +1/2\Delta x$. In equation (18) the discrete values f_{i+j} can be written in terms of the Taylor series expansion about $x = x_i$ as

$$f_{i+j} = f_i + j\Delta x f_i' + \frac{(j\Delta x)^2}{2} f_i'' + ... \tag{21}$$

$$= f_i + \sum_{k=1}^{\infty} \frac{(j\Delta x)^k}{k!} f_i^{(k)}\,. \tag{22}$$

Using this Taylor series approximation with $m+2$ terms for the f_{i+j} in equation (18), where m is the order of accuracy of the finite difference formula, we can substitute these values into equation (17) and solve for the coefficients a_{j+N_l} to derive the appropriate finite difference formula.

As an example, suppose we would like to determine a second order accurate approximation to the second derivative of a function $f(x)$ at $x = x_i$ using the data at x_{i-1}, x_i, and

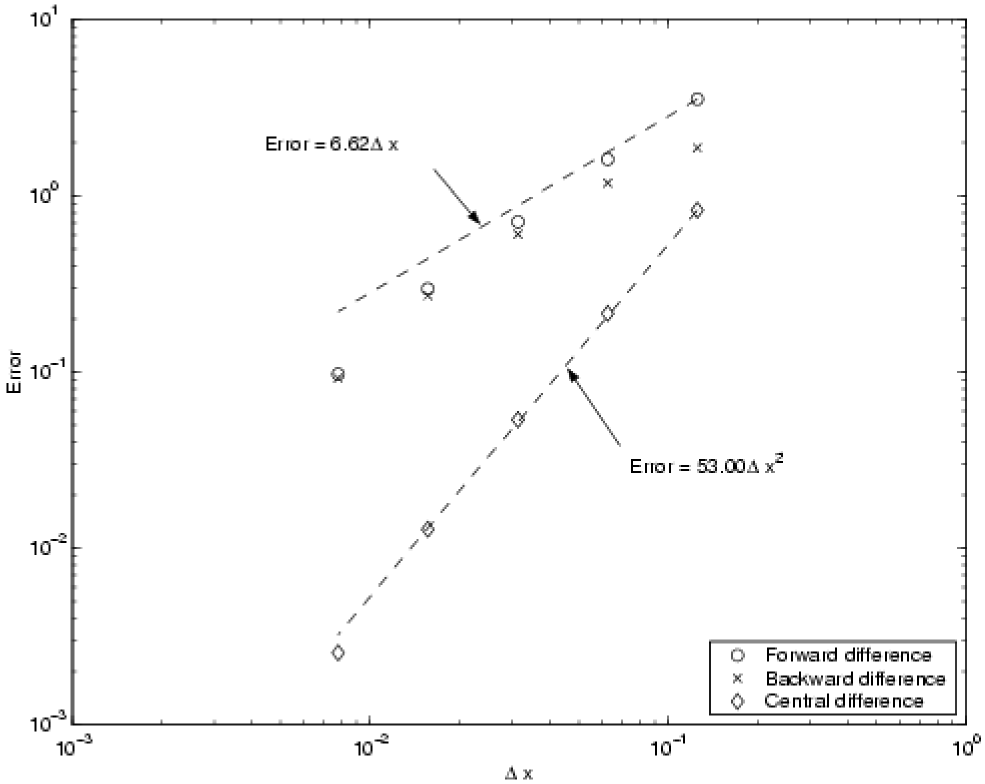

Figure 5: Depiction of the error in computing the first derivative for the forward, backward, and central difference formulas

x_{i+1}. Writing this in the form of equation (17) yields

$$\frac{d^2 f}{dx^2} = \frac{\delta f}{\delta x} + \mathcal{O}\left(\Delta x^2\right) , \tag{23}$$

where, from equation (18),

$$\frac{\delta f}{\delta x} = a_0 f_{i-1} + a_1 f_i + a_2 f_{i+1} \, . \tag{24}$$

The Taylor series approximations to f_{i-1} and f_{i+1} to $\mathcal{O}\left(\Delta x^4\right)$ are given by

$$\begin{aligned} f_{i-1} &\approx f_i - \Delta x f_i' + \frac{\Delta x^2}{2} f_i'' - \frac{\Delta x^3}{6} f_i''' + \frac{\Delta x^4}{24} f_i^{iv} \, , && (25) \\ f_{i+1} &\approx f_i + \Delta x f_i' + \frac{\Delta x^2}{2} f_i'' + \frac{\Delta x^3}{6} f_i''' + \frac{\Delta x^4}{24} f_i^{iv} \, , && (26) \end{aligned}$$

Rather than substitute these into equation (24), we create a **Taylor table**, which requires much less writing, as follows. If we add the columns in the table then we have

$$\begin{aligned} a_0 f_{i-1} + a_1 f_i + a_2 f_{i+1} &= (a_0 + a_1 + a_2) f_i + (-a_0 + a_2) \Delta x f_i' + (a_0 + a_2) \frac{\Delta x^2}{2} f_i'' \\ &+ (-a_0 + a_2) \frac{\Delta x^3}{6} f_i''' + (a_0 + a_2) \frac{\Delta x^4}{24} f_i^{iv} \, . \end{aligned} \tag{27}$$

Term in (24)	f_i	$\Delta x f_i'$	$\Delta x^2 f_i''$	$\Delta x^3 f_i'''$	$\Delta x^4 f_i^{iv}$
$a_0 f_{i-1}$	a_0	$-a_0$	$a_0/2$	$-a_0/6$	$a_0/24$
$a_1 f_i$	a_1	0	0	0	0
$a_2 f_{i+1}$	a_2	a_2	$a_2/2$	$a_2/6$	$a_2/24$
	0	0	1	?	?

Because we would like the terms containing f_i and f_i' on the right hand side to vanish, then we must have $a_0 + a_1 + a_2 = 0$ and $-a_0 + a_2 = 0$. Furthermore, since we want to retain the second derivative on the right hand side, then we must have $a_0 + a_2 = 1$. This yields three equations in three unknowns for a_0, a_1, and a_2, namely,

$$\begin{array}{ccccccc} a_0 & + & a_1 & + & a_2 & = & 0 \\ -a_0 & & & + & a_2 & = & 0 \\ a_0/2 & & & + & a_2/2 & = & 1 \end{array} \,, \tag{28}$$

in which the solution is given by $a_0 = a_2 = 1$ and $a_1 = -2$. Substituting these values into equation (27) results in

$$f_{i-1} - 2f_i + f_{i+1} = \Delta x^2 f_i'' + \frac{\Delta x^4}{12} f_i^{iv} \,, \tag{29}$$

which, after rearranging, yields the second order accurate finite difference formula for the second derivative as

$$f_i'' = \frac{f_{i-1} - 2f_i + f_{i+1}}{\Delta x^2} + \mathcal{O}\left(\Delta x^2\right) \,, \tag{30}$$

where the error term is given by

$$\text{Error} = -\frac{\Delta x^2}{12} f_i^{iv} \,. \tag{31}$$

As another example, let us compute the second order accurate one-sided difference formula for the first derivative of $f(x)$ at $x = x_i$ using x_i, x_{i-1}, and x_{i-2}. The Taylor table for this example is given below. By requring that $a_0 + a_1 + a_2 = 0$, $-2a_0 - a_1 = 1$, and

Term	f_i	$\Delta x f_i'$	$\Delta x^2 f_i''$	$\Delta x^3 f_i'''$	$\Delta x^4 f_i^{iv}$
$a_0 f_{i-2}$	a_0	$-2a_0$	$2a_0$	$-4a_0/3$	$2a_0/3$
$a_1 f_{i-1}$	a_1	$-a_1$	$+a_1/2$	$-a_1/6$	$a_1/24$
$a_2 f_i$	a_2	0	0	0	0
	0	1	0	?	?

$2a_0 + a_1/2 = 0$, we have $a_0 = 1/2$, $a_1 = -2$, and $a_2 = 3/2$. Therefore, the second order accurate one-sided finite difference formula for the first derivative is given by

$$\frac{df}{dx} = \frac{f_{i-2} - 4f_{i-1} + 3f_i}{2\Delta x} + \mathcal{O}\left(\Delta x^2\right) \,, \tag{32}$$

where the error term is given by

$$\text{Error} = \frac{\Delta x^2}{3} f_i''' \,. \tag{33}$$

Higher order finite difference formulas can be derived using the Taylor table method described in this section. These are shown in Applied numerical analysis, sixth edition, by C. F. Gerald & P. O. Wheatley, Addison-Welsley, 1999., pp. 373-374.