Module 9 – Numerical Differentiation

Lesson goals

1. Understanding the application of high-accuracy numerical differentiation formulas for equi-spaced data.
2. Knowing how to evaluate derivatives for unequally spaced data.
3. Recognizing the sensitivity of numerical differentiation to data error.
4. Knowing how to evaluate derivatives in MATLAB with the `diff` and `gradient` functions.

Introduction

Mathematically, the derivative, which serves as the fundamental vehicle for differentiation, represents the rate of change of a dependent variable with respect to an independent variable. The derivative of $f(x)$ at the point $x = x_i$ is defined as:

$$f'(x_i) = \left.\frac{dy}{dx}\right|_{x=x_i} = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

which is going to be the *slope of the tangent line* to the curve at $x = x_i$. Therefore, for small values of Δx,

$$f'(x_i) \approx \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

Although this may be obvious, it is not very successful, due to round-off error. But it is certainly the place to start.

The second derivative represents the derivative of the first derivative,

$$\frac{d^2y}{dx^2} = \frac{d}{dx}\left(\frac{dy}{dx}\right)$$

which is going to be the rate of change in the slope of tangent line and is commonly referred to as curvature.

Partial derivatives for a function with more than one independent variable can be thought of as taking the derivative of the function at a point with all but one variable held constant. For example, for the function $f(x,y)$, we have:

$$\frac{\partial f(x,y)}{\partial x} = \lim_{\Delta x \to 0} \frac{f(x+\Delta x, y) - f(x,y)}{\Delta x}$$

$$\frac{\partial f(x,y)}{\partial y} = \lim_{\Delta y \to 0} \frac{f(x, y+\Delta y) - f(x,y)}{\Delta y}$$

Example. *Fourier's law of heat conduction* quantifies the observation that heat flows from regions of high to low temperature. For the one-dimensional case, this can be expressed mathematically as

$$q = -k\frac{dT}{dx}$$

where $q(x)$ = heat flux (W/m^2), k = coefficient of thermal conductivity [W/(m.K)], T = temperature (K), and x = distance (m). Thus, the derivative, or gradient, provides a measure of the intensity of the spatial temperature change, which drives the transfer of heat.

$h =$ Step Size $\quad x_{i-1} = x_i - h \quad x_i \quad x_i + h = x_{i+1}$

Numerical Differentiation Formulas

Numerical differentiations are mainly based on the Taylor expansion (series) of a function around a given point or based on interpolating polynomials for a tabular function. We first consider the case where the points are equally spaced.

For the given consecutive points x_i and x_{i+1}, let $h = x_{i+1} - x_i$. Using Taylor expansion, we have:

$f'(x_i)$

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

$$\Rightarrow \; f(x_i + h) = f(x_i) + f'(x_i)h + \frac{f''(\mu)}{2}h^2$$

where $\mu \in (x_{i+1}, x_i)$ and the third term is called the remainder (truncation error) of the expansion. By solving this equation for $f'(x_i)$, we get:

$$f'(x_i) = \frac{f(x_i + h) - f(x_i)}{h} - \frac{f''(\mu)}{2}h$$

Thus, the *forward-difference* (or forward finite difference) approximation

$$f'(x_i) \approx \frac{f(x_i + h) - f(x_i)}{h}$$

has the truncation error as $E_a = -\frac{f''(\mu)}{2}h$ or simply an error of order $O(h)$.

In a similar fashion, we can get *backward-difference* approximation.

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

where $h = x_i - x_{i-1}$. Thus, the *backward-difference* (or backward finite difference) approximation

$$f'(x_i) \approx \frac{f(x_i) - f(x_i - h)}{h}$$

has the truncation error as $E_a = -\frac{f''(\mu)}{2}h$ or simply an error of order $O(h)$.

Now, consider the following two equations:

$$f(x_i + h) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2}h^2 + \frac{f^{(3)}(\mu)}{3!}h^3 \qquad (1)$$

$$f(x_i - h) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2}h^2 - \frac{f^{(3)}(\mu)}{3!}h^3 \qquad (2)$$

Subtracting (2) from (1) yields:

$$f(x_i + h) - f(x_i - h) = 2hf'(x_i) + \frac{f^{(3)}(\hat{\mu})}{3!}h^3$$

Thus, the *centered-difference* (or centered finite difference) approximation

$$f'(x_i) \approx \frac{f(x_i + h) - f(x_i - h)}{2h}$$

has the truncation error as $E_a = -\frac{f^{(3)}(\hat{\mu})}{6}h^2$ or simply an error of order $O(h^2)$.

Note. The truncation error in the centered-difference is of the order of h^2 in contrast to the forward and backward approximations that were of the order of h. Consequently, the Taylor series analysis yields the practical information that the centered difference is a more accurate representation of the first derivative.

For example, if we halve the step size h using a forward or backward difference, we would approximately halve the truncation error, whereas for the central difference, the error would be *quartered*.

Example. Use forward, backward and centered difference approximations to estimate the first derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at $x = 0.5$ using a step size $h = 0.5$. Repeat the computation using $h = 0.25$. Note that the derivative can be calculated directly as

$$f'(x) = -0.4x^3 - 0.45x^2 - 1.0x - 0.25$$

and can be used to compute the true value as $f'(0.5) = -0.9125$.

$h = 0.5$

$f'(0.5) \simeq$

$x_i = 0.5 \qquad x_{i+1} = x_i + h = 1$

forward-diff. $\quad f'(0.5) \simeq \dfrac{f_{i+1} - f_i}{h} = \dfrac{0.2 - 0.925}{0.5} = -1.45 \qquad |\text{error}| = 0.5375$

backward-diff $\quad x_{i-1} = x_i - h = 0 \qquad x_i = 0.5$

$f'(0.5) \simeq \dfrac{f_i - f_{i-1}}{h} = \dfrac{0.925 - 1.2}{0.5} = -0.55 \qquad |\text{error}| = 0.3625$

Centered-diff $\quad x_{i-1} = 0 \qquad x_i = 0.5 \qquad x_{i+1} = 1$

$f'(0.5) \simeq \dfrac{f_{i+1} - f_{i-1}}{2h} = \dfrac{0.2 - 1.2}{2(0.5)} = -1 \qquad |\text{error}| = 0.0875$

For $h = 0.25 \qquad x_{i-1} = 0.25 \qquad x_i = 0.5 \qquad x_{i+1} = 0.75$

Forward: $\quad f'(0.5) \simeq \dfrac{f_{i+1} - f_i}{h} = -1.1547 \qquad |\text{error}| = 0.2422$

back: $\quad f'(0.5) \simeq \dfrac{f_i - f_{i-1}}{h} = -0.7141 \qquad |\text{error}| = 0.1984$

Centered. $\quad f'(0.5) \simeq \dfrac{f_{i+1} - f_{i-1}}{2h} = -0.9344 \qquad |\text{error}| = 0.0214$

$$f(x) = f(x_i) + \frac{f'(x_i)}{1!}(x - x_i) + \frac{f''(x_i)}{2!}(x - x_i)^2 + \frac{f'''(x_i)}{3!}(x - x_i)^3 + \cdots$$

Second-order derivatives.

This above procedure can be used to numerically estimate higher order derivatives. As an example, for the second derivative at $x = x_i$, we have:

$h \quad h$

$x_i \quad x_{i+1} \quad x_{i+2}$

$$f(x_{i+2}) = f(x_i) + f'(x_i)(2h) + \frac{f''(x_i)}{2!}(2h)^2 + \frac{f^{(3)}(x_i)}{3!}(2h)^3 + \cdots$$

$$2\times \quad f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f^{(3)}(x_i)}{3!}h^3 + \cdots$$

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

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

Thus, the *second forward difference* approximation

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

has the truncation error of order $O(h)$. In similar fashion, we can get the second backward difference approximation

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

that has the same truncation error of order $O(h)$. Finally, the second centered difference approximation

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

has the truncation error of order $O(h^2)$.

Example. Use the second centered difference approximations to estimate the first derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at $x = 0.5$ using a step size $h = 0.5$.

$x = 0.5, \quad h = 0.5$

$x_{i-2} = -0.5 \quad x_{i-1} = 0 \quad x_i = 0.5 \quad x_{i+1} = 1 \quad x_{i+2} = 1.5$

Forward: $f''(0.5) \simeq \dfrac{f_{i+2} - 2f_{i+1} + f_i}{h^2} = -3.15 \qquad O(h)$

back: $f''(0.5) \simeq \dfrac{f_i - 2f_{i-1} + f_{i-2}}{h^2} = -1.05 \qquad O(h)$

Centered: $f''(0.5) \simeq \dfrac{f_{i+1} - 2f_i + f_{i-1}}{h^2} = -1.8 \qquad O(h^2)$

$f'(x_i) \simeq \dfrac{f_{i+1} - f_i}{h}$ $\quad O(h)$ $\quad f''(x_i) = \dfrac{f_{i+2} - 2f_{i+1} + f_i}{h^2}$

High-Accuracy Differentiation Formulas

By combining the first and second forward differences formulas, we can improve the accuracy for the forward difference formula from $O(h)$ to $O(h^2)$.

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

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

On the other hand, we know that

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

By substituting this equation in the formula for $f'(x_i)$, we get

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

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

Thus, the approximation

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

has the truncation error of order $O(h^2)$.

In a similar fashion, we can develop an improved formula for the backward and centered differences.

The following tables provide some higher-accuracy formulas for the derivatives of the function $f(x)$ at the equally spaced points.

First Derivative		Error
$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_i)}{h}$	3-points	$O(h)$
$f'(x_i) = \dfrac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}$	5-points	$O(h^2)$
Second Derivative		
$f''(x_i) = \dfrac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2}$	5-points	$O(h)$
$f''(x_i) = \dfrac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2}$	7-points	$O(h^2)$
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		
$f''''(x_i) = \dfrac{f(x_{i+4}) - 4f(x_{i+3}) + 6f(x_{i+2}) - 4f(x_{i+1}) + f(x_i)}{h^4}$		$O(h)$
$f''''(x_i) = \dfrac{-2f(x_{i+5}) + 11f(x_{i+4}) - 24f(x_{i+3}) + 26f(x_{i+2}) - 14f(x_{i+1}) + 3f(x_i)}{h^4}$		$O(h^2)$

Table 1. Forward difference formulas

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

Table 2. Backward difference formulas

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

Table 3. Centered difference formulas

Example. Use the higher accuracy forward, backward and centered difference approximations to estimate the first derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at $x = 0.5$ using a step size $h = 0.25$. Report the relative errors.

$x_{i-2} = 0$ $\quad x_{i-1} = 0.25$ $\quad x_i = 0.5$ $\quad x_{i+1} = 0.75$ $\quad x_{i+2} = 1$

Forward: $f'(0.5) \simeq \frac{-f_{i+2} + 4f_{i+1} - 3f_i}{2h} = -0.8594$

Back: $f'(0.5) \simeq \frac{3f_i - 4f_{i-1} + f_{i-2}}{2h} = -0.8781$

Centered: $f'(0.5) \simeq \frac{-f_{i+2} + 8f_{i+1} - 8f_{i-1} + f_{i-2}}{12h} = -0.9125$

Derivatives of Unequally Spaced Data

To handle nonequispaced data, we fit a Lagrange interpolating polynomial to a set of adjacent points that bracket the location value at which you want to evaluate the derivative. The polynomial can then be differentiated analytically to yield a formula that can be used to estimate the derivative.

For example, you can fit a second-order Lagrange polynomial to three adjacent points $(x_1, f_1), (x_2, f_2),$ and (x_3, f_3).

$$f(x) \approx P_2(x) = \overbrace{\frac{(x - x_2)(x - x_3)}{(x_1 - x_2)(x_1 - x_3)}}^{L_1(x)} f_1 + \overbrace{\frac{(x - x_1)(x - x_3)}{(x_2 - x_1)(x_2 - x_3)}}^{L_2(x)} f_2 + \overbrace{\frac{(x - x_2)(x - x_1)}{(x_3 - x_2)(x_3 - x_1)}}^{L_3(x)} f_3$$

Differentiating the polynomial yields:

$$f'(x) \approx P'_2(x) = \frac{2x - x_2 - x_3}{(x_1 - x_2)(x_1 - x_3)} f_1 + \frac{2x - x_1 - x_3}{(x_2 - x_1)(x_2 - x_3)} f_2 + \frac{2x - x_1 - x_2}{(x_3 - x_2)(x_3 - x_1)} f_3$$

Although it seems a bit complicated, it has some important advantages:

1. It can provide estimates anywhere within the range prescribed by the three points.
2. The points themselves do not have to be equally spaced.
3. The derivative estimate is of the same accuracy as the centered difference for equispaced points.

$$x_1 \xleftrightarrow{h} x_2 \xleftrightarrow{h} x_3$$

Example. Estimate the first derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at $x = 0.5$ using the function values at $x = 0.2, 0.6, 0.7$.

x_i	0.2	0.6	0.7
f_i	1.1286	0.8246	$\underbrace{0.7045}_{f_3}$

$f'(0.5)$

$$P_2(x) = L_1(x) f_1 + L_2(x) f_2 + L_3(x) f_3$$

$$= \frac{(x-0.6)(x-0.7)}{(0.2-0.6)(0.2-0.7)}(1.1286) + \frac{(x-0.2)(x-0.7)}{(0.6-0.2)(0.6-0.7)}(0.8246) + \frac{(x-0.2)(x-0.6)}{(0.7-0.2)(0.7-0.6)} f_3$$

$$P_2'(x) = 5.643(2x-1.3) + (-20.615)(2x-0.9) + (14.09)(2x-0.8)$$

$$f'(0.5) \simeq P_2'(0.5) = -0.9364$$

actual value $= -0.9125$

MATLAB built-in functions for differentiation

Two built-in function diff and gradient can be used. Give a try to the following using Matlab command window:

```
>> f = @(x) 0.2+25*x-200*x.^2+675*x.^3-900*x.^4+400*x.^5;
>> x = 0:0.1:0.8;
>> y = f(x);
>> d = diff(y)./diff(x)
```

$\frac{y_2-y_1}{x_2-x_1} = f'(0.1)$

$[y_1 \quad y_2 \quad y_3 \cdots y_n]$

$[x_1 \quad x_2 \quad x_3 \cdots x_n]$

The vector d now contains derivative estimates corresponding to the midpoint between adjacent elements.

$\frac{y_3-y_2}{x_3-x_2} = f'(0.2)$

The gradient function also returns differences. However, it does so in a manner that is more compatible with evaluating derivatives at the values themselves rather than in the intervals between values. Give a try to the following using Matlab command window:

$[0, 0.8]$

```
>> f = @(x) 0.2+25*x-200*x.^2+675*x.^3-900*x.^4+400*x.^5;
>> x = 0:0.1:0.8;
>> y = f(x);
>> dy = gradient(y,0.1)
```

gradient(y)

(spacing =0.1 , default spacing = 1)

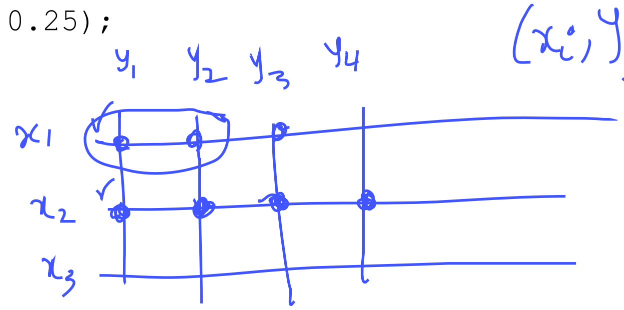
This function can be used to evaluate the gradient vector (partial derivatives vector) for the multivariate function as well.

```
>> f = @(x,y) y - x - 2*x.^2 - 2.*x.*y - y.^2;
>> [x,y] = meshgrid(-2:.25:0, 1:.25:3);
>> z = f(x,y);
>> [fx,fy] = gradient(z,0.25);
```

$\frac{\partial f}{\partial y}(x_1,y_1) = \frac{f(x_1,y_2)-f(x_1,y_1)}{h}$

(x_i, y_j)

$\frac{\partial f}{\partial x}(x_1,y_1) \approx \frac{f(x_2,y_1)-f(x_1,y_1)}{h}$



References

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