# Finite Difference Methods: Differentiation, Interpolation and Integration (I)

## Differentiation: Finite Differences

The definition of derivative is:

> $$\left.\frac{df}{dx}\right|_{x=x_0} = f'(x_0) = \lim_{h\to 0}\frac{f(x_0+h)-f(x_0)}{h}$$

Therefore, it is reasonable to think that:

> For small enough $h$:
>
> $$f'(x_0) \approx \frac{f(x_0+h)-f(x_0)}{h}$$

In this way, we approximate the differential operator $D = \frac{d}{dx}$ by an expression involving the values of the function at a discrete set of points. This kind of formula is called a **Finite Difference Formula**. The discrete set of points is called the **Stencil** of the formula.

All *finite difference formulas* are based on the concept of the *Taylor Series*:

> A function $f(x)$ continuous and differentiable in the interval $[x_0, x]$ can be approximated by:
>
> $$f(x) = \sum_{k=0}^{\infty}\frac{f^{(k)}(x_0)}{k!}(x-x_0)^k = \sum_{k=0}^{n}\frac{f^{(k)}(x_0)}{k!}(x-x_0)^k + R_n$$
>
> Where $R_n = \frac{1}{(n+1)!}(x-x_0)^{n+1}f^{(n+1)}(\xi)$, usually abbreviated as $O(h^{n+1})$.

The exponent of $O(h^{n+1})$ is the order of the finite difference formula. It means that the error made when approximating the derivative with a certain formula with $O(h^p)$ will have an error of the order of $h^p$. As we normally use $h << 1$, the error will be smaller for larger order formulas.

The choice of stencil is very important. Normally we use equispaced stencils, which means that all consecutive points are spaced by a constant amount $(x_{i+n} = x_i + nh)$. A general stencil would be:

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| $x$ | $x_{i-n}$ | $\cdots$ | $x_{i-1}$ | $x_i$ | $x_{i+1}$ | $\cdots$ | $x_{i+m}$ |
| $y = f(x)$ | $y_{i-n}$ | $\cdots$ | $y_{i-1}$ | $y_i$ | $y_{i+1}$ | $\cdots$ | $y_{i+m}$ |

In order to derive the dinite difference formulas, it is useful to define a set of linear differential operators:

> **Difference Operators:**
> Forward Difference:

> $$\Delta u = u_{i+1} - u_i$$
>
> Backward Difference:
>
> $$\nabla u = u_i - u_{i-1}$$
>
> Central Difference:
>
> $$\delta u = u_{i+1/2} - u_{i-1/2}$$

## Finite Forward Difference Formulas

Forward difference formulas are those that enable us to compute the value $y_i'$ of the derivative of a function $y$ at a certain point $x_i$ based on the value $y_i$ of the function at that same point $x_i$ and a certain number of points larger than $x_i$ $(y_{i+1}, y_{i+2}, \dots)$.

These formulas derive from the taylor expansion of $y$ around $x_i$ up to order $N$:

$$y_{i+n} = \sum_{k=0}^{N} \frac{(x_{i+n} - x_i)^k}{k!} y_i^{(k)} + O(h^{N+1})$$

The order up to which the expansion is used, $N$, is the order of the finite difference formula. If we consider $x_{i+1} - x_i = h$, then $x_{i+n} - x_i = nh$, and the formula is simplified to:

$$y_{i+n} = \sum_{k=0}^{N} \frac{(nh)^k}{k!} y_i^{(k)} + O(h^{N+1})$$

If we want to find the expression of the derivative $y_i^{(r)}$, then we need to find the previous expansion up to $N \geq r$ and evaluate it at $n = 0, 1, \dots, N$. This will allow us to build a system of equations with enough equations to find the coefficients $a_n$ of:

$$y_i^{(r)} = a_0 y_i + a_1 y_{i+1} + \cdots + a_N y_{i+N} + O(h^N)$$

The order of forward finite difference formulas is usually equal to $k - 1$, where $k$ is the number of points of the function $y$ on which the formula depends.

**Example: Second Order Finite Forward Difference Formula for the First Derivative**

We want to find the second order finite difference formula, so $N = 2$. We know this is possible because, as we want the first derivative ($r = 1$), we can verify that $N = 2 > 1 = r$.

As $N = 2$, we need to expand $y_{i+n}$ up to the second order and evaluate for $n = 0, 1, 2$ :

$$y_{i+n} = \sum_{k=0}^{2} \frac{(nh)^k}{k!} y_i^{(k)} + O(h^3) = y_i + nhy_i' + \frac{1}{2}(nh)^2 y_i'' + O(h^3)$$

Then:

$$y_i = y_i$$

$$y_{i+1} = y_i + hy_i' + \frac{1}{2}h^2 y_i'' + O(h^3)$$

$$y_{i+2} = y_i + 2hy_i' + 2h^2 y_i'' + O(h^3)$$

Now we have a system of equations to solve:

$$y_i' = a_0 y_i + a_1 y_{i+1} + a_2 y_{i+2} + O(h^2)$$

Substituting:

$$\begin{gathered} y_i' = a_0 y_i + a_1 \left( y_i + hy_i' + \frac{1}{2}h^2 y_i'' + O(h^3) \right) + \\ a_2 \left( y_i + 2hy_i' + 2h^2 y_i'' + O(h^3) \right) + O(h^2) = \\ = (a_0 + a_1 + a_2) y_i + h(a_1 + 2a_2) y_i' + \frac{h^2}{2}(a_1 + 4a_2) y_i'' \end{gathered}$$

Finally, $y_i' = (a_0 + a_1 + a_2) y_i + h(a_1 + 2a_2) y_i' + \frac{h^2}{2}(a_1 + 4a_2) y_i''$ requires:

$$a_0 + a_1 + a_2 = 0$$

$$h(a_1 + 2a_2) = 1$$

$$\frac{h^2}{2}(a_1 + 4a_2) = 0$$

yielding $a_0 = -\frac{3}{2h}$, $a_1 = \frac{2}{h}$ and $a_2 = -\frac{1}{2h}$:

> The *Second Order Finite Forward Difference Formula for the First Derivative* is:
>
> $$y_i' = \frac{-3y_i + 4y_{i+1} - y_{i+2}}{2h} + O(h^2)$$

## Finite Backward Difference Formulas

Backward difference formulas are those that enable us to compute the value $y_i'$ of the derivative of a function $y$ at a certain point $x_i$ based on the value $y_i$ of the function at that same point $x_i$ and a certain number of points smaller than $x_i$ $(y_{i-1}, y_{i-2}, \ldots)$.

Again, these formulas derive from the taylor expansion of $y$ around $x_i$ up to order $N$ that we simplified before to:

$$y_{i+n} = \sum_{k=0}^{N} \frac{(nh)^k}{k!} y_i^{(k)} + O(h^{N+1})$$

If we want to find the expression of the derivative $y_i^{(r)}$, then we need to find the previous expansion up to $N \geq r$ and evaluate it at $n = 0, -1, \ldots, -N$. This will allow us to build a system of equations with enough equations to find the coefficients $a_n$ of:

$$y_i^{(r)} = a_0 y_i + a_1 y_{i-1} + \cdots + a_N y_{i-N} + O(h^N)$$

The order of backward finite difference formulas is usually equal to $k-1$, where $k$ is the number of points of the function $y$ on which the formula depends.

**Example: Second Order Finite Backward Difference Formula for the First Derivative**

We want to find the second order finite difference formula, so $N=2$. We know this is possible because, as we want the first derivative ($r=1$), we can verify that $N=2>1=r$.

As $N=2$, we need to expand $y_{i+n}$ up to the second order and evaluate for $n=0,1,2$ :

$$y_{i+n} = \sum_{k=0}^{2} \frac{(nh)^k}{k!} y_i^{(k)} + O(h^3) = y_i + nhy_i' + \frac{1}{2}(nh)^2 y_i'' + O(h^3)$$

Then:

$$y_i = y_i$$

$$y_{i-1} = y_i - hy_i' + \frac{1}{2}h^2 y_i'' + O(h^3)$$

$$y_{i-2} = y_i - 2hy_i' + 2h^2 y_i'' + O(h^3)$$

Now we have a system of equations to solve:

$$y_i' = a_0 y_i + a_1 y_{i+1} + a_2 y_{i+2} + O(h^2)$$

Substituting:

$$\begin{aligned} y_i' &= a_0 y_i + a_1 \left( y_i - hy_i' + \frac{1}{2}h^2 y_i'' + O(h^3) \right) + \\ &a_2 \left( y_i - 2hy_i' + 2h^2 y_i'' + O(h^3) \right) + O(h^2) = \\ &= (a_0 + a_1 + a_2) y_i - h(a_1 + 2a_2) y_i' + \frac{h^2}{2}(a_1 + 4a_2) y_i'' \end{aligned}$$

Finally, $y_i' = (a_0 + a_1 + a_2) y_i - h(a_1 + 2a_2) y_i' + \frac{h^2}{2}(a_1 + 4a_2) y_i''$ requires:

$$a_0 + a_1 + a_2 = 0$$

$$h(a_1 + 2a_2) = -1$$

$$\frac{h^2}{2}(a_1 + 4a_2) = 0$$

yielding $a_0 = \frac{3}{2h}$, $a_1 = -\frac{2}{h}$ and $a_2 = \frac{1}{2h}$:

> The *Second Order Finite Backward Difference Formula for the First Derivative* is:

$$y_i' = \frac{3y_i - 4y_{i-1} + y_{i-2}}{2h} + O(h^2)$$

Notice that this is just the formula for the forward difference but substituting $h$ by $-h$ and substituting $i$ by $i-2$.

## Finite Centered Difference Formulas

Centered difference formulas are those that enable us to compute the value $y_i'$ of the derivative of a function $y$ at a certain point $x_i$ based on the value $y_i$ of the function at that same point $x_i$ and a certain number of points of which half are smaller than $x_i$ ($y_{i-1}, y_{i-2}, \ldots$) and the other half are larger than $x_i$ ( $y_{i+1}, y_{i+2}, \ldots$).

Again, these formulas derive from the taylor expansion of $y$ around $x_i$ up to order $N$ that we simplified before to:

$$y_{i+n} = \sum_{k=0}^{N} \frac{(nh)^k}{k!} y_i^{(k)} + O(h^{N+1})$$

If we want to find the expression of the derivative $y_i^{(r)}$, then we need to find the previous expansion up to even $N \geq r$ and evaluate it at $n = -N/2, \ldots, -10, 1, \ldots, N/2$. This will allow us to build a system of equations with enough equations to find the coefficients $a_n$ of:

$$y_i^{(r)} = a_{-N/2} y_{i-N/2} + \ldots + a_{-1} y_{i-1} + \\ + a_0 y_i + a_1 y_{i+1} + \cdots + a_{N/2} y_{i+N/2} + O(h^{N+1})$$

The order of centered finite difference formulas is usually equal to the number of points of the function $y$ on which the formula depends.

#### Example: Second Order Finite Centered Difference Formula for the First Derivative

We want to find the second order finite difference formula, so $N = 2$. We know this is possible because, as we want the first derivative ($r = 1$), we can verify that $N = 2 > 1 = r$.

As $N = 2$, we need to expand $y_{i+n}$ up to the second order and evaluate for $n = 0, 1, 2$ :

$$y_{i+n} = \sum_{k=0}^{2} \frac{(nh)^k}{k!} y_i^{(k)} + O(h^3) = y_i + nhy_i' + \frac{1}{2}(nh)^2 y_i'' + O(h^3)$$

Then:

$$y_i = y_i$$

$$y_{i+1} = y_i + hy_i' + \frac{1}{2}h^2 y_i'' + O(h^3)$$

$$y_{i-1} = y_i - hy_i' + \frac{1}{2}h^2 y_i'' + O(h^3)$$

Now we have a system of equations to solve:

$$y_i' = a_{-1} y_{i-1} + a_0 y_i + a_1 y_{i+1} + O(h^3)$$

Substituting:

$$y'_i = a_{-1}\left(y_i - hy'_i + \frac{1}{2}h^2 y''_i + O(h^3)\right) + a_0 y_i +$$
$$+ a_1\left(y_i + hy'_i + \frac{1}{2}h^2 y''_i + O(h^3)\right) + O(h^3) =$$

$$= (a_{-1} + a_0 + a_1)y_i + h(-a_{-1} + a_0 + a_1)y'_i + \frac{h^2}{2}(a_{-1} + a_1)y''_i + O(h^3)$$

Finally, $y'_i = (a_{-1} + a_0 + a_1)y_i + h(-a_{-1} + a_0 + a_1)y'_i + \frac{h^2}{2}(a_{-1} + a_1)y''_i$ requires:

$$a_{-1} + a_0 + a_1 = 0$$

$$h(-a_{-1} + a_0 + a_1) = 1$$

$$\frac{h^2}{2}(a_{-1} + a_1) = 0$$

yielding $a_{-1} = -\frac{1}{2h}$, $a_0 = 0$ and $a_1 = \frac{1}{2h}$:

> The *Second Order Finite Centered Difference Formula for the First Derivative* is:
>
> $$y'_i = \frac{y_{i+1} - y_{i-1}}{2h} + O(h^3)$$

Online finite differences calculator here.