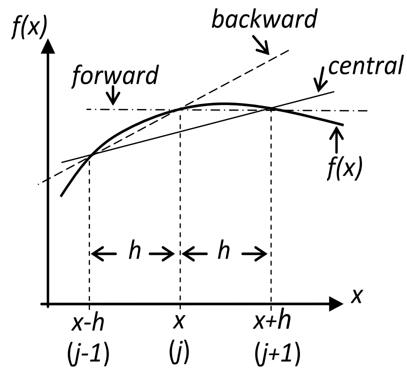
5- Numerical Differentiation
(Finite Difference Calculus)

Introduction

Numerical differentiation is the process of finding the numerical value of a derivative of a given function at a given point. In numerical analysis, numerical differentiation describes algorithms for estimating the derivative of a mathematical function using values of the function and perhaps other knowledge about the function.

Forward and backward differences

Consider a function $f(x)$ which is analytical (can be expanded by Taylor series) in the neighborhood of a point *x* as shown in the figure. We can find $f(x+h)$ by expanding $f(x)$ in a Taylor series about *x*:



$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \ldots\ldots,$$

solving for $f'(x)$ yields:

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2!}f''(x) - \frac{h^2}{3!}f'''(x) - \ldots\ldots,$$

or $$f'(x) = \frac{f(x+h) - f(x)}{h} + O(h).$$

This equation represents the first derivative of $f(x)$ with respect to *x* which is accurate to within an error of order *h*. employing the subscript notation:

$f(x) = f_j$ and $f(x+h) = f_{j+1}$, then

$$f'_j = \frac{f_{j+1} - f_j}{h} + O(h) \quad \text{or} \quad f'_j = \frac{\Delta f_j}{h} + O(h),$$

where Δf_j is the first forward difference of *f* at *j*, and $\frac{\Delta f_j}{h}$ is the first forward difference approximation to f' at *j* with an error order of *h*.

Similarly, we can find $f(x-h)$ by expanding $f(x)$ in a Taylor series about *x*:

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f'''(x) + \ldots\ldots,$$

solving for $f'(x)$ yields:

$$f'(x) = \frac{f(x) - f(x-h)}{h} + \frac{h}{2!} f''(x) - \frac{h^2}{3!} f'''(x) - \ldots\ldots,$$

or simply $f'_j = \dfrac{f_j - f_{j-1}}{h} + O(h)$ or $f'_j = \dfrac{\nabla f_j}{h} + O(h)$,

where ∇f_j is the first backward difference of *f* at *j*, and $\dfrac{\nabla f_j}{h}$ is the first backward difference approximation to f' at *j* with an error order of *h*.

How to find higher order derivatives

To find $f''(x)$, using Taylor series expansion of $f(x+h)$ and $f(x+2h)$ about *x* gives:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) + \ldots\ldots, \qquad \ldots\ldots\ldots\ldots (1)$$

$$f(x+2h) = f(x) + 2hf'(x) + \frac{4h^2}{2!} f''(x) + \frac{8h^3}{3!} f'''(x) + \ldots\ldots \qquad \ldots\ldots\ldots\ldots (2)$$

Multiplying Eq.1 by 2 and subtracting Eq.1 from Eq.2, then solving for $f''(x)$ yields:

$$f''(x) = \frac{f(x+2h) - 2f(x+h) + f(x)}{h^2} - hf'''(x) - \ldots\ldots,$$

or simply, $f''_j = \dfrac{f_{j+2} - 2f_{j+1} + f_j}{h^2} + O(h)$ or $f''_j = \dfrac{\Delta^2 f_j}{h^2} + O(h)$,

where $\Delta^2 f_j$ is the second forward difference of *f* at *j*.

Similarly, by using the Taylor series expansion of $f(x-h)$ and $f(x-2h)$ about *x*, we can get:

$$f_j'' = \frac{f_j - 2f_{j-1} + f_{j-2}}{h^2} + O(h) \quad \text{or} \quad f_j'' = \frac{\nabla^2 f_j}{h^2} + O(h),$$

where $\nabla^2 f_j$ is the second backward difference of f at j.

Generally, any forward or backward difference may be obtained starting from the first forward or backward difference by using the following recurrence formulae:

$$\Delta^n f_j = \Delta(\Delta^{n-1} f_j) \quad \text{and} \quad \nabla^n f_j = \nabla(\nabla^{n-1} f_j).$$

For example,

$$\Delta^2 f_j = \Delta(\Delta f_j) = \Delta(f_{j+1} - f_j) = \Delta f_{j+1} - \Delta f_j = (f_{j+2} - f_{j+1}) - (f_{j+1} - f_j)$$

$$= f_{j+2} - 2f_{j+1} + f_j.$$

Thus, the derivatives of any order, with an error of order h, are given by:

$$\frac{d^n f_j}{dx^n} = \frac{\Delta^n f_j}{h^n} + O(h), \quad \text{or} \quad \frac{d^n f_j}{dx^n} = \frac{\nabla^n f_j}{h^n} + O(h).$$

Note: The 1st forward and backward difference approximations of $O(h)$ are exact for 1st polynomials (straight lines), and the 2nd forward and backward difference approximations of $O(h)$ are exact for 2nd degree polynomials. Generally, the nth difference approximations of $O(h)$ for $f^n(x)$ are exact for polynomials of *n*-degree.

How to find more accurate approximations

More accurate expressions for derivatives may be found by taking more terms in the Taylor series expansion. For example, to find $f'(x)$ with $O(h)^2$:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) + \ldots ,$$

but $f''(x) = \dfrac{f(x+2h) - 2f(x+h) + f(x)}{h^2} + O(h)$, substituting above:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}\left[\frac{f(x+2h) - 2f(x+h) + f(x)}{h^2} + O(h)\right] + \frac{h^3}{3!}f'''(x) + ..,$$

solving for $f'(x)$ yields:

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

or simply, $$f'_j = \frac{-f_{j+2} + 4f_{j+1} - 3f_j}{2h} + O(h)^2 .$$

Note: This expression is exact for polynomials of degree 2 and lower (since the error involves only third and higher derivatives).

Central differences

Using Taylor series expansion of $f(x+h)$ and $f(x-h)$ about x gives:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + ... , \qquad .... (3)$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + ... \qquad .... (4)$$

Subtracting Eq.4 from Eq.3 and solving for $f'(x)$ yields:

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{3!}f'''(x) - ...... ,$$

or simply, $$f'_j = \frac{f_{j+1} - f_{j-1}}{2h} + O(h)^2 .$$

Note: This expression is exact for polynomials of degree 2 and lower.

To obtain $f''(x)$, one additional Taylor series expansion in each direction is required. In general:

$$\frac{d^n f_j}{dx^n} = \frac{\nabla^n f_{j+n/2} + \Delta^n f_{j-n/2}}{2h^n} + O(h)^2 \qquad n \text{ is even,}$$

$$\frac{d^n f_j}{dx^n} = \frac{\nabla^n f_{j+(n-1)/2} + \Delta^n f_{j-(n-1)/2}}{2h^n} + O(h)^2 \qquad n \text{ is odd.}$$

Note: The following table gives the most used finite difference approximations:

FORWARD DIFFERENCES	BACKWARD DIFFERENCES	Error
First Derivative	First Derivative	
$f'_j = \frac{-f_j + f_{j+1}}{h}$	$f'_j = \frac{f_j - f_{j-1}}{h}$	$O(h)$
$f'_j = \frac{-3f_j + 4f_{j+1} - f_{j+2}}{2h}$	$f'_j = \frac{3f_j - 4f_{j-1} + f_{j-2}}{2h}$	$O(h)^2$
Second Derivative	Second Derivative	
$f''_j = \frac{f_j - 2f_{j+1} + f_{j+2}}{h^2}$	$f''_j = \frac{f_j - 2f_{j-1} + f_{j-2}}{h^2}$	$O(h)$
$f''_j = \frac{2f_j - 5f_{j+1} + 4f_{j+2} - f_{j+3}}{h^2}$	$f''_j = \frac{2f_j - 5f_{j-1} + 4f_{j-2} - f_{j-3}}{h^2}$	$O(h)^2$
Third Derivative	Third Derivative	
$f'''_j = \frac{-f_j + 3f_{j+1} - 3f_{j+2} + f_{j+3}}{h^3}$	$f'''_j = \frac{f_j - 3f_{j-1} + 3f_{j-2} - f_{j-3}}{h^3}$	$O(h)$
$f'''_j = \frac{-5f_j + 18f_{j+1} - 24f_{j+2} + 14f_{j+3} - 3f_{j+4}}{2h^3}$	$f'''_j = \frac{5f_j - 18f_{j-1} + 24f_{j-2} - 14f_{j-3} + 3f_{j-4}}{2h^3}$	$O(h)^2$
Fourth Derivative	Fourth Derivative	
$f^{iv}_j = \frac{f_j - 4f_{j+1} + 6f_{j+2} - 4f_{j+3} + f_{j+4}}{h^4}$	$f^{iv}_j = \frac{f_j - 4f_{j-1} + 6f_{j-2} - 4f_{j-3} + f_{j-4}}{h^4}$	$O(h)$
$f^{iv}_j = \frac{3f_j - 14f_{j+1} + 26f_{j+2} - 24f_{j+3} + 11f_{j+4} - 2f_{j+5}}{h^4}$	$f^{iv}_j = \frac{3f_j - 14f_{j-1} + 26f_{j-2} - 24f_{j-3} + 11f_{j-4} - 2f_{j-5}}{h^4}$	$O(h)^2$

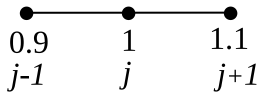
CENTRAL DIFFERENCES	Error
First Derivative	
$f'_j = \frac{-f_{j-1} + f_{j+1}}{2h}$	$O(h)^2$
$f'_j = \frac{f_{j-2} - 8f_{j-1} + 8f_{j+1} - f_{j+2}}{12h}$	$O(h)^4$
Second Derivative	
$f''_j = \frac{f_{j-1} - 2f_j + f_{j+1}}{h^2}$	$O(h)^2$
$f''_j = \frac{-f_{j-2} + 16f_{j-1} - 30f_j + 16f_{j+1} - f_{j+2}}{12h^2}$	$O(h)^4$
Third Derivative	
$f'''_j = \frac{-f_{j-2} + 2f_{j-1} - 2f_{j+1} + f_{j+2}}{2h^3}$	$O(h)^2$
$f'''_j = \frac{f_{j-3} - 8f_{j-2} + 13f_{j-1} - 13f_{j+1} + 8f_{j+2} - f_{j+3}}{8h^3}$	$O(h)^4$
Fourth Derivative	
$f^{iv}_j = \frac{f_{j-2} - 4f_{j-1} + 6f_j - 4f_{j+1} + f_{j+2}}{h^4}$	$O(h)^2$
$f^{iv}_j = \frac{-f_{j-3} + 12f_{j-2} - 39f_{j-1} + 56f_j - 39f_{j+1} + 12f_{j+2} - f_{j+3}}{6h^4}$	$O(h)^4$

Example 1: Find $f'(x)$ at $x=1$ for the function $f(x)=e^x$. Compare with the exact answer. (Use $h=0.1$)

Solution:

By central difference approximations with $O(h)^2$,

$$f'_j = \frac{-f_{j-1} + f_{j+1}}{2h} + O(h)^2,$$



At $x=1 \Rightarrow j=1, \quad j+1 = x+h = 1+0.1 = 1.1,$ and $j-1 = x-h = 1-0.1 = 0.9$.

$$f'(1) \approx \frac{-f(0.9)+f(1.1)}{2(0.1)} \quad \Rightarrow \quad f'(1) \approx \frac{-e^{0.9}+e^{1.1}}{0.2} \approx 2.722815.$$

The (exact) value is $e^1 = 2.718282$ (from the scientific calculator).

Percent relative error $P= \left|\frac{exact - approx.}{exact}\right| \times 100 = \left|\frac{2.718282 - 2.722815}{2.718282}\right| \times 100 = 0.17\%$

Notes:

* If we use forward difference approximations with $O(h)$,

$$f'_j = \frac{-f_j + f_{j+1}}{h} + O(h),$$

$$f'(1) \approx \frac{-f(1)+f(1.1)}{0.1} \quad \Rightarrow \quad f'(1) \approx \frac{-e^{1}+e^{1.1}}{0.1} \approx 2.858842.$$

The (exact) value is $e^1 = 2.718282$ (from the scientific calculator).

Percent relative error $P= \left|\frac{2.718282 - 2.858842}{2.718282}\right| \times 100 = 5.17\%$.

* If we use backward difference approximations with $O(h)$,

$$f'_j = \frac{f_j - f_{j-1}}{h} + O(h),$$

$$f'(1) \approx \frac{f(1)-f(0.9)}{0.1} \quad \Rightarrow \quad f'(1) \approx \frac{e^{1}-e^{0.9}}{0.1} \approx 2.586787.$$

Percent relative error $P= \left|\frac{2.718282 - 2.586787}{2.718282}\right| \times 100 = 4.8\%$.

Example 2: Given the function $f(x)=(x+1)^x$, find $f'(2)$ correct to three decimals.

Solution:

Use central difference approximations with $O(h)^2$,

$$f'_j = \frac{-f_{j-1} + f_{j+1}}{2h} + O(h)^2 .$$

1.8 2 2.2
j-1 j j+1

1st iteration: Take $h_1 = 0.2$,

At $x=2 \Rightarrow j=2$, $j+1 = x+h_1 = 2+0.2 = 2.2$, and $j-1 = x-h_1 = 2-0.2 = 1.8$.

$$f'(2) \approx \frac{-f(1.8)+f(2.2)}{2(0.2)} \approx \frac{-(1.8+1)^{1.8}+(2.2+1)^{2.2}}{0.4} \approx 16.352674 .$$

1.9 2 2.1
j-1 j j+1

2nd iteration: Take $h_2 = \frac{h_1}{2} = \frac{0.2}{2} = 0.1$,

$j+1 = x+h_2 = 2+0.1 = 2.1$, and $j-1 = x-h_2 = 2-0.1 = 1.9$.

$$f'(2) \approx \frac{-f(1.9)+f(2.1)}{2(0.1)} \approx \frac{-(1.9+1)^{1.9}+(2.1+1)^{2.1}}{0.2} \approx 16.002864 .$$

The calculations must be continued until $\Delta \le \varepsilon$.

No. of Iteration (i)	h_i	f'_i	$\Delta_i = \left\| f'_i - f'_{i-1} \right\|$
1	0.2	16.352674	----
2	0.1	16.002864	0.34….
3	0.05	15.916291	0.08….
4	0.025	15.894702	0.02….
5	0.0125	15.889308	5.3×10^{-3}
6	0.00625	15.887960	1.3×10^{-3}
7	0.003125	15.887623	$3.3\times10^{-4} < \varepsilon$

$\therefore \quad f'(2) \approx 15.887623$.