Mathematical Methods for Engineers

by
Sourabh V. Apte
Computational Flow Physics Laboratory
Oregon State University
Corvallis, OR 97331

Contents

Chapter 3

Taylor Series Expansion

Consider a function $f(x)$. Let's assume that we know the value of the function at $x = a$ (i.e. $f(a)$ is known). We also assume that first $(n+1)$ derivatives of $f(x)$ at $x = a$ are continuous on an interval containing a and x. Then the function at any point x *is* given by the following Taylor Series expansion, [1]

$$f(x) = f(a) + f'(a)(x-a) + \frac{f''(x-a)^2}{2!} + \frac{f'''(a)(x-a)^3}{3!} + ... + \frac{f^{(n)}(a)(x-a)^n}{n!} + R_n, \tag{3.0.1}$$

where f', f'', $f^(n)$ represent the first, second and the nth derivative of $f(x)$ and R_n is the remainder of the infinite series,

$$R_n = \frac{(x-a)^{n+1}}{(n+1)!} f^{n+1}(x^*), \tag{3.0.2}$$

where x^* is some value such that $x^* \in [a, x]$.

This is called the Taylor series expansion of $f(x)$ about a point $x = a$. This also tells us that a smooth function $f(x)$ can be approximated by an infinite series based on higher degree polynomials. If we truncate the Taylor series to a few terms (say first two terms), we get an "approximate" value of f at some point x, using properties at a neighboring point $x = a$. For example, truncating the series after the first two terms gives,

$$f(x) \approx f(a) + f'(a)(x-a). \tag{3.0.3}$$

Here we are assumming that we know the values of the function f and its derivatives at the point $x = a$. Knowing that, we can approximate $f(x)$. This is an approximation because we neglected all the other terms in the series. Such approximations will lead to error in the evaluation of $f(x)$. This error introduced by truncating the Taylor series is termed as 'truncation error'.

3.1 Order of Expansion and Truncation Error

Let us say we have a function $f(x)$. The curve $f(x)$ versus x is shown by the solid line in figure 3.1. Let us assume that we know the value of $f(x)$ at $x = x_i$ as well as all the

[1] Taylor series concept was first formulated by Scottish mathematicial James Gregory and formally introduced by the English mathematicial Brook Taylor. If the Taylor series is centered at zero, then it is called the Maclaurin series. For more information on history read more at `https://en.wikipedia.org/wiki/Taylor_series`

higher derivatives of this function at $x = x_i$. Here we also implicitly assume that the function is continuous and all its derivatives are continuous too. We can use the Taylor series to estimate the value at $x = x_{i+1}$, a point in the neighborhood of x_i, such that $x_{i+1} = x_i + h$. Writing a Taylor series expansion around the point x_i, we get,

$$f(x_{i+1}) = f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)(x_{i+1} - x_i)^2}{2!} + \frac{f'''(x_i)(x_{i+1} - x_i)^3}{3!} + \text{h.o.t.} \tag{3.1.1}$$

$$f(x_{i+1}) = f(x_i) + hf'(x_i) + \frac{h^2}{2!}f''(x_i) + \frac{h^3}{3!}f'''(x_i) + ..\text{h.o.t.} \tag{3.1.2}$$

where 'h.o.t.' stands for higher order terms or the remainder terms.

Now let us truncate the Taylor series at different locations and see the effect of these approximations or truncations.

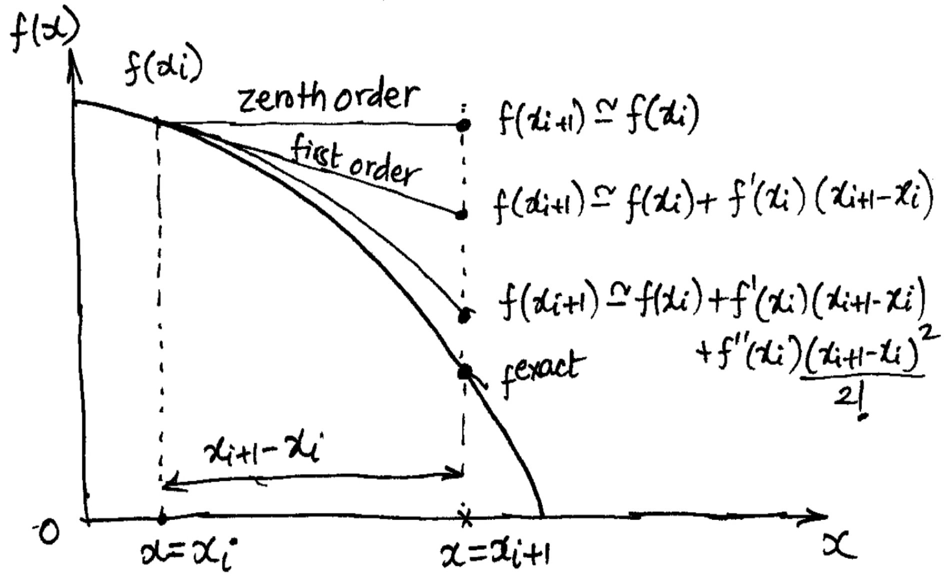

Figure 3.1: Taylor series order of expansion.

3.1.1 Zeroth Order Expansion

Let us truncate the series after the first term. This is called the zeroth order Taylor series expansion,

$$f(x_{i+1}) \approx f(x_i). \tag{3.1.3}$$

This tells us that value of $f(x_{i+1})$ is the same as the value of $f(x_i)$ and represents a horizontal line in the figure 3.1.This is the least accurate approximation (see the graph). Note that the error in the zeroth order approximation is zero if the function $f(x)$ is constant (or horizontal line). That is if we have a function $f(x)$ = constant, then the zeroth-order approximation is an exact approximation without any truncation error. But for a general non-constant function it does introduce an error. Since the given function is not a constant, there is an error owing to not including all the terms in the Taylor series expansion. As can be seen from the figure 3.1, this error can be calculated by using the exact value of the function at x_{i+1} and using the zeroth-order expansion value. The magnitude of the difference between the two (ϵ^{zeroth}) will be equal to the magnitude of the truncation error, R_0.

$$\epsilon^{zeroth} = |f(x_{i+1}) - f^{exact}_{x_{i+1}}| = |R_0|.$$

Note that the remainder of the Taylor series is also given as,

$$R_0 = hf'(x^*), \tag{3.1.4}$$

where x^* is some value of x between x_i and x_{i+1}. To understand this truncation error better, notice that $f'(x^*) = R_0/h$, denotes the slope of the line joining the two points $(x_i, f(x_i))$ and $(x_{i+1}, f(x_{i+1}))$. The point x^* then denotes the point between x_i and x_{i+1} such that the slope of (given by the first derivative) of the curve at that point is exactly equal to the slope of the straight line joining the points between $f(x_i)$ and $f(x_{i+1})$.

The above approximation then **represents the zeroth-order Taylor series expansion** approximating the function $f(x)$. The **truncation error incurred in such an approximation, R_0 is of order h^1, or first-order, written as $\mathcal{O}(h)$.**

3.1.2 First Order Expansion

Let us keep the first two terms in our Taylor series $f(x_{i+1}) \approx f(x_i) + f'(x_i)(x_{i+1} - x_i)$. In this case, we also need the value of the first derivate of $f(x)$ at $x = x_i$. This first derivative is basically the "slope" of the curve at $x = x_i$. Hence this approximation is called a"linear" approximation (a straight line drawn at $x = x_i$, as in the graph, is the slope of the curve at $x = x_i$). Then the approximate value of $f(x_{i+1})$ is a little bit closer to $f^{exact}(x_{i+1})$ as shown in the curve. The error obtained from this first order expansion is thus smaller than that in the zeroth order expansion for the case shown. With first order expansions, we can represent "linear functions" exactly (with zero error). The truncation error for the first-order expansion is,

$$R_1 = \frac{h^2}{2!} f''(x^*), \tag{3.1.5}$$

and it is of the order h to the second power, or second-order. Similarly, we can continue to keep more and more terms in our Taylor series and our approximation will get better with smaller errors. To illustrate this, let us look at the following example.

3.1.3 Example Evaluating Truncation Errors

Consider a function $f(x) = \cos(x)$. Let us assume that we know $f(x)$ and its derivatives at $x_i = \pi/4$ (i.e. use $\cos(x)$ to find these values). Our goal is to estimate $f(x)$ at $x_{i+1} = \pi/3$ using Taylor series expansion. Find the first 6^{th} order estimates, and the errors using the exact value at $\pi/3$, which is, $f^{exact}(\pi/3) = 0.5$.

Let us find $f(\pi/3)$ using zeroth order expansion.

$$f(x_{i+1}) \approx f(x_i) \rightarrow f(\pi/3) \approx f(\pi/4) = 0.707106$$

$\therefore$ Relative error in the zeroth order expansion is
$\epsilon^{rel} = \frac{f^{exact} - f^{appr}}{f^{exact}} \times 100 = \frac{0.5 - 0.707106}{0.5} \times 100 = -41.4\%$

Table 3.1: Truncation Error in Taylor Series Expansion.

Expansion Order n	$f^{(n)}(x)$	$f^{appr}(\pi/3)$	ϵ^{rel} %
0	$\cos(x)$	0.707106	-41.4
1	$-\sin(x)$	0.521986	-4.4
2	$-\cos(x)$	0.49775	0.449
3	$\sin(x)$	0.499869	2.62×10^{-2}
4	$\cos(x)$	0.500007	-1.51×10^{-3}
5	$-\sin(x)$	0.5000003	-6.08×10^{-5}
6	$-\cos(x)$	0.499999	2.44×10^{-6}

Likewise, first order expansion will give, $f(x_{i+1}) \approx f(x_i)+f'(x_i)(x_{i+1}-x_i)$, $x_{i+1} = \pi/3$, $x_i = \pi/4$, $f(x) = \cos(x)$, $f'(x) = \sin(x)$. This gives, $f(\pi/3) \approx 0.521986$ with relative error $\epsilon^{rel} = -4.4\%$.

Error decreases as more terms are included in the Taylor series expansion. Let $h = x_{i+1} - x_i$. We are then usually interested in how the error in our approximation changes (or depends) on h.

For example, for zeroth order expansion, $f(x_{i+1}) \approx f(x_i) + O(h)$. Here the error (truncation error) is proportional to the step size (h). We typically are interested in how the "leading" order trunction error changes with the step size. First order expansion using Taylor series gives, $f(_{x_{i+1}}) \approx f(x_i) + hf'(x_i)$. The leading order truncation error is proportional to h^2. This also means that, as we decrease h, the truncation error goes down. If the truncation error is of first order, i.e. is proportional to h, then if h is reduced by a factor of 1/2, the error will also reduce by a factor of half. If the truncation error is of the second order, then it is proportional to h^2, then if h is reduced by a factor of 1/2, the error is reduced by a factor of $1/4^{\text{th}}$.

Taylor series expansion forms a basis for several finite difference methods used in numerical analysis. When using Taylor series we implicitly assume continuous functions with continuous derivatives.

3.2 Taylor Series for Error Propagation and Uncertainty Quantification

Taylor series can be used to study error propagation in a given problem. Consider a function of a single variable $f(x)$. Assume $\tilde{x}$ is an approximation of x (potentially because of uncertainty in measuring x accurately). We would like to asses the effect of this approximation on the function value. That is we would like to get $\Delta f(\tilde{x}) = |f(x) - f(\tilde{x})|$. This is the absolute of the difference between the true value and the estimated value. It is not straightforward to estimate this, since the true x is unknown (we only know it with some uncertainty).

Consider a function $f(x) = x^3$. If a value of $\tilde{x} = 2.5$ is measured with an error of $\Delta\tilde{x} = 0.01$, estimate the resulting error in $f(x)$. That is, we want to estimate $\Delta f(\tilde{x}) = |f(x) - f(\tilde{x})|$ at $\tilde{x} = 2.5$. If we assume that $f(\hat{x})$ is a continuous and differentiable function, from Taylor series we know that,

$$f(x) = f(\tilde{x}) + (x-\tilde{x})f'(\tilde{x}) + \frac{(x-\tilde{x})^2}{2!}f''(\tilde{x}) + ... \quad (3.2.1)$$

$$\therefore |f(x) - f(\tilde{x})| = \Delta f(\tilde{x}) \approx |f'(\tilde{x})|\Delta\tilde{x} \text{ (truncated after first derivative)}, \quad (3.2.2)$$

where $\Delta\hat{x} = |x - \hat{x}|$ represents the 'error' in x, and $\Delta f(\hat{x}) = |f(x) - f(\hat{x})|$ represents the 'estimation' of error in the function value $f(x)$. Evaluating the derivatives,

$$f'(\tilde{x} = 2.5) == 2\hat{x}^2 = 3 \times 2.5^2 \quad (3.2.3)$$

$$\Delta\tilde{x} = |x - \tilde{x}| = 0.01(\text{given}) \quad (3.2.4)$$

$$\therefore \Delta f(\tilde{x}) = 3 \times 2.5^2 \times 0.01 = 0.1875. \quad (3.2.5)$$

Because $f(2.5) = 15.625$ we get, $f(2.5) = 15.625 \pm 0.1875$. Thus an error of 0.01 in measurement of x results in almost 18 times more error in $f(x)$ due to the non-linearity of the function $f(x)$. Note that, this error in function value is just an estimate, and not the true error as shown in figure 3.2.

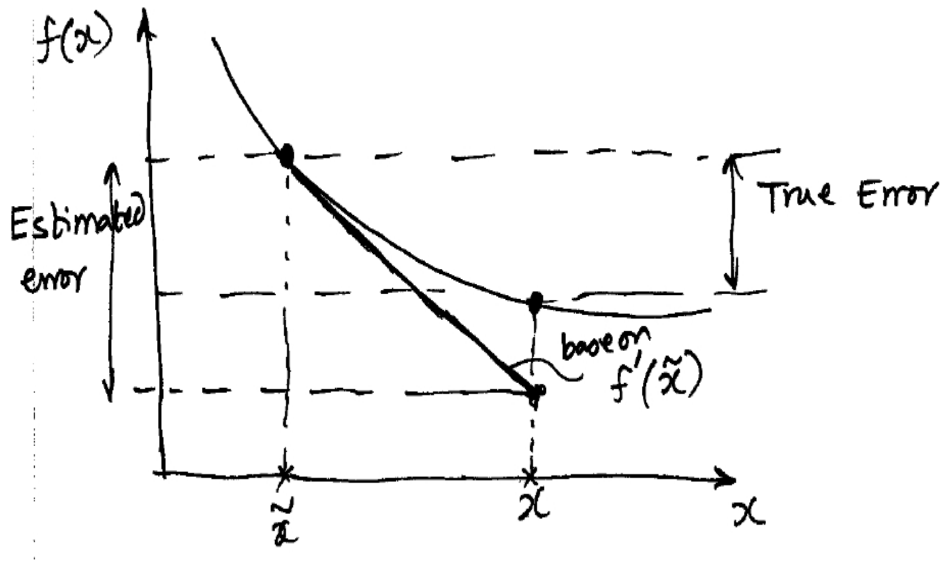

Figure 3.2: Estimation of error propagation.

3.3 Taylor Series and Error Propagation for Multiple Variables

Taylor series expression that we have seen so far is for a function of one indepdenent variable. It can, however, be generalized to multiple independent variables. Let $f(x, y, z)$ be a function in three-dimensions. Then knowing the function value and all derivatives at (x_i, y_i, z_i), and assuming that the function and its derivatives are continuous, one can evaluate the function value at a neighboring point $(x_{i+1}, y_{i+1}, z_{i+1})$ using the Taylor series as,

$$f(x_{i+1}, y_{i+1}, z_{i+1}) = f(x_i, y_i, z_i) + \left.\frac{\partial f}{\partial x}\right|_i (x_{i+1} - x_i) + \left.\frac{\partial f}{\partial y}\right|_i (y_{i+1} - y_i) + \left.\frac{\partial f}{\partial z}\right|_i (z_{i+1} - z_i) + ...(h.o.t) \quad (3.3.1)$$

The above equation only retains the first derivative terms, but one can continue writing higher-order terms in a similar fashion. This is the Taylor series expansion in multiple variables.

The above expansion can also be used for uncertainty analysis and error propagation due to errors in multiple variables. For example, let us say we want to evaluate the function value at some location $(\tilde{x}, \tilde{y}, \tilde{z})$. However, there are errors in measuring the location itself, i.e. $\Delta\tilde{x}$, $\Delta\tilde{y}$, and $\Delta\tilde{z}$. Then, these errors will propagate into the function evaluation and we are interested in calculating the error in the function. This can be achieved by using the same Taylor series expansion, truncated after the first-order terms, and writing,

$$\Delta f(\tilde{x}, \tilde{y}, \tilde{z}) \approx \left|\frac{\partial f}{\partial x}\right|_{\tilde{x},\tilde{y},\tilde{z}} \times \Delta\tilde{x} + \left|\frac{\partial f}{\partial y}\right|_{\tilde{x},\tilde{y},\tilde{z}} \times \Delta\tilde{y} + \left|\frac{\partial f}{\partial z}\right|_{\tilde{x},\tilde{y},\tilde{z}} \times \Delta\tilde{z}. \tag{3.3.2}$$

This will then give us an error in the function value due to the combined effect of the measurement errors in all the three variables.

3.4 Taylor Series for Numerical Differentiation

In the systems we are interested in, we encouter differential equations with derivatives. We need to know how to numerically approximate these. Taylor series is commonly used to derive numerical approximations for ordinary and partial derivatives. Let us look at approximations for the first derivatives. Consider a function $f(x)$, where x is the independent variable. Let us divide the x coordinate into uniformly spaced grid with step size h. Note that it is not necessary to divide the independent variable using uniform step sizes. Non-uniform step sizes are used to save number of points used in the calculation. However, the approximations derived below are valid for uniformly spaced points. Starting with $x = 0$, the x coordinates of each discrete point can be written as $x_i = ih$, where $i = 0, 1, 2, 3, ...$. Notice that, $x_{i+1} = (i + 1)h = x_i + h$ and likewise, $x_{i-1} = x_i - h$, and so on. We are interested in finding approximate alebraic expressions for df/dx, d^2f/dx^2 etc. at the point x_i, using the function values at neighboring points.

3.4.1 Forward Difference

Now consider Taylor series expansion for $f(x_{i+1})$ around the point x_i.

$$f(x_{i+1}) = f(x_i) + hf'(x_i) + \frac{h^2}{2!}f''(x_i) + ... \tag{3.4.1}$$

If we truncate the above series after the first two terms,

$$f(x_{i+1}) = f(x_i) + hf'(x_i) + \mathcal{O}(h^2) \tag{3.4.2}$$

We could use this equation to get an approximate expression for $f'(x_i)$ or the derivative of $f(x)$ i.e. $\frac{df}{dx}$ at point x_i. Rearranging we get,

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + \mathcal{O}(h) \tag{3.4.3}$$

$$f'(x_i) \approx \frac{f(x_{i+1}) - f(x_i)}{h} \quad \text{(after truncation)}, \tag{3.4.4}$$

where the leading order truncation (L.O.T.) term is given as

$$\text{L.O.T} = -\frac{h}{2!} f''(x_i). \tag{3.4.5}$$

Notice that the negative sign is included in the L.O.T. The truncation error in the first derivative approximation is then said to be proportional to the h^1, that is it is first-order with respect to the step size. In other words, if the step size is reduced by a factor of 2, the truncation error will reduce by a factor of 2, as it is linearly proportional to the step size. It is also important to notice that, equation 3.4.4 involves the function values at x_i and a neighboring point in the *forward* x direction at x_{i+1}. Hence, this approximation is called Forward Differencing. It is important to notice that the left hand side of equation 3.4.4 represents the first derivative of the function f evaluated at the point x_i. The right-hand side represents the slope of the straight line joining the points x_i and x_{i+1}. This slope is also evaluated at the point x_i (see figure 3.3). Thus, the forward differencing formula for the first derivative of the function $f(x)$ at the point x_i is obtained by calculating the slope of the line joining the point x_i and a neighboring point at a distance of h in the forward x direction.

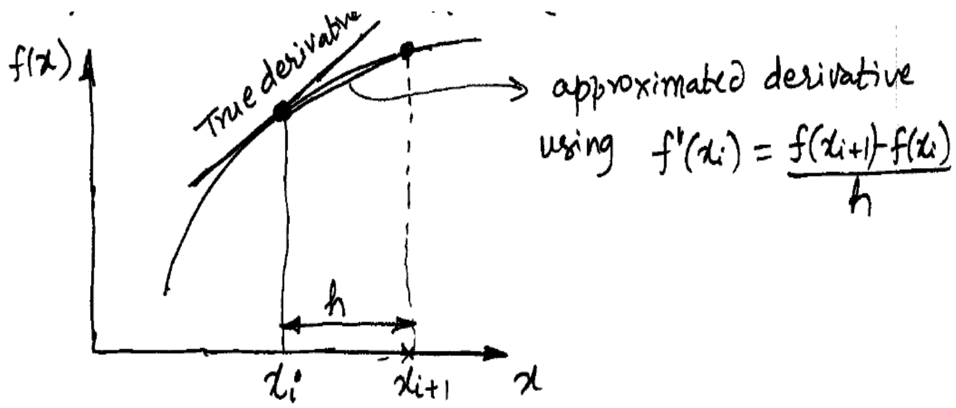

Figure 3.3: Forward differencing for the first derivative.

3.4.2 Backward Differencing

In the above forward differencing approximation, we made use of the information at the points x_i and x_{i+1} and the function values at these points to approximate the first derivative at point x_i. In a similar manner, one can use points x_i and x_{i-1} together with the function values at these two points to approximate the derivative at x_i. The formula obtained will then be called as Backward Differencing, as we use the point backward in x compared to the point at which we are trying to evaluate the first derivative. In general, the two values, obtained from forwarding differencing and backward differencing will be different as they represent different approximations to the slope at x_i. To find the Backward Differencing formula, consider the Taylor Series expansion for $f(x_{i-1})$ around x_i,

$$f(x_{i-1}) = f(x_i) + f'(x_i)(x_{i-1} - x_i) + f''(x_i)\frac{(x_{i-1} - x_i)^2}{2!} + ... \tag{3.4.6}$$

Here, $x_{i-1} - x_i = -h$, the negative sign comes in because we know $x_{i-1} < x_i$ based on the direction of x.

$$\therefore f(x_{i-1}) = f(x_i) - hf'(x_i) + \frac{h^2}{2!}f''(x_i) - \frac{h^3}{3!}f'''(x_i) + ... \tag{3.4.7}$$

If we plan to keep the first two terms on the right hand side and truncate the series after that, we can rewrite this by including the leading order truncation (L.O.T.) term as,

$$\begin{aligned}
f(x_{i-1}) &= f(x_i) - hf'(x_i) + \frac{h^2}{2!}f''(x_i) - ... \\
f'(x_i) &= -\frac{f(x_{i-1}) - f(x_i)}{h} + \frac{h}{2!}f''(x_i) - . \\
f'(x_i) &= \frac{f(x_i) - f(x_{i-1})}{h} + \frac{h}{2!}f''(x_i) - ... \\
\therefore f'(x_i) &\approx \frac{f(x_i) - f(x_{i-1})}{h},
\end{aligned}$$

where we dropped the leading order truncation term in the last step. The above formula is called the backward differencing formula. Notice that the approximate formula has the truncation error of

$$\text{L.O.T.} = +\frac{h}{2!}f''(x_i) = \mathcal{O}(h). \tag{3.4.8}$$

Notice that the magnitude of the leading order truncation term for the forward and backward differencing is same, but the signs are different. Both approximations have errors that are *linearly* proportional to the step size h, and thus they both are first-order accurate. This formula can be visualized as shown in figure 3.4.

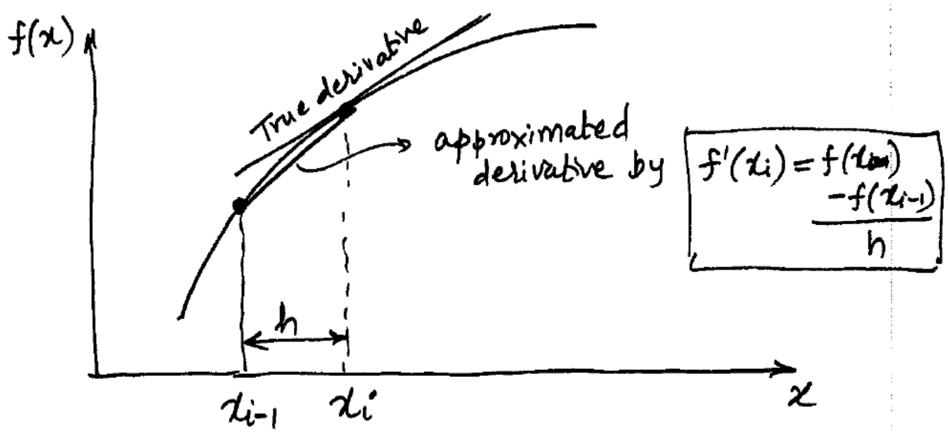

Figure 3.4: Backward differencing formula.

3.4.3 Centered Differencing

Instead of using data from one side of the point x_i, one can use data on either side of the point to approximate the derivative at x_i. If this is done, one can obtain a formula based on the points x_{i-1}, x_i, and x_{i+1} and the function values at these points. This formula will be called as centered differencing, as we will be evaluating the first derivative at the point x_i which is centered around the points x_{i-1} and x_{i+1}. Consider the Taylor series expansions of $f(x_{i+1})$ and $f(x_{i-1})$ around the point x_i. Here we have $x_{i+1} - x_i = x_i - x_{i-1} = h$.

$$f(x_{i+1}) = f(x_i) + hf'(x_i) + \frac{h^2}{2!}f''(x_i) + .. \tag{3.4.9}$$

$$f(x_{i-1}) = f(x_i) - hf'(x_i) + \frac{h^2}{2!}f''(x_i) + .. \tag{3.4.10}$$

Subtracting the second equation from the first one, and only keeping the leading order truncation term after the f' term in the series, we get,

$$f(x_{i+1}) - f(x_{i-1}) = 2hf'(x_i) + \frac{2h^3}{3!}f'''(x_i) + ... \tag{3.4.11}$$

$$\therefore f'(x_i) = \frac{f(x_{i+1} - f(x_{i-1})}{2h} - \frac{h^2}{3!}f'''(x_i) + ... \tag{3.4.12}$$

$$\therefore f'(x_i) \approx \frac{f(x_{i+1}) - f(x_{i-1})}{2h}, \tag{3.4.13}$$

where we dropped the leading order truncation term in the last step to obtain an approximate formula. The leading order truncation term is,

$$\text{L.O.T.} = -\frac{h^2}{3!}f'''(x_i) = \mathcal{O}(h^2). \tag{3.4.14}$$

Therefore, the central differencing formula is second-order accurate. We find that, by using the points on either side of x_i, there is cancellation of some of the terms in the Taylor series and this results in higher order accuracy. Notice that the formula consists of the function values at x_{i+1} and x_{i-1}, but it approximates the derivative at the mid-way between the two points, that is at x_i. Figure 3.5 shows the graphic representation of the slope of the curve approximated by using the central differencing.

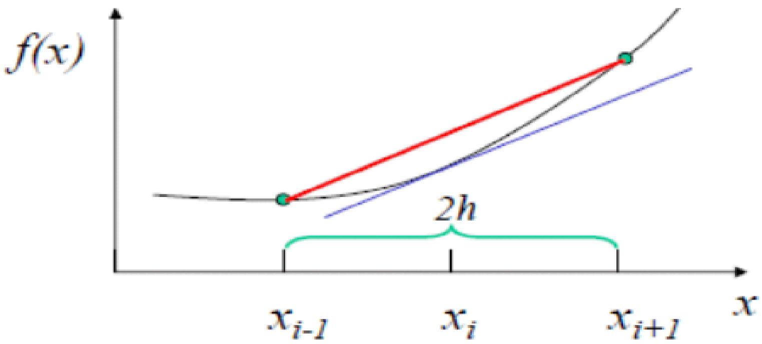

Figure 3.5: Central differencing for first derivative.

Another way to look at the three approximations, Forward, Backward and Central differencing and their accuracy, is to think of the fact that, if we have two points, the highest order accurate polynomial we can fit is a straight-line. However, if we have three points, one can fit a quadratic function. The accuracy of the three formulas are also related to this.

Notice that if we has added the two Taylor series expansions for $f(x_{i+1})$ and $f(x_{i-1})$ (equations 3.4.9 and 3.4.10), we will get rid of the first derivative term. Then, we can derive a formula for the second derivative at $f''(x_i)$.

$$
\begin{aligned}
f''(x_i) &= \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2} - 2\frac{h^2}{4!}f''''(x_i) - .....\\
\therefore f''(x_i) &= \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2} - \mathcal{O}(h^2)\\
\therefore f''(x_i) &\approx \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2},
\end{aligned}
$$

with the leading order truncation term as

$$\text{L.O.T.} = -\frac{h^2}{12}f''''(x_i) = \mathcal{O}(h^2). \tag{3.4.15}$$

The formula for the second derivative of the function at x_i also uses information at the points x_{i-1}, x_i and x_{i+1} and provides a central difference approximation that is second-order accurate.

3.4.4 Other Differencing Formulae

Using the method outline above, it is possible to have a number of different approximations for the first as well as second derivatives. For example, instead of using only one point on either side of x_i, one can use two points on either side. That is, if we use the function values at x_{i-2}, x_{i-1}, x_i, x_{i+1}, and x_{i+2}, we will be using more information, and thus we should be able to obtain a higher order approximation for the first derivative. With five points, we can fit a fourth-order polynomial, and thus we will get a fourth-order approximation for the first derivative. This can be done by simply writing Taylor series expansions for $f(x_{i-2})$, $f(x_{i-1})$, $f(x_{i+1})$, and $f(x_{i+2})$ around the point x_i. Then we can manipulate these four expansions such that we get the highest possible order of accuracy for the first derivative. In other words, we should manipulate the expansions such that we can get rid of as many of the higher-order terms (after the first derivative term, we want to keep this as we are interested in finding the first derivative) as possible.

$$f(x_{i+2}) = f(x_i) + (2h)f'(x_i) + \frac{(2h)^2}{2!}f''(x_i) + \frac{(2h)^3}{3!}f'''(x_i) + \frac{(2h)^4}{4!}f'''(x_i) + \frac{(2h)^5}{5!}f''''(x_i).. \tag{3.4.16}$$

$$f(x_{i+1}) = f(x_i) + hf'(x_i) + \frac{h^2}{2!}f''(x_i) + \frac{h^3}{3!}f'''(x_i) + \frac{h^4}{4!}f'''(x_i) + \frac{h^5}{5!}f''''(x_i).. \tag{3.4.17}$$

$$f(x_{i-1}) = f(x_i) - hf'(x_i) + \frac{h^2}{2!}f''(x_i) - \frac{h^3}{3!}f'''(x_i) + \frac{h^4}{4!}f'''(x_i) - \frac{h^5}{5!}f''''(x_i).. \tag{3.4.18}$$

$$f(x_{i-2}) = f(x_i) - (2h)f'(x_i) + \frac{(2h)^2}{2!}f''(x_i) - \frac{(2h)^3}{3!}f'''(x_i) + \frac{(2h)^4}{4!}f'''(x_i) - \frac{(2h)^5}{5!}f''''(x_i).. \tag{3.4.19}$$

Now, we want an expression for $f'(x_i)$ of highest possible order of accuracy using the above four equations. Notice that, if we subtract equation 3.4.19 from equation 3.4.16 the even powered terms cancel out, and the odd powered terms double. Likewise, same thing will happen if we subtract equation 3.4.18 from equation 3.4.17. Now, if we want the highest possible accuracy, we should also try to get rid of the cubic term. This can be done if we do [eq. 3.4.16 - eq. 3.4.19 - 8 × (eq. 3.4.17 - eq. 3.4.18)]. Then, we get,

$$f(x_{i+2}) - 8f(x_{i+1}) + 8f(x_{i-1}) - f(x_{i-2}) = -12hf'(x_i) + 48\frac{h^5}{5!}f'''''(x_i) + ...$$

Dividing the whole equation by $(-12h)$ and rearranging,

$$
\begin{aligned}
\therefore f'(x_i) &= \frac{f(x_{i+2}) - 8f(x_{i+1}) + 8f(x_{i-1}) - f(x_{i-2})}{(-12h)} - \frac{48}{(-12h)}\frac{h^5}{5!}f'''''(x_i) + ... \\
\therefore f'(x_i) &= \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h} + \frac{h^4}{30}f'''''(x_i) + ... \\
\therefore f'(x_i) &= \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h} + \mathcal{O}(h^4) \\
\therefore f'(x_i) &\approx \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h}.
\end{aligned}
$$

This gives us a fourth-order accurate formula for the first derivative at the point x_i with the leading order truncation term as

$$
\text{L.O.T.} = +\frac{h^4}{30}f'''''(x_i) = \mathcal{O}(h^4). \tag{3.4.20}
$$

Notice that due to the symmetry of the data (two on either side of x_i), we got a symmetric fourth-order formula.

If on the other hand, we wanted to use information only on one-side of the point x_i (say only on the backward side), wherein we use the points x_i, x_{i-1}, and x_{i-2}, we will get a one-sided differencing formula. Since we are using three points, we can fit a quadratic through the points, and one can expect a second-order accurate approximation for the first derivative,

$$
\begin{aligned}
f'(x_i) &= \frac{f_{i-2} - 4f_{i-1} + 3f_i}{2h} + \frac{h^2}{3}f'''(x_i) + ... \\
f'(x_i) &= \frac{f_{i-2} - 4f_{i-1} + 3f_i}{2h} + \mathcal{O}(h^2)
\end{aligned}
$$

Similarly, using three points on the right side, we can get another one-sided differencin formula that is second-order accurate,

$$
\begin{aligned}
f'(x_i) &= \frac{-f_{i-2} + 4f_{i-1} - 3f_i}{2h} - \frac{h^2}{3}f'''(x_i) + ... \\
f'(x_i) &= \frac{-f_{i-2} + 4f_{i-1} - 3f_i}{2h} - \mathcal{O}(h^2)
\end{aligned}
$$