Universidad Nacional Agraria la Molina

Escuela de Postgrado

Maestría en Ingeniería de Recursos Hídricos

Métodos Numéricos en Recursos Hídricos

Sesión 8:
Diferenciación Numérica

Eusebio Ingol Blanco, Ph.D., A.M.ASCE

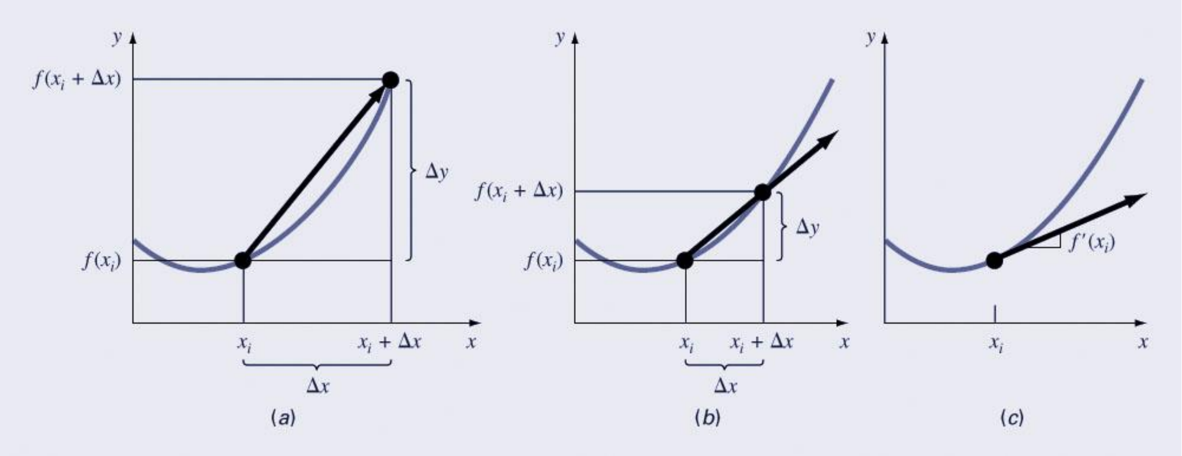
Diferenciación

- The mathematical definition of a derivative begins with a difference approximation:

$$\frac{\Delta y}{\Delta x} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

and as Δx is allowed to approach zero, the difference becomes a derivative:

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$



Backward Finite-Difference

First Derivative | Error

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} \qquad O(h)$$

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

Second Derivative

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

$$f''(x_i) = \frac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3})}{h^2} \qquad O(h^2)$$

Third Derivative

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

$$f'''(x_i) = \frac{5f(x_i) - 18f(x_{i-1}) + 24f(x_{i-2}) - 14f(x_{i-3}) + 3f(x_{i-4})}{2h^3} \qquad O(h^2)$$

Fourth Derivative

$$f''''(x_i) = \frac{f(x_i) - 4f(x_{i-1}) + 6f(x_{i-2}) - 4f(x_{i-3}) + f(x_{i-4})}{h^4} \qquad O(h)$$

$$f''''(x_i) = \frac{3f(x_i) - 14f(x_{i-1}) + 26f(x_{i-2}) - 24f(x_{i-3}) + 11f(x_{i-4}) - 2f(x_{i-5})}{h^4} \qquad O(h^2)$$

High-Accuracy Differentiation Formulas

- Taylor series expansion can be used to generate high-accuracy formulas for derivatives by using linear algebra to combine the expansion around several points.
- Three categories for the formula include ***forward finite-difference***, ***backward finite-difference***, and ***centered finite-difference***.

Forward Finite-Difference

First Derivative	Error
$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_i)}{h}$	$O(h)$
$f'(x_i) = \dfrac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}$	$O(h^2)$
Second Derivative	
$f''(x_i) = \dfrac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2}$	$O(h)$
$f''(x_i) = \dfrac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2}$	$O(h^2)$
Third Derivative	
$f'''(x_i) = \dfrac{f(x_{i+3}) - 3f(x_{i+2}) + 3f(x_{i+1}) - f(x_i)}{h^3}$	$O(h)$
$f'''(x_i) = \dfrac{-3f(x_{i+4}) + 14f(x_{i+3}) - 24f(x_{i+2}) + 18f(x_{i+1}) - 5f(x_i)}{2h^3}$	$O(h^2)$
Fourth Derivative	
$f''''(x_i) = \dfrac{f(x_{i+4}) - 4f(x_{i+3}) + 6f(x_{i+2}) - 4f(x_{i+1}) + f(x_i)}{h^4}$	$O(h)$
$f''''(x_i) = \dfrac{-2f(x_{i+5}) + 11f(x_{i+4}) - 24f(x_{i+3}) + 26f(x_{i+2}) - 14f(x_{i+1}) + 3f(x_i)}{h^4}$	$O(h^2)$

Centered Finite-Difference

First Derivative	Error
$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_{i-1})}{2h}$	$O(h^2)$
$f'(x_i) = \dfrac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h}$	$O(h^4)$
Second Derivative	
$f''(x_i) = \dfrac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2}$	$O(h^2)$
$f''(x_i) = \dfrac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2}$	$O(h^4)$
Third Derivative	
$f'''(x_i) = \dfrac{f(x_{i+2}) - 2f(x_{i+1}) + 2f(x_{i-1}) - f(x_{i-2})}{2h^3}$	$O(h^2)$
$f'''(x_i) = \dfrac{-f(x_{i+3}) + 8f(x_{i+2}) - 13f(x_{i+1}) + 13f(x_{i-1}) - 8f(x_{i-2}) + f(x_{i-3})}{8h^3}$	$O(h^4)$
Fourth Derivative	
$f''''(x_i) = \dfrac{f(x_{i+2}) - 4f(x_{i+1}) + 6f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{h^4}$	$O(h^2)$
$f''''(x_i) = \dfrac{-f(x_{i+3}) + 12f(x_{i+2}) + 39f(x_{i+1}) + 56f(x_i) - 39f(x_{i-1}) + 12f(x_{i-2}) + f(x_{i-3})}{6h^4}$	$O(h^4)$

Richardson Extrapolation

- The Richardson extrapolation can be used to combine two lower-accuracy estimates of the derivative to produce a higher-accuracy estimate.
- For the cases where there are two $O(h^2)$ estimates and the interval is halved ($h_2=h_1/2$), an improved $O(h^4)$ estimate may be formed using:

$$D = \frac{4}{3}D(h_2) - \frac{1}{3}D(h_1)$$

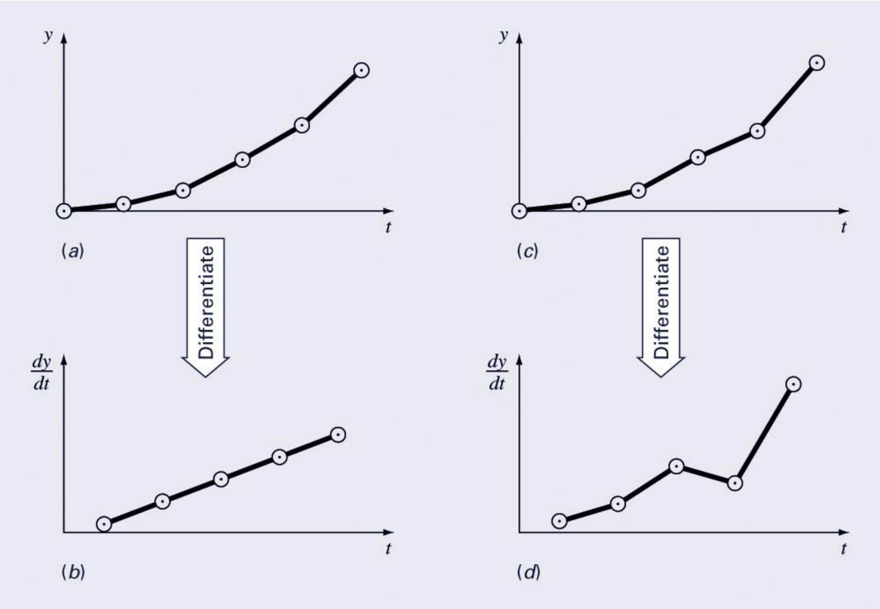
Unequally Spaced Data

- One way to calculated derivatives of unequally spaced data is to determine a polynomial fit and take its derivative at a point.
- As an example, using a second-order Lagrange polynomial to fit three points and taking its derivative yields:

$$f'(x) = f(x_0)\frac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} + f(x_1)\frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} + f(x_2)\frac{2x - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}$$

Derivatives and Integrals for Data with Errors

- A shortcoming of numerical differentiation is that it tends to amplify errors in data, whereas integration tends to smooth data errors.
- One approach for taking derivatives of data with errors is to fit a smooth, differentiable function to the data and take the derivative of the function.



Numerical Differentiation with MATLAB

- MATLAB has two built-in functions to help take derivatives, diff and gradient:
- diff(x)
  - Returns the difference between adjacent elements in x
- diff(y)./diff(x)
  - Returns the difference between adjacent values in y divided by the corresponding difference in adjacent values of x

Numerical Differentiation with MATLAB

- *fx* = gradient(*f*, *h*)
  Determines the derivative of the data in f at each of the points. The program uses forward difference for the first point, backward difference for the last point, and centered difference for the interior points. h is the spacing between points; if omitted h=1.
- The major advantage of gradient over diff is gradient's result is the same size as the original data.
- Gradient can also be used to find partial derivatives for matrices:
  [*fx*, *fy*] = gradient(*f*, *h*)

Visualization

- MATLAB can generate contour plots of functions as well as vector fields. Assuming x and y represent a meshgrid of x and y values and z represents a function of x and y,
  - contour(x, y, z) can be used to generate a contour plot
  - [fx, fy]=gradient(z,h) can be used to generate partial derivatives and
  - quiver(x, y, fx, fy) can be used to generate vector fields