Numerical Differentiation - Lecture 02

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Outline

In this lecture:

- We will develop an approximation to the first derivative using central differences
- We will generalize the central difference approximation for the n^{th} derivative
- We will show how to obtain higher order approximations using Lagrange Polynomials

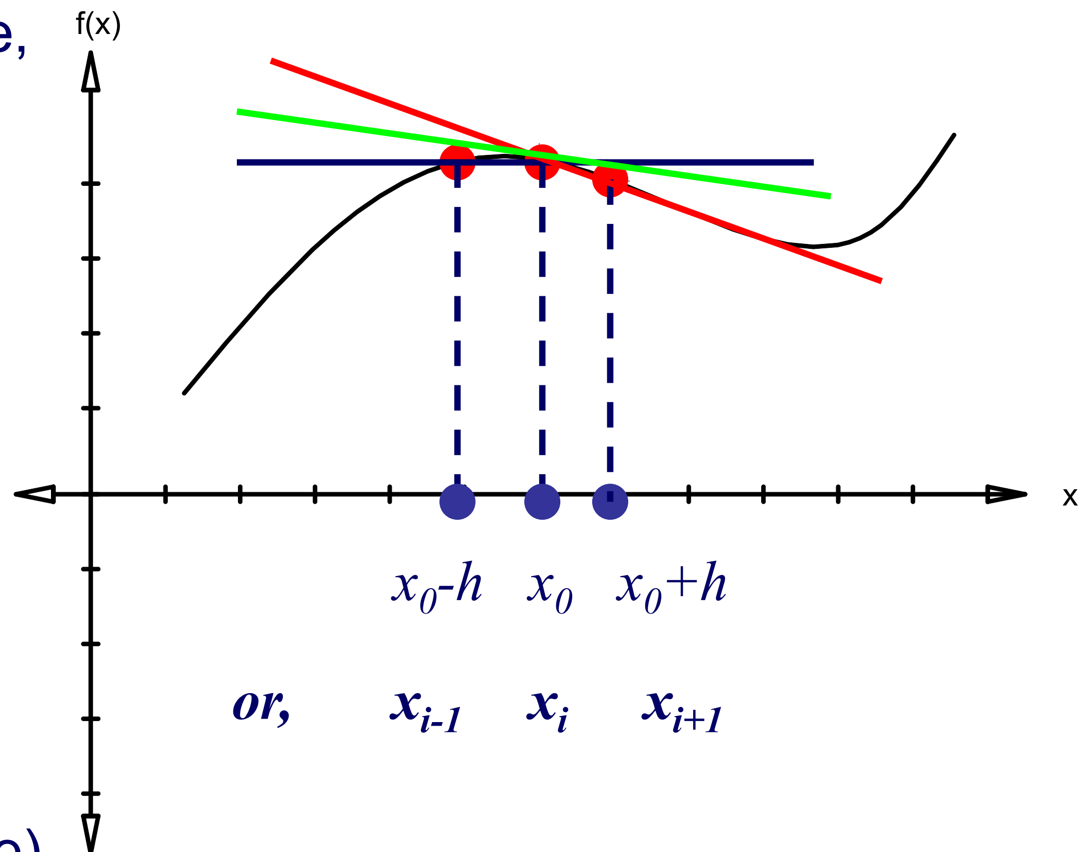
Generalization of one sided approximation to the n^{th} derivative

Generalizing to the n^{th} derivative,

$$f_i^{(n)} = \frac{\Delta^n f_i}{h^n} + \vartheta(h)$$

Using the Backward Difference operator, one obtains,

$$f_i^{(n)} = \frac{\nabla^n f_i}{h^n} + \vartheta(h)$$



The principle of the 1st order forward (red) and backward (blue) difference is depicted in the adjacent figure. We notice that the centered scheme (in green) approximates the slope better.

Central Difference Schemes (1st Derivative)

Numerical differences obtained from data symmetric about the expansion point are called **central difference formula**.

Obtain f_i' and f_i'' using 2nd order accurate central difference schemes

$$\mathrm{f}_{\mathrm{i+1}} = \mathrm{f}_{\mathrm{i}} + hf_i' + \frac{h^2}{2} f_i'' + \frac{h^3}{6} f_i''' + \frac{h^4}{24} f_i^{iv} + \ldots \rightarrow (1)$$

$$\mathrm{f}_{\mathrm{i-1}} = \mathrm{f}_{\mathrm{i}} - hf_i' + \frac{h^2}{2} f_i'' - \frac{h^3}{6} f_i''' + \frac{h^4}{24} f_i^{iv} - \ldots \rightarrow (2)$$

Perform the Subtract : $(1)-(2) \Rightarrow$

$$\mathrm{f}_{\mathrm{i+1}} - \mathrm{f}_{\mathrm{i-1}} = 2hf_i' + \frac{h^3}{3} f_i''' + \vartheta(h^5)$$

$$f_i' \approx \frac{\mathrm{f}_{\mathrm{i+1}} - \mathrm{f}_{\mathrm{i-1}}}{2\mathrm{h}} \qquad \text{The error is } -\frac{h^2}{6} f_i''' + \vartheta(h^4) = \vartheta(h^2)$$

This expression represents a second-order accurate central difference approximation to a first derivative.

Central Difference Schemes (2nd Derivative)

Adding (1) and (2) will result in a central difference approximation of f′′

$$(1)\ f_{i+1} = f_i + hf_i' + \frac{h^2}{2} f_i'' + \frac{h^3}{6} f_i''' + \frac{h^4}{24} f_i^{iv} + \dots$$

$$(2)\ f_{i-1} = f_i - hf_i' + \frac{h^2}{2} f_i'' - \frac{h^3}{6} f_i''' + \frac{h^4}{24} f_i^{iv} - \dots$$

Add $(1)+(2) \Rightarrow$

$$f_{i+1} + f_{i-1} = 2f_i + h^2 f_i'' + \frac{h^4}{12} f_i^{iv} + \vartheta(h^6)$$

$$f_i'' = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} - \frac{h^2}{12} f_i^{iv}$$

The error is $\vartheta(h^2)$

Using the operator notation

$$f_i'' \approx \frac{\Delta f_i - \nabla f_i}{h^2}$$

Central Difference Generalization

It can be shown that this generalizes to

$$\left.\frac{d^n f}{dx^n}\right|_i = \frac{\nabla^n f_{i+n/2} + \Delta^n f_{i-n/2}}{2h^n} + \vartheta(h^2) \text{ when } n \text{ is even}$$

$$\left.\frac{d^n f}{dx^n}\right|_i = \frac{\nabla^n f_{i+(n-1)/2} + \Delta^n f_{i-(n-1)/2}}{2h^n} + \vartheta(h^2) \text{ when } n \text{ is odd}$$

For example:

$$\left.\frac{d^2 f}{dx^2}\right|_i = \frac{\nabla^2 f_{i+1} + \Delta^2 f_{i-1}}{2h^2} = \frac{\nabla(f_{i+1} - f_i) + \Delta(f_i - f_{i-1})}{2h^2}$$

$$= \frac{2f_{i+1} - 4f_i + 2f_{i-1}}{2h^2} = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2}$$

and the error is $\vartheta(h^2)$

Obtaining Higher Order Approximations Using Lagrange Polynomials

Pass a Lagrange Polynomial through the given points (for example if you have $n+1$ data pairs):

$$f(x) = P_n(x) + Error(x) = \left[\sum_{k=0}^{n} f(x_k) L_{n,k}(x)\right] + \frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x-x_0)....(x-x_n)$$

Differentiate both sides (Here we consider the first derivative)

$$f'(x) = P_n'(x) + Error'(x) = \left[\sum_{k=0}^{n} f(x_k) \frac{d[L_{n,k}(x)]}{dx}\right] +$$

$$\frac{d}{dx}\left[\frac{(x-x_0)(x-x_1)....(x-x_n)}{(n+1)!}\right] f^{(n+1)}(\xi(x)) + \frac{(x-x_0)(x-x_1)...(x-x_n)}{(n+1)!} \frac{d}{dx}\left[f^{(n+1)}(\xi(x))\right]$$

Evaluate the derivative at the point of interest $x=x_j$

$$f'(x_j) = P_n'(x_j) + Error'(x_j) = \left[\sum_{k=0}^{n} f(x_k) \left.\frac{d[L_{n,k}(x)]}{dx}\right|_{x=x_j}\right] + f^{(n+1)}(\xi(x)) \prod_{\substack{k=0 \\ k\neq j}}^{n} (x_j - x_k)$$

The above expression is called the $(n+1)^{th}$ formula to approximate df/dx at $x=x_j$

2^{nd} Order Approximation to the First Derivative Using Lagrange Polynomials (1)

Use (x_{i+2}, f_{i+2}), (x_{i+1}, f_{i+1}), and (x_i, f_i) to find an approximation to the first derivative of f(x) at $x=x_i$ using the Lagrange Polynomial methods

$$P_2(x) = \sum_{k=0}^{2} f(x_{i+k}) L_{2,(i+k)}(x) \quad \& \quad P_2'(x) = \sum_{k=0}^{2} f(x_{i+k}) L'_{2,(i+k)}(x)$$

$$L_{2,i}(x) = \frac{(x - x_{i+1})(x - x_{i+2})}{(x_i - x_{i+1})(x_i - x_{i+2})} \quad \& \quad L'_{2,i}(x) = \frac{2x - x_{i+1} - x_{i+2}}{(x_i - x_{i+1})(x_i - x_{i+2})}$$

$$L_{2,i+1}(x) = \frac{(x - x_i)(x - x_{i+2})}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})} \quad \& \quad L'_{2,i+1}(x) = \frac{2x - x_i - x_{i+2}}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})}$$

$$L_{2,i+2}(x) = \frac{(x - x_i)(x - x_{i+1})}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} \quad \& \quad L'_{2,i+2}(x) = \frac{2x - x_i - x_{i+1}}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})}$$

2nd Order Approximation to the First Derivative Using Lagrange Polynomials (2)

$$f'(x_i) \approx P_2'(x_i) = \sum_{k=0}^{2} f(x_{i+k}) L'_{2,(i+k)}(x_i)$$

$$P_2'(x_i) = f(x_i)\left[\frac{2x_i - x_{i+1} - x_{i+2}}{(x_i - x_{i+1})(x_i - x_{i+2})}\right] + f(x_{i+1})\left[\frac{2x_i - x_i - x_{i+2}}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})}\right] +$$

$$f(x_{i+2})\left[\frac{2x_i - x_i - x_{i+1}}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})}\right]$$

$$and\ error = \frac{1}{6} f'''(\xi_i)(x_i - x_{i+1})(x_i - x_{i+2})$$

$$for\ x_{i+1} = x_i + h \quad and \quad x_{i+2} = x_i + 2h$$

$$f'(x_i) \approx \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}$$

$$Error = \frac{h^2}{3} f'''(\xi_i) \quad where \quad x_i \le \xi_i \le x_{i+2}$$

Note that this is the same approximation and the error term we have obtained using other two methods (see the previous lecture)

Summary

We have

- developed an approximation to the first derivative using central differences and generalized the approximation for the nth derivative

- shown how to obtain higher order approximations using Lagrange Polynomials and obtained a second order approximation to the first derivative. A similar approach can be used to approximate the other derivatives with desired order of accuracy