Numerical Methods

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Syllabus (part of PHSDSC405P: Mathematical Methods II Lab)

Reference
J. Mathews and R. L. Walker, *Mathematical Methods of Physics*

I. INTERPOLATION

Suppose we have a two-column data set with equally spaced x values, where $x_i = x_0 + ih$.

x_0	x_1	x_2	$\cdots$	x_{n-2}	x_{n-1}	x_n
y_0	y_1	y_2	$\cdots$	y_{n-2}	y_{n-1}	y_n

A. Forward Differences

We define the difference operator Δ such that,

$$\Delta y_i = y_{i+1} - y_i \Rightarrow y_{i+1} = (1+\Delta)y_i \Rightarrow y_i = (1+\Delta)^i y_0, \tag{1}$$

which we can expand using,

$$\begin{aligned} \Delta^2 y_i &= \Delta(\Delta y_i) = \Delta y_{i+1} - \Delta y_i, \ldots, \\ \Delta^n y_i &= \Delta(\Delta^{n-1} y_i) = \Delta^{n-1} y_{i+1} - \Delta^{n-1} y_i. \end{aligned} \tag{2}$$

To interpolate the value of y at some intermediate value x, such that $x_0 < x < x_n$, we use the same formula as the one used for points where data is available. I.e.,

$$y(x) = (1+\Delta)^\alpha y_0, \tag{3}$$

where, $x = x_0 + \alpha h \Rightarrow \alpha = \dfrac{x - x_0}{h}$. Expanding, we get,

$$y(x) = y_0 + \alpha \Delta y_0 + \frac{\alpha(\alpha-1)}{2!}\Delta^2 y_0 + \cdots + \frac{\alpha(\alpha-1)\cdots(\alpha-n+1)}{n!}\Delta^n y_0. \tag{4}$$

Note that even for non-integer α the series terminates since differences of the order greater than n are undefined for a data set with n entries. The above relation also simplifies to,

$$y(x) = y_0 + \frac{(x-x_0)}{h}\Delta y_0 + \frac{(x-x_0)(x-x_1)}{2!h^2}\Delta^2 y_0 + \cdots + \frac{(x-x_0)(x-x_1)\cdots(x-x_{n-1})}{n!h^n}\Delta^n y_0. \tag{5}$$

This is the Newton-Gregory forward difference interpolation formula.
When using this formula using pen and paper, it is useful to construct a table similar to the one shown below (5 data points are used for illustration).

x_0	y_0				
		Δy_0			
x_1	y_1		$\Delta^2 y_0$		
		Δy_1		$\Delta^3 y_0$	
x_2	y_2		$\Delta^2 y_1$		$\Delta^4 y_0$
		Δy_2		$\Delta^3 y_1$	
x_3	y_3		$\Delta^2 y_2$		
		Δy_3			
x_4	y_4				

TABLE I: Sample forward difference table for a data set with five entries.

B. Backward Differences

In the same way as above, we may define the backward difference operator ∇ such that,

$$\nabla y_i = y_i - y_{i-1} \Rightarrow y_{i-1} = (1-\nabla)y_i \Rightarrow y_{n-i} = (1-\nabla)^i y_n, \tag{6}$$

which we can expand using,

$$\begin{aligned} \nabla^2 y_i &= \nabla(\nabla y_i) = \nabla y_i - \nabla y_{i-1}, \ldots, \\ \nabla^n y_i &= \nabla(\nabla^{n-1} y_i) = \nabla^{n-1} y_i - \nabla^{n-1} y_{i-1}. \end{aligned} \tag{7}$$

To interpolate the value of y at some intermediate value x, such that $x_0 < x < x_n$, we use the same formula as the one used for points where data is available. We write $x = x_n + \alpha h \Rightarrow \alpha = \dfrac{x - x_n}{h}$. Thus,

$$y(x) = (1-\nabla)^{-\alpha} y_n. \tag{8}$$

Expanding, we get,

$$y(x) = y_n + \alpha \nabla y_n + \frac{\alpha(\alpha+1)}{2!}\nabla^2 y_n + \cdots + \frac{\alpha(\alpha+1)\cdots(\alpha+n-1)}{n!}\nabla^n y_0. \tag{9}$$

As before, the above relation also simplifies to,

$$y(x) = y_n + \frac{(x-x_n)}{h}\nabla y_n + \frac{(x-x_n)(x-x_{n-1})}{2!h^2}\nabla^2 y_n + \cdots + \frac{(x-x_n)(x-x_{n-1})\cdots(x-x_1)}{n!h^n}\nabla^n y_n. \tag{10}$$

This is the Newton-Gregory backward difference interpolation formula.

x_0	y_0				
		∇y_1			
x_1	y_1		$\nabla^2 y_3$		
		∇y_2		$\nabla^3 y_3$	
x_2	y_2		$\nabla^2 y_3$		$\nabla^4 y_4$
		∇y_3		$\nabla^3 y_4$	
x_3	y_3		$\nabla^2 y_4$		
		∇y_4			
x_4	y_4				

TABLE II: Sample backward difference table for a data set with five entries.

II. NUMERICAL DIFFERENTIATION

The forward, backward and central approximations for the numerical derivative of $f(x)$ at $x = x_0$ are given by,

$$f'(x_0) \approx \frac{f(x_0+\delta x) - f(x_0)}{\delta x} \text{ (forward)}, \tag{11}$$

$$f'(x_0) \approx \frac{f(x_0) - f(x_0-\delta x)}{\delta x} \text{ (backward), and,} \tag{12}$$

$$f'(x_0) \approx \frac{f(x_0+\delta x) - f(x_0-\delta x)}{2\delta x} \text{ (central).} \tag{13}$$

The errors in the forward and backward formulae are of the order of δx (i.e., the ratio of the error to δx is neither negligible nor large compared to one). The error in the central difference formula is of the order of $(\delta x)^2$. Check these by doing Taylor expansions of $f(x_0 \pm \delta x)$ in the above expressions.
The numerical derivative may be calculated using the interpolation formulae. Differentiating Eq. 5, we get,

$$y'(x) = \frac{\Delta y_0}{h} + \Big((x-x_0)+(x-x_1)\Big)\frac{\Delta^2 y_0}{2!h^2} + \cdots + (x-x_0)(x-x_1)\cdots(x-x_{n-1})\left(\sum_{i=0}^{n-1}\frac{1}{x-x_i}\right)\frac{\Delta^n y_0}{n!h^n}, \tag{14}$$

$$y'(x_0) = \frac{1}{h}\left(\Delta y_0 - \frac{\Delta^2 y_0}{2} + \cdots + (-1)^{n-1}\frac{\Delta^n y_0}{n}\right). \tag{15}$$

This formula may be applied to any of the tabulated x-values to give,

$$y'(x_i) = \frac{1}{h}\left(\Delta y_i - \frac{\Delta^2 y_i}{2} + \cdots + (-1)^{n-i-1}\frac{\Delta^{n-i} y_i}{n-i}\right). \tag{16}$$

Similarly, using the backward interpolation formula, Eq. 10, we have,

$$y'(x_n) = \frac{1}{h}\left(\nabla y_n + \frac{\nabla^2 y_n}{2} + \cdots + \frac{\nabla^n y_n}{n}\right), \tag{17}$$

$$\Rightarrow y'(x_i) = \frac{1}{h}\left(\nabla y_i + \frac{\nabla^2 y_i}{2} + \cdots + \frac{\nabla^i y_i}{i}\right). \tag{18}$$