ChE 205 — Formulas for Numerical Differentiation

Consider a set of data points $\{x_i, f_i\} = \{x_i, f(x_i)\}$ $(i = 1, \ldots, N)$ that represent a function $f(x)$. Here are finite-difference formulas for approximating the slope at the data points.

$$\text{First:} \quad f'(x_1) \approx \left[\frac{2x_1 - x_2 - x_3}{(x_2 - x_1)(x_3 - x_1)}\right] f_1 + \left[\frac{x_3 - x_1}{(x_2 - x_1)(x_3 - x_2)}\right] f_2 + \left[\frac{x_1 - x_2}{(x_3 - x_2)(x_3 - x_1)}\right] f_3$$

$$\text{Last:} \quad f'(x_N) \approx \left[\frac{x_N - x_{N-1}}{(x_N - x_{N-2})(x_{N-1} - x_{N-2})}\right] f_{N-2} + \left[\frac{x_{N-2} - x_N}{(x_{N-1} - x_{N-2})(x_N - x_{N-1})}\right] f_{N-1} + \left[\frac{2x_N - x_{N-1} - x_{N-2}}{(x_N - x_{N-1})(x_N - x_{N-2})}\right] f_N$$

$$\text{Intermediate:} \quad f'(x_i) \approx \left[\frac{x_i - x_{i+1}}{(x_{i+1} - x_{i-1})(x_i - x_{i-1})}\right] f_{i-1} + \left[\frac{2x_i - x_{i-1} - x_{i+1}}{(x_i - x_{i-1})(x_i - x_{i+1})}\right] f_i + \left[\frac{x_i - x_{i-1}}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)}\right] f_{i+1} \qquad (i = 2, \ldots, N-1)$$

When the data points are evenly spaced (i.e., $x_i - x_{i-1} = h$ for all $i = 2, \ldots, N$) then these formulas simplify considerably.

$$\text{First:} \quad f'(x_1) \approx \frac{-3f_1 + 4f_2 - f_3}{2h}$$

$$\text{Last:} \quad f'(x_N) \approx \frac{f_{N-2} - 4f_{N-1} + 3f_N}{2h}$$

$$\text{Intermediate:} \quad f'(x_i) \approx \frac{f_{i+1} - f_{i-1}}{2h} \qquad (i = 2, \ldots, N-1)$$

These are second-order formulas, because the errors scale like h^2. An equally accurate estimate for the second derivative is as follows.

$$f''(x_i) \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} \qquad (i = 2, \ldots, N-1)$$

5.1. Finite Differences.

In general, a *finite difference* approximate to the value of some derivative of a function $u(x)$ at a point x_0 in its domain, say $u'(x_0)$ or $u''(x_0)$, relies on a suitable combination of sampled function values at nearby points. The underlying formalism used to construct these approximation formulae is known as the *calculus of finite differences*. Its development has a long and influential history, dating back to Newton.

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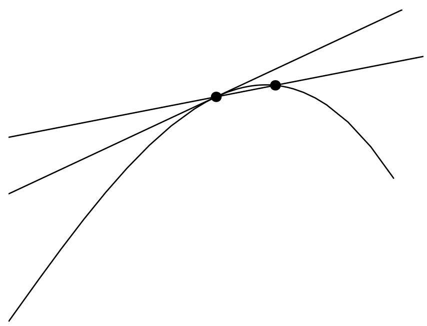
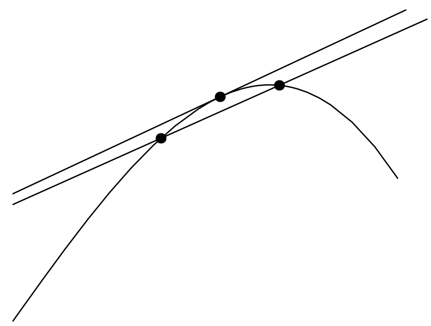


Forward Difference



Central Difference

Figure 5.1. Finite Difference Approximations.

We begin with the first order derivative. The simplest finite difference approximation is the ordinary *difference quotient*

$$\frac{u(x+h)-u(x)}{h} \approx u'(x) \tag{5.1}$$

that appears in the original calculus definition of the derivative. Indeed, if u is differentiable at x, then $u'(x)$ is, by definition, the limit, as $h \to 0$ of the finite difference quotients. Geometrically, the difference quotient measures the slope of the secant line through the two points $(x, u(x))$ and $(x+h, u(x+h))$ on the graph of the function. For small h, this should be a reasonably good approximation to the slope of the tangent line, $u'(x)$, as illustrated in the first picture in Figure 5.1. Throughout our discussion, h, the *step size*, which may be either positive or negative, is assumed to be small: $|\,h\,| \ll 1$. When $h > 0$, (5.1) is referred to as a *forward difference*, while $h < 0$ yields a *backward difference*.

How close an approximation is the difference quotient? To answer this question, we assume that $u(x)$ is at least twice continuously differentiable, and examine its first order Taylor expansion

$$u(x+h) = u(x) + u'(x)\,h + \tfrac{1}{2}\,u''(\xi)\,h^2 \tag{5.2}$$

at the point x. We have used the Cauchy form for the remainder term, [**7**, **129**], in which ξ, which depends on both x and h, is a point lying between x and $x+h$. Rearranging (5.2), we find

$$\frac{u(x+h)-u(x)}{h} \; - \; u'(x) = \tfrac{1}{2}\,u''(\xi)\,h.$$

Thus, the *error* in the finite difference approximation (5.1) can be bounded by a multiple of the step size:

$$\left|\, \frac{u(x+h)-u(x)}{h} \; - \; u'(x) \,\right| \le C\,|\,h\,|,$$

where $C = \max \frac{1}{2}\,|\,u''(\xi)\,|$ depends on the magnitude of the second derivative of the function over the interval in question. Since the error is proportional to the first power of h, we say that the finite difference quotient (5.1) is a *first order* approximation to the derivative $u'(x)$. When the precise formula for the error is not so important, we will write

$$u'(x) = \frac{u(x+h)-u(x)}{h} + \mathrm{O}(h). \tag{5.3}$$

The "big Oh" notation $\mathrm{O}(h)$ refers to a term that is proportional to h, or, more rigorously, bounded by a constant multiple of h as $h \to 0$.

Example 5.1. Let $u(x) = \sin x$. Let us try to approximate

$$u'(1) = \cos 1 = .5403023\ldots$$

by computing finite difference quotients

$$\cos 1 \approx \frac{\sin(1+h) - \sin 1}{h}.$$

The result for smaller and smaller (positive) values of h is listed in the following table.

h	.1	.01	.001	.0001
approximation	.497364	.536086	.539881	.540260
error	$-.042939$	$-.004216$	$-.000421$	$-.000042$

We observe that reducing the step size by a factor of $\frac{1}{10}$ reduces the size of the error by approximately the same factor. Thus, to obtain 10 decimal digits of accuracy, we anticipate needing a step size of about $h = 10^{-11}$. The fact that the error is more or less proportional to the step size confirms that we are dealing with a first order numerical approximation.

To approximate higher order derivatives, we need to evaluate the function at more than two points. In general, an approximation to the n^{th} order derivative $u^{(n)}(x)$ requires at least $n+1$ distinct sample points. For simplicity, we restrict our attention to equally spaced sample points, leaving the general case to the exercises.

For example, let us try to approximate $u''(x)$ by sampling u at the particular points x, $x+h$ and $x-h$. Which combination of the function values $u(x-h), u(x), u(x+h)$ should be used? The answer to such a question can be found by consideration of the relevant Taylor expansions[†]

$$\begin{aligned} u(x+h) &= u(x) + u'(x)\,h + u''(x)\,\frac{h^2}{2} + u'''(x)\,\frac{h^3}{6} + \mathrm{O}(h^4), \\ u(x-h) &= u(x) - u'(x)\,h + u''(x)\,\frac{h^2}{2} - u'''(x)\,\frac{h^3}{6} + \mathrm{O}(h^4), \end{aligned} \tag{5.4}$$

where the error terms are proportional to h^4. Adding the two formulae together gives

$$u(x+h) + u(x-h) = 2\,u(x) + u''(x)\,h^2 + \mathrm{O}(h^4).$$

Dividing by h^2 and rearranging terms, we arrive at the *centered finite difference approximation* to the second derivative of a function:

$$u''(x) = \frac{u(x+h) - 2\,u(x) + u(x-h)}{h^2} + \mathrm{O}(h^2). \tag{5.5}$$

Since the error is proportional to h^2, this forms a second order approximation.

[†] Throughout, the function $u(x)$ is assumed to be sufficiently smooth in order that the derivatives that appear are well defined and the expansion formula is valid.

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Example 5.2. Let $u(x) = e^{x^2}$, with $u''(x) = (4x^2 + 2)\,e^{x^2}$. Let us approximate

$$u''(1) = 6\,e = 16.30969097\ldots$$

by using the finite difference quotient (5.5):

$$u''(1) = 6\,e \;\approx\; \frac{e^{(1+h)^2} - 2\,e + e^{(1-h)^2}}{h^2}\,.$$

The results are listed in the following table.

h	.1	.01	.001	.0001
approximation	16.48289823	16.31141265	16.30970819	16.30969115
error	.17320726	.00172168	.00001722	.00000018

Each reduction in step size by a factor of $\frac{1}{10}$ reduces the size of the error by a factor of about $\frac{1}{100}$, thus gaining two new decimal digits of accuracy. This confirms that the centered finite difference approximation is of second order.

However, this prediction is not completely borne out in practice. If we take $h = .00001$ then the formula produces the approximation 16.3097002570, with an error of .0000092863 — which is *less* accurate than the approximation with $h = .0001$. The problem is that round-off errors due to the finite precision of numbers stored in the computer (in the preceding computation we used single precision floating point arithmetic) have now begun to affect the computation. This highlights the inherent difficulty with numerical differentiation: Finite difference formulae inevitably require dividing very small quantities, and so round-off inaccuracies may lead to noticeable numerical errors. Thus, while finite difference formulae typically produce reasonably good approximations to the derivatives for moderately small step sizes, achieving high accuracy requires switching to higher precision computer arithmetic. Indeed, a similar comment applies to the previous computation in Example 5.1. Our expectations about the error were not, in fact, fully justified, as you may have discovered had you tried an extremely small step size.

Another way to improve the order of accuracy of finite difference approximations is to employ more sample points. For instance, if the first order approximation (5.3) to $u'(x)$ based on the two points x and $x+h$ is not sufficiently accurate, one can try combining the function values at three points, say x, $x+h$, and $x-h$. To find the appropriate combination of function values $u(x-h), u(x), u(x+h)$, we return to the Taylor expansions (5.4). To solve for $u'(x)$, we subtract† the two formulae, and so

$$u(x+h) - u(x-h) = 2\,u'(x)\,h + u'''(x)\,\frac{h^3}{3} + \mathrm{O}(h^4).$$

Rearranging the terms, we are led to the well-known *centered difference formula*

$$u'(x) = \frac{u(x+h) - u(x-h)}{2\,h} + \mathrm{O}(h^2), \tag{5.6}$$

† *Important*: The terms $\mathrm{O}(h^4)$ do *not* cancel, since they represent potentially different multiples of h^4.

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which is a second order approximation to the first derivative. Geometrically, the centered difference quotient represents the slope of the secant line passing through the two points $(x-h, u(x-h))$ and $(x+h, u(x+h))$ on the graph of u centered symmetrically about the point x. Figure 5.1 illustrates the two approximations; the advantages in accuracy of the centered difference version are graphically evident. Higher order approximations can be found by evaluating the function at yet more sample points, say, $x+2h, x-2h$, etc.

Example 5.3. Return to the function $u(x) = \sin x$ considered in Example 5.1. The centered difference approximation to its derivative $u'(1) = \cos 1 = .5403023\ \ldots$ is

$$\cos 1 \approx \frac{\sin(1+h) - \sin(1-h)}{2h}.$$

The results are tabulated as follows:

h	.1	.01	.001	.0001
approximation	.53940225217	.54029330087	.54030221582	.54030230497
error	−.00090005370	−.00000900499	−.00000009005	−.00000000090

As advertised, the results are much more accurate than the one-sided finite difference approximation used in Example 5.1 at the same step size. Since it is a second order approximation, each reduction in the step size by a factor of $\frac{1}{10}$ results in two more decimal places of accuracy — up until the point where the effects of round-off error kick in.

Many additional finite difference approximations can be constructed by similar manipulations of Taylor expansions, but these few very basic formulae, plus some derived in the exercises, will suffice for our purposes. In the following sections, we will employ the finite difference formulae to devise numerical solution schemes for a variety of partial differential equations. Applications to the numerical integration of ordinary differential equations can be found, for example, in [**24**, **73**, **80**].

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 $\Delta x_i \neq \Delta x_{i+1}$.

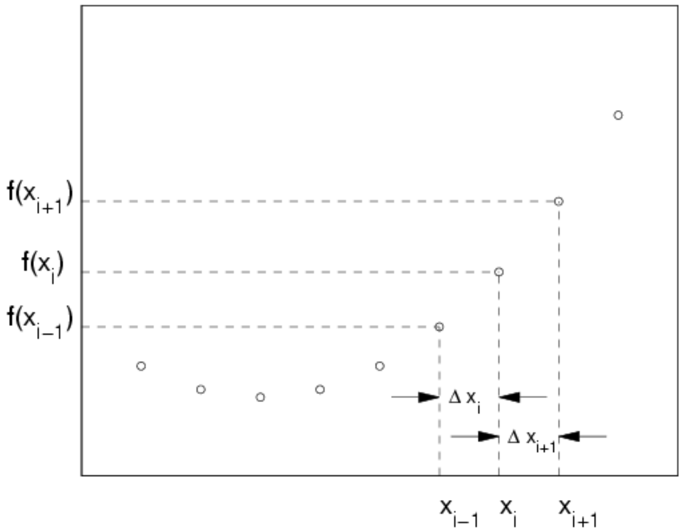

Figure 1: Data set of N points at $x = x_i$ with values $f(x_i)$

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

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

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

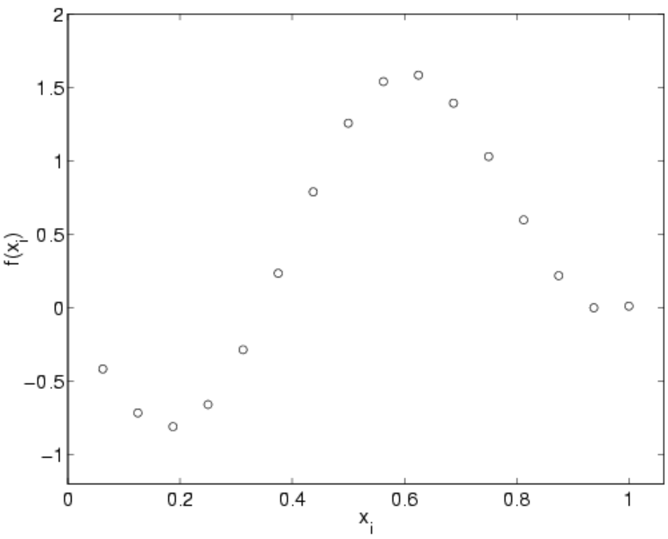

Figure 2: A data set consisting of $N = 16$ points.

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

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

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

$$\text{Error} = k\Delta x^n\,, \tag{15}$$

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

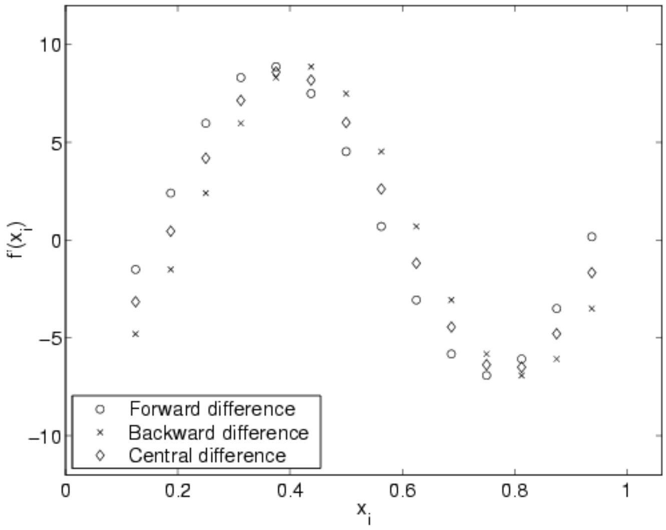

Figure 3: Approximation to the first derivative of the data shown in Figure 2 using three different approximations.

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,

$$f_i' = -\frac{1}{2\Delta x} f_{i-1} + 0 f_i + \frac{1}{2\Delta x} f_{i+1} + \mathcal{O}\left(\Delta x^2\right)\,, \tag{19}$$

$$= a_0 f_{i-1} + a_1 f_i + a_2 f_{i+1} + \mathcal{O}\left(\Delta x^2\right)\,. \tag{20}$$

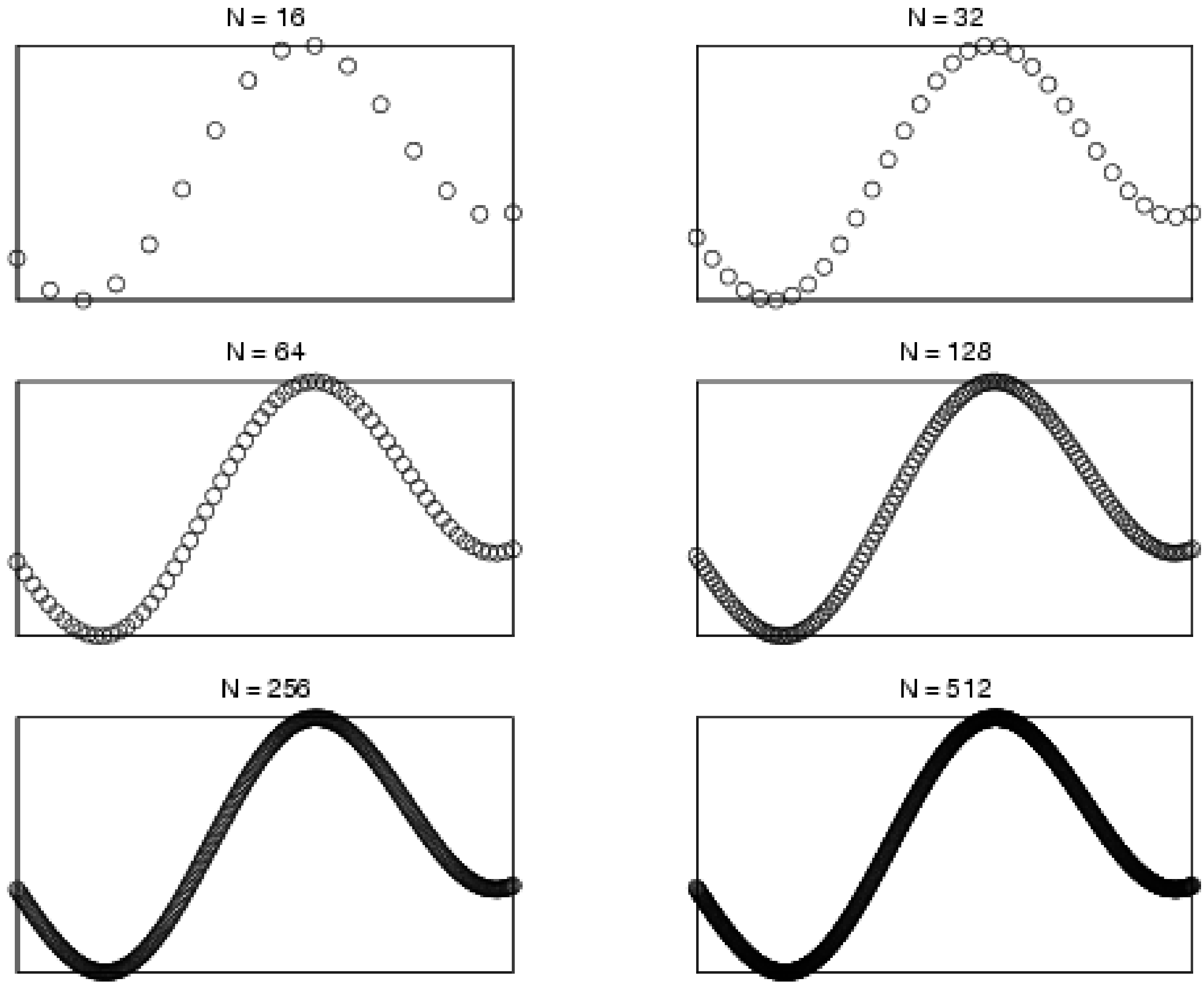

Figure 4: The original data set and 5 more, each with twice as many grid points as the previous one.

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

$$\begin{aligned} f_{i+j} &= f_i + j\Delta x f_i' + \frac{(j\Delta x)^2}{2} f_i'' + \ldots && (21) \\ &= f_i + \sum_{k=1}^{\infty} \frac{(j\Delta x)^k}{k!} f_i^{(k)}\,. && (22) \end{aligned}$$

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

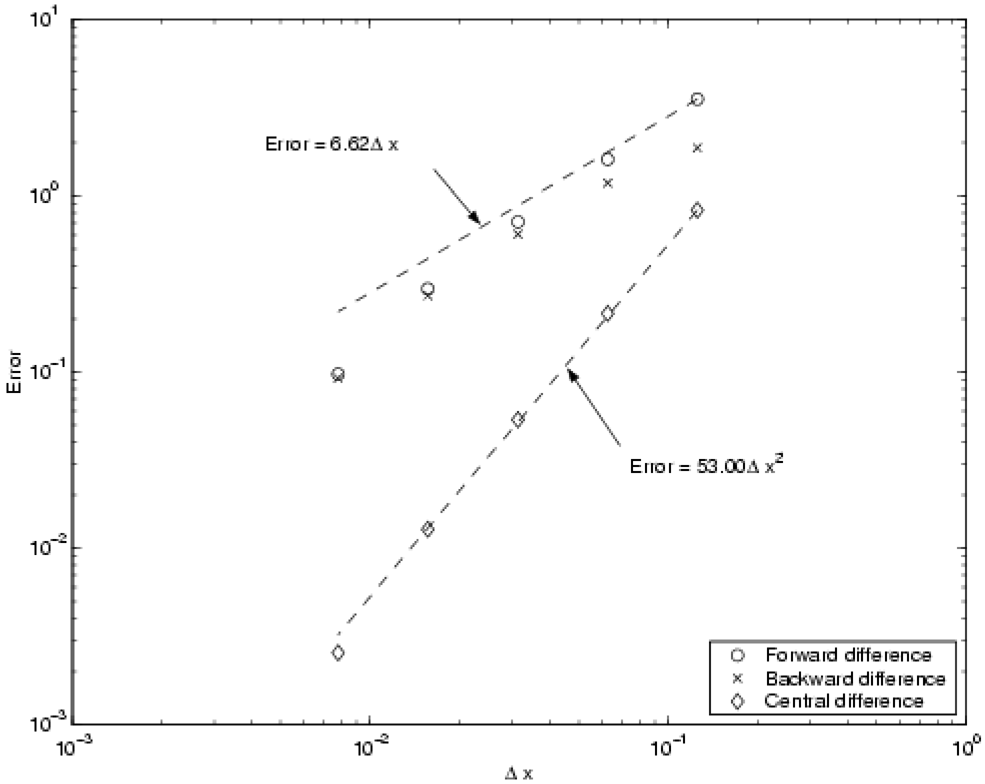

Figure 5: Depiction of the error in computing the first derivative for the forward, backward, and central difference formulas

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

$$f_{i-1} \approx f_i - \Delta x f_i' + \frac{\Delta x^2}{2} f_i'' - \frac{\Delta x^3}{6} f_i''' + \frac{\Delta x^4}{24} f_i^{iv} , \tag{25}$$

$$f_{i+1} \approx f_i + \Delta x f_i' + \frac{\Delta x^2}{2} f_i'' + \frac{\Delta x^3}{6} f_i''' + \frac{\Delta x^4}{24} f_i^{iv} , \tag{26}$$

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.