NUMERICAL DIFFERENTIATION

1 Introduction

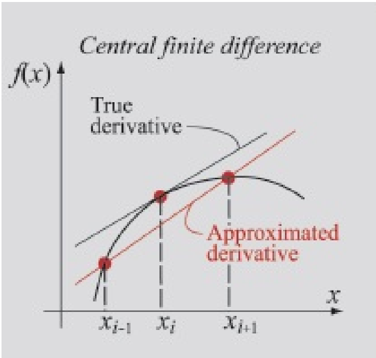
Differentiation is a method to compute the rate at which a dependent output y changes with respect to the change in the independent input x. This rate of change is called the derivative of y with respect to x. In more precise language, the dependence of y upon x means that y is a function of x. This functional relationship is often denoted $y = f(x)$, where f denotes the function.

- If x and y are real numbers, and if the graph of y is plotted against x, the derivative measures the slope of this graph at each point.
- When the functional dependence is given as a simple mathematical expression, the derivative can be determined analytically. When analytical differentiation of the expression is difficult or not possible, numerical differentiation has to be used.
- When the functional dependence is specified as a set of discrete points, differentiation is completed using a numerical method.

For a given set of points two approaches can be used to calculate a numerical approximation of the derivative at one of the points

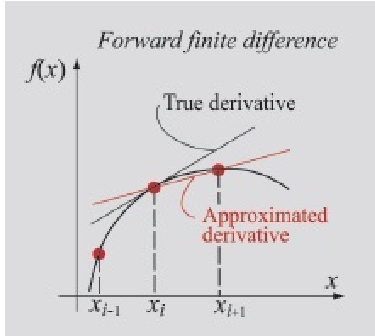
- **Finite difference approximation:** In this approach we approximate the derivative based on values of points in the neighborhood of the point. **The accuracy of a finite difference approximation depends on the accuracy of the data points, the spacing between the point, and the specific formula used for the approximation**. In the example below, the first derivative at x_i is approximated by the slope of the line connecting the points adjacent to x_i. This approximation is called **Two points central difference approximation**.

$$\frac{df}{dx}|_{x=x_i} = \frac{f(x_{i+1}) - f(x_{i-1})}{x_{i+1} - x_{i-1}}$$



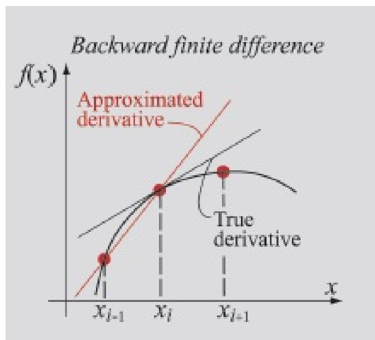
- Two additional two points finite difference approximations:
  - **Two points forward difference approximation** where the first derivative x_i is approximated by the slope of the line connecting x_i and $x_i + 1$

$$\frac{df}{dx}|_{x=x_i} = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}$$

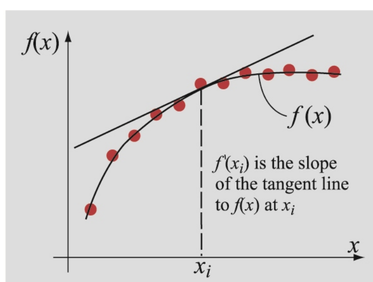


- **Two points backward difference approximation** where the first derivative x_i is approximated by the slope of the line connecting x_i and $x_i - 1$

$$\frac{df}{dx}|_{x=x_i} = \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}}$$

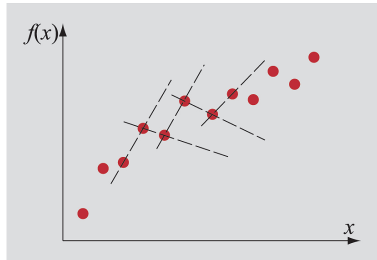


- The second approach is to approximate the points with an analytical expression that can be easily differentiated and then to calculate the derivative by differentiating the analytical expression. The approximate analytical expression can be derived using curve fitting.



Note:

- Sometimes when the measured data contain scatter as shown in the figure below, using one of the two points finite difference approximation may be erroneous and better results may be obtained using a higher order finite difference approximation as will be discussed later in this chapter or by using a curve fit. This eliminates the problem of wrongly amplified slopes between successive points.



2 Finite difference formulas using Taylor series expansion

2.1 Taylor series expansion of a function

Taylor series expansion of a function is a way to find the value of a function near a known point, that is, a point where the value of the function is known. The function is represented by a sum of terms of a convergent series. In some cases (if the function is a polynomial), the Taylor series can give the exact value of the function. In most cases, however, a sum of an infinite number of terms is required for the exact value. If only a few terms are used, the value of the function that is obtained from the Taylor series is an approximation.

Given a function that is differentiable $(n+1)$ times in an interval containing a point x_o, Taylor's theorem states that for each x in the interval, there exists a value η between x and x_o such that:

$$f(x) = f(x_o) + (x - x_o)\frac{df}{dx}|_{x=x_o} + \frac{(x-x_o)^2}{2!}\frac{d^2f}{dx^2}|_{x=x_o} + ... + \frac{(x-x_o)^n}{n!}\frac{d^nf}{dx^n}|_{x=x_o} + R_n(\eta)$$

where the remainder $R_n(x)$ is given by

$$R_n(\eta) = \frac{(x-x_o)^{n+1}}{(n+1)!}\frac{d^{n+1}f}{dx^{n+1}}|_{x=\eta}$$

2.2 Finite difference formulas of first derivatives

Several finite difference formulas, including the two points finite difference approximations can be derived from the Taylor series expansion of the function. These approximations varies in the number of points involved in the approximation, the spacing and accuracy of the measured values. We assume the spacing between adjacent points to be fixed and equal to h

- Two points forward difference approximation

$$f(x_{i+1}) = f(x_i) + (x_{i+1} - x_i)\frac{df}{dx}|_{x=x_i} + \frac{(x_{i+1}-x_i)^2}{2!}\frac{d^2f}{dx^2}|_{x=\eta}$$

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

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{h}{2!}f''(\eta)$$

  - If the second term is ignored, the previous expression reduces to the two points forward difference approximation.

– Ignoring the second term introduces a truncation error that is proportional to h. The truncation error is said to be of on the order of h

$$\mathit{truncation\ error} = -\frac{h}{2!} f''(\eta) = O(h)$$

- Two points backward difference approximation

$$f(x_{i-1}) = f(x_i) + (x_{i-1} - x_i)\frac{df}{dx}|_{x=x_i} + \frac{(x_{i-1} - x_i)^2}{2!}\frac{d^2 f}{dx^2}|_{x=\eta}$$

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

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} + \frac{h}{2!} f''(\eta)$$

  – If the second term is ignored, the previous expression reduces to the two points backward finite difference approximation.
  – Ignoring the second term introduces a truncation error that is proportional to h. The truncation error is said to be of on the order of h

$$\mathit{truncation\ error} = -\frac{h}{2!} f''(\eta) = O(h)$$

- Two points central difference approximation

$$f(x_{i+1}) = f(x_i) + (x_{i+1} - x_i)\frac{df}{dx}|_{x=x_i} + \frac{(x_{i+1} - x_i)^2}{2!}\frac{d^2 f}{dx^2}|_{x=x_i} + \frac{(x_{i+1} - x_i)^3}{3!}\frac{d^3 f}{dx^3}|_{x=\eta_1}$$

$$f(x_{i-1}) = f(x_i) + (x_{i-1} - x_i)\frac{df}{dx}|_{x=x_i} + \frac{(x_{i-1} - x_i)^2}{2!}\frac{d^2 f}{dx^2}|_{x=x_i} + \frac{(x_{i+1} - x_i)^3}{3!}\frac{d^3 f}{dx^3}|_{x=\eta_2}$$

$$f(x_{i+1}) = f(x_i) + hf'(x_i) + \frac{h^2}{2!} f''(x_i) + \frac{h^3}{3!} f'''(\eta_1)$$

$$f(x_{i-1}) = f(x_i) - hf'(x_i) + \frac{h^2}{2!} f''(x_i) - \frac{h^3}{3!} f'''(\eta_2)$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{h} + \frac{h^2}{3!} f'''(\eta_1) - \frac{h^2}{3!} f'''(\eta_2)$$

  – If the second term is ignored, the previous expression reduces to the two points central finite difference approximation.
  – Ignoring the second term introduces a truncation error that is proportional to h^2. The truncation error is said to be of on the order of h^2

$$\mathit{truncation\ error} = \frac{h^3}{3!} f'''(\eta_1) - \frac{h^2}{3!} f'''(\eta_2) = O(h^2)$$

  – A comparison between the last three approximations show that for small h, the central difference approximation gives better approximation that the forward or backward approximations.
  – The central difference approximation is useful only for interior points and not for the end points x_1 or x_n

- Three points forward difference approximation

$$f(x_{i+1}) = f(x_i) + hf'(x_i) + \frac{h^2}{2!}f''(x_i) + \frac{h^3}{3!}f'''(\eta_1)$$

$$f(x_{i+2}) = f(x_i) + 2hf'(x_i) + \frac{(2h)^2}{2!}f''(x_i) + \frac{(2h)^3}{3!}f'''(\eta_2)$$

$$f'(x_i) = \frac{-3f(x_i) + 4f(x_{i+1}) - f(x_{i+2})}{2h} - \frac{2h^2}{3!}f'''(\eta_1) + \frac{4h^2}{3!}f'''(\eta_2)$$

  - If the second term is ignored, the previous expression reduces to the three points forward finite difference approximation.
  - Ignoring the second term introduces a truncation error that is proportional to h^2. The truncation error is said to be of on the order of h^2

$$truncation\ error = -\frac{2h^2}{3!}f'''(\eta_1) + \frac{4h^2}{3!}f'''(\eta_2) = O(h^2)$$

  - The three points forward difference approximation is only useful for points $i = 1$ to $i = n - 2$

- Three points backward difference approximation

$$f(x_{i-1}) = f(x_i) - hf'(x_i) + \frac{h^2}{2!}f''(x_i) - \frac{h^3}{3!}f'''(\eta_1)$$

$$f(x_{i-2}) = f(x_i) - 2hf'(x_i) + \frac{(2h)^2}{2!}f''(x_i) - \frac{(2h)^3}{3!}f'''(\eta_2)$$

$$f'(x_i) = \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h} - \frac{2h^2}{3!}f'''(\eta_1) + \frac{4h^2}{3!}f'''(\eta_2)$$

  - If the second term is ignored, the previous expression reduces to the three points forward finite difference approximation.
  - Ignoring the second term introduces a truncation error that is proportional to h^2. The truncation error is said to be of on the order of h^2

$$truncation\ error = \frac{2h^2}{3!}f'''(\eta_1) - \frac{4h^2}{3!}f'''(\eta_2) = O(h^2)$$

  - The three points backward difference approximation is only useful for points $i = n$ to $i = 2$

- The same approach can be used to derive the four points central difference approximation

$$f'(x_i) = \frac{f(x_{i-2}) - 8f(x_{i-1}) + 8f(x_{i+1}) - f(x_{i+2})}{12h} + O(h^4)$$

First Derivative		
Method	**Formula**	**Truncation Error**
Two-point forward difference	$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_i)}{h}$	$O(h)$
Three-point forward difference	$f'(x_i) = \dfrac{-3f(x_i) + 4f(x_{i+1}) - f(x_{i+2})}{2h}$	$O(h^2)$
Two-point backward difference	$f'(x_i) = \dfrac{f(x_i) - f(x_{i-1})}{h}$	$O(h)$
Three-point backward difference	$f'(x_i) = \dfrac{f(x_{i-2}) - 4f(x_{i-1}) + 3f(x_i)}{2h}$	$O(h^2)$
Two-point central difference	$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_{i-1})}{2h}$	$O(h^2)$
Four-point central difference	$f'(x_i) = \dfrac{f(x_{i-2}) - 8f(x_{i-1}) + 8f(x_{i+1}) - f(x_{i+2})}{12h}$	$O(h^4)$

2.3 Finite difference formulas of second derivatives

- Three points forward difference approximation

$$f(x_{i+1}) = f(x_i) + hf'(x_i) + \frac{h^2}{2!}f''(x_i) + \frac{h^3}{3!}f'''(\eta_1)$$

$$f(x_{i+2}) = f(x_i) + 2hf'(x_i) + \frac{(2h)^2}{2!}f''(x_i) + \frac{(2h)^3}{3!}f'''(\eta_2)$$

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} - \frac{8h}{3!}f'''(\eta_2) + \frac{h}{3!}f'''(\eta_1)$$

  - If the second term is ignored, the previous expression reduces to the three points forward finite difference approximation.
  - Ignoring the second term introduces a truncation error that is proportional to h. The truncation error is said to be of on the order of h

$$truncation\ error = -\frac{8h}{3!}f'''(\eta_2) + \frac{h}{3!}f'''(\eta_1) = O(h)$$

- Three points backward difference approximation

$$f(x_{i-1}) = f(x_i) - hf'(x_i) + \frac{h^2}{2!}f''(x_i) - \frac{h^3}{3!}f'''(\eta_1)$$

$$f(x_{i-2}) = f(x_i) - 2hf'(x_i) + \frac{(2h)^2}{2!}f''(x_i) - \frac{(2h)^3}{3!}f'''(\eta_2)$$

$$f''(x_i) = \frac{f(x_{i-2}) - 2f(x_{i-1}) + f(x_i)}{h^2} + \frac{8h}{3!}f'''(\eta_2) - \frac{h}{3!}f'''(\eta_1)$$

  - If the second term is ignored, the previous expression reduces to the three points backward finite difference approximation.

– Ignoring the second term introduces a truncation error that is proportional to h. The truncation error is said to be of on the order of h

$$truncation\ error = \frac{8h}{3!}f'''(\eta_2) - \frac{h}{3!}f'''(\eta_1) = O(h)$$

- Three points central difference approximation

$$f(x_{i+1}) = f(x_i) + hf'(x_i) + \frac{h^2}{2!}f''(x_i) + \frac{h^3}{3!}f'''(x_i) + \frac{h^4}{4!}f''''(\eta_1)$$

$$f(x_{i-1}) = f(x_i) - hf'(x_i) + \frac{h^2}{2!}f''(x_i) - \frac{h^3}{3!}f'''(x_i) - \frac{h^4}{4!}f''''(\eta_2)$$

$$f''(x_i) = \frac{f(x_{i+1}) + f(x_{i-1}) - 2f(x_i)}{h^2} + \frac{h^2}{4!}f''''(\eta_2) - \frac{h^2}{4!}f''''(\eta_1)$$

  – If the second term is ignored, the previous expression reduces to the three points central difference approximation.
  – Ignoring the second term introduces a truncation error that is proportional to h^2. The truncation error is said to be of on the order of h^2

$$truncation\ error = \frac{h^2}{4!}f''''(\eta_2) - \frac{h^2}{4!}f''''(\eta_1) = O(h^2)$$

- The same procedure can be used to develop higher order finite difference approximations. The result is summarized in the table below

Second Derivative		
Method	**Formula**	**Truncation Error**
Three-point forward difference	$f''(x_i) = \frac{f(x_i) - 2f(x_{i+1}) + f(x_{i+2})}{h^2}$	$O(h)$
Four-point forward difference	$f''(x_i) = \frac{2f(x_i) - 5f(x_{i+1}) + 4f(x_{i+2}) - f(x_{i+3})}{h^2}$	$O(h^2)$
Three-point backward difference	$f''(x_i) = \frac{f(x_{i-2}) - 2f(x_{i-1}) + f(x_i)}{h^2}$	$O(h)$
Four-point backward difference	$f''(x_i) = \frac{-f(x_{i-3}) + 4f(x_{i-2}) - 5f(x_{i-1}) + 2f(x_i)}{h^2}$	$O(h^2)$
Three-point central difference	$f''(x_i) = \frac{f(x_{i-1}) - 2f(x_i) + f(x_{i+1})}{h^2}$	$O(h^2)$
Five-point central difference	$f''(x_i) = \frac{-f(x_{i-2}) + 16f(x_{i-1}) - 30f(x_i) + 16f(x_{i+1}) - f(x_{i+2})}{12h^2}$	$O(h^4)$

2.4 Finite difference formulas of third and fourth

Third Derivative		
Method	**Formula**	**Truncation Error**
Four-point forward difference	$f'''(x_i) = \dfrac{-f(x_i) + 3f(x_{i+1}) - 3f(x_{i+2}) + f(x_{i+3})}{h^3}$	$O(h)$
Five-point forward difference	$f'''(x_i) = \dfrac{-5f(x_i) + 18f(x_{i+1}) - 24f(x_{i+2}) + 14f(x_{i+3}) - 3f(x_{i+4})}{2h^3}$	$O(h^2)$
Four-point backward difference	$f'''(x_i) = \dfrac{-f(x_{i-3}) + 3f(x_{i-2}) - 3f(x_{i-1}) + f(x_i)}{h^3}$	$O(h)$
Five-point backward difference	$f'''(x_i) = \dfrac{3f(x_{i-4}) - 14f(x_{i-3}) + 24f(x_{i-2}) - 18f(x_{i-1}) + 5f(x_i)}{2h^3}$	$O(h^2)$
Four-point central difference	$f'''(x_i) = \dfrac{-f(x_{i-2}) + 2f(x_{i-1}) - 2f(x_{i+1}) + f(x_{i+2})}{2h^3}$	$O(h^2)$
Six-point central difference	$f'''(x_i) = \dfrac{f(x_{i-3}) - 8f(x_{i-2}) + 13f(x_{i-1}) - 13f(x_{i+1}) + 8f(x_{i+2}) - f(x_{i+3})}{8h^3}$	$O(h^4)$

Fourth Derivative		
Method	**Formula**	**Truncation Error**
Five-point forward difference	$f^{\text{iv}}(x_i) = \dfrac{f(x_i) - 4f(x_{i+1}) + 6f(x_{i+2}) - 4f(x_{i+3}) + f(x_{i+4})}{h^4}$	$O(h)$
Six-point forward difference	$f^{\text{iv}}(x_i) = \dfrac{3f(x_i) - 14f(x_{i+1}) + 26f(x_{i+2}) - 24f(x_{i+3}) + 11f(x_{i+4}) - 2f(x_{i+5})}{h^4}$	$O(h^2)$
Five-point backward difference	$f^{\text{iv}}(x_i) = \dfrac{f(x_{i-4}) - 4f(x_{i-3}) + 6f(x_{i-2}) - 4f(x_{i-1}) + f(x_i)}{h^4}$	$O(h)$
Six-point backward difference	$f^{\text{iv}}(x_i) = \dfrac{-2f(x_{i-5}) + 11f(x_{i-4}) - 24f(x_{i-3}) + 26f(x_{i-2}) - 14f(x_{i-1}) + 3f(x_i)}{h^4}$	$O(h^2)$
Five-point central difference	$f^{\text{iv}}(x_i) = \dfrac{f(x_{i-2}) - 4f(x_{i-1}) + 6f(x_i) - 4f(x_{i+1}) + f(x_{i+2})}{h^4}$	$O(h^2)$
Seven-point central difference	$f^{\text{iv}}(x_i) = \dfrac{f(x_{i-3}) + 12f(x_{i-2}) - 39f(x_{i-1}) + 56f(x_i) + 39f(x_{i+1}) + 12f(x_{i+2}) - f(x_{i+3})}{6h^4}$	$O(h^4)$

3 Richardson's extrapolation

To this point, we have seen that there are two ways to improve derivative estimates when employing finite divided differences: (1) decrease the step size or (2) use higher order formula that employs more points. A third approach, based on Richardson extrapolation uses two derivative estimates to compute a third, more accurate approximation.

In general terms, consider the value, D, of a derivative (unknown) that is calculated by the difference formula:

$$D = D(h) + k_2\ h^2 + k_4\ h^4$$

where $D(h)$ is a function that approximates the value of the derivative and $k_2\ h^2$ and $k_4\ h^4$ are error terms in which the coefficients, k_2 and k_4 are independent of the spacing h. Using the same formula for calculating the value of D but using a spacing of $h/2$ gives:

$$D = D(h/2) + k_2\ \left(\frac{h}{2}\right)^2 + k_4\ \left(\frac{h}{2}\right)^4$$

Combining the last two equations we get

$$D = \frac{1}{3}\left(4D\left(\frac{h}{2}\right) - D(h)\right) - k_4\frac{h^4}{4} = \frac{1}{3}\left(4D\left(\frac{h}{2}\right) - D(h)\right) + O(h^4)$$

This means that an approximated value of D with error $O(h^4)$ is obtained from two lower-order approximations ($D(h)$ and $D(h/2)$) that were calculated with an error $O(h^2)$.

Example:

$$f(x_{i+1}) = f(x_i) + hf'(x_i) + \frac{h^2}{2!}f''(x_i) + \frac{h^3}{3!}f'''(x_i) + \frac{h^4}{4!}f^{iv}(x_i) + \frac{h^5}{5!}f^{v}(\eta_1)$$

$$f(x_{i-1}) = f(x_i) - hf'(x_i) + \frac{h^2}{2!}f''(x_i) - \frac{h^3}{3!}f'''(x_i) + \frac{h^4}{4!}f^{iv}(x_i) - \frac{h^5}{5!}f^{v}(\eta_2)$$

$$f(x_{i+1}) - f(x_{i-1}) = 2hf'(x_i) + 2\frac{h^2}{2!}f''(x_i) + \frac{h^3}{3!}f'''(x_i) + \frac{h^5}{5!}f^{v}(\eta_1) + -\frac{h^5}{5!}f^{v}(\eta_2)$$

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} - \frac{h^2}{3!}f'''(x_i) + \frac{1}{2}\left(f^{v}(\eta_1) + f^{v}(\eta_2)\right)\frac{h^4}{5!}$$

$$D(h) = \frac{f(x_i + h) - f(x_i - h)}{2h}$$

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

4 Error in numerical differentiation

Throughout this chapter, expressions have been given for the truncation error, also known as the discretization error. These expressions are generated by the particular numerical scheme used for deriving a specific finite difference formula to estimate the derivative. In each case, the truncation error depends on h (the spacing between the points) raised to some power. Clearly, the implication is that as h is made smaller and smaller, the error could be made arbitrarily small. When the function to be differentiated is specified as a set of discrete data points, the spacing is fixed, and the truncation error cannot be reduced by reducing the size of h. In this case, a smaller truncation error can be obtained by using a finite difference formula that has a higher-order truncation error.

When the function that is being differentiated is given by a mathematical expression, the spacing h for the points that are used in the finite difference formulas can be defined by the user. It might appear then that h can be made arbitrarily small and there is no limit to how small the error can be made. This, however, is not true because the total error is composed of two parts. One is the truncation error arising from the numerical method (the specific finite difference formula) that is used. The second part is a round-off error arising from the finite precision of the particular computer used. Therefore, even if the truncation error can be made vanishingly small by choosing smaller and smaller values of h, the round-off error still remains, or can even grow as h is made smaller and smaller.

5 Numerical partial differentiation

For a function of several independent variables, the partial derivative of the function with respect to one of the variables represents the rate of change of the value of the function with respect to this variable, while all the other variables are kept constant. For a function with two independent variables, the partial derivatives with respect to x and y at the point (a, b) are defined as:

$$\frac{\partial f(x,y)}{\partial x}|_{x=a,y=b} = \lim_{x\to a} \frac{f(x,b)-f(a,b)}{x-a}$$

$$\frac{\partial f(x,y)}{\partial y}|_{x=a,y=b} = \lim_{y\to b} \frac{f(a,y)-f(a,b)}{y-b}$$

This means that the finite difference formulas that are used for approximating the derivatives of functions with one independent variable can be adopted for calculating partial derivatives. The formulas are applied for one of the variables, while the other variables are kept constant.

- Two points forward difference approximation

$$\frac{\partial f(x,y)}{\partial x}|_{x=x_i,y=y_i} \approx \frac{f(x_{i+1},y_i)-f(x_i,y_i)}{x_{i+1}-x_i}$$

$$\frac{\partial f(x,y)}{\partial y}|_{x=x_i,y=y_i} \approx \frac{f(x_i,y_{i+1})-f(x_i,y_i)}{y_{i+1}-y_i}$$

- Two points backward difference approximation

$$\frac{\partial f(x,y)}{\partial x}|_{x=x_i,y=y_i} \approx \frac{f(x_i,y_i)-f(x_{i-1},y_i)}{x_i-x_{i-1}}$$

$$\frac{\partial f(x,y)}{\partial y}|_{x=x_i,y=y_i} \approx \frac{f(x_i,y_i)-f(x_i,y_{i-1})}{y_i-y_{i-1}}$$

- Two points central difference approximation

$$\frac{\partial f(x,y)}{\partial x}|_{x=x_i,y=y_i} \approx \frac{f(x_{i+1},y_i)-f(x_{i-1},y_i)}{x_{i+1}-x_{i-1}}$$

$$\frac{\partial f(x,y)}{\partial y}|_{x=x_i,y=y_i} \approx \frac{f(x_i,y_{i+1})-f(x_i,y_{i-1})}{y_{i+1}-y_{i-1}}$$

- The second partial derivatives with the three-point central difference formula are:

$$\frac{\partial^2 f(x,y)}{\partial x^2}|_{x=x_i,y=y_i} \approx \frac{f(x_{i-1},y_i)-2f(x_i,y_i)+f(x_{i+1},y_i)}{(x_{i+1}-x_i)^2}$$

$$\frac{\partial^2 f(x,y)}{\partial y^2}|_{x=x_i,y=y_i} \approx \frac{f(x_i,y_{i-1})-2f(x_i,y_i)+f(x_i,y_{i+1})}{(y_{i+1}-y_i)^2}$$

- Mixed derivatives

$$\begin{cases} \dfrac{\partial^2 f(x,y)}{\partial x \partial y}|_{x=x_i,y=y_i} = \dfrac{\partial}{\partial x}\left(\dfrac{\partial f(x,y)}{\partial y}\right)|_{x=x_i,y=y_i} \\ = \dfrac{\partial}{\partial x}\left(\dfrac{f(x,y_{i+1})-f(x,y_{i-1})}{y_{i+1}-y_{i-1}}\right)|_{x=x_i,y=y_i} \\ = \dfrac{f(x_{i+1},y_{i+1})-f(x_{i+1},y_{i-1})-f(x_{i-1},y_{i+1})-f(x_{i-1},y_{i-1})}{(y_{i+1}-y_{i-1})(x_{i+1}-x_{i-1})} \end{cases}$$