~ Numerical Differentiation and Integration ~

Numerical Differentiation

Chapter 23

High Accuracy Differentiation Formulas

- High-accuracy divided-difference formulas can be generated by including additional terms from the Taylor series expansion.

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

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

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

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

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

- Inclusion of the 2nd derivative term has improved the accuracy to $O(h^2)$.
- Similar improved versions can be developed for the *backward* and *centered* formulas

Forward finite-divided-difference formulas

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

Backward finite-divided-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	Error
$f''(x_i) = \dfrac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2}$	**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)**

Centered finite-divided-difference formulas

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	Error
$f''(x_i) = \dfrac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2}$	$O(h^2)$
$f''(x_i) = \dfrac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2}$	$O(h^4)$

Derivation of the centered formula for *f''*(x_i)

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

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

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

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

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

Differentiation Using MATLAB

	x	f(x)
i-2	0	1.2
i-1	0.25	1.1035
i	0.50	0.925
i+1	0.75	0.6363
i+2	1	0.2

First, create a file called **fx1.m** which contains y=f(x):

```
function y = fx1(x)
    y = 1.2 - .25*x - .5*x.^2 - .15*x.^3 -.1*x.^4 ;
```

Command window:

```
>> x=0:.25:1
     0     0.25     0.5     0.75     1
>> y = fx1(x)

     1.2   1.1035   0.925   0.6363   0.2

>> d = diff(y) ./ diff(x)     % diff() takes differences between
                              % consecutive vector elements

     d =   -0.3859   -0.7141   -1.1547   -1.7453
```

Forward: x = 0 0.25 0.50 0.75 1

Backward: x = 0.25 0.50 0.75 1

Example :

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$
$$f'(x) = -0.4x^3 - 0.45x^2 - x - 0.25$$

At **x = 0.5** **True value** for First Derivative = **-0.9125**

Using finite divided differences and a step size of **h = 0.25** we obtain:

	x	$f(x)$
$i-2$	0	1.2
$i-1$	0.25	1.1035
i	0.50	0.925
$i+1$	0.75	0.6363
$i+2$	1	0.2

	Forward ***O(h)***	**Backward** ***O(h)***
Estimate	**-1.155**	**-0.714**
ε_t (%)	**26.5**	**21.7**

Forward difference of accuracy $O(h^2)$ is computed as:

$$f'(0.5) = \frac{-0.2 + 4(0.6363) - 3(0.925)}{2(0.25)} = -0.8593 \qquad \varepsilon_t = 5.82\%$$

Backward difference of accuracy $O(h^2)$ is computed as:

$$f'(0.5) = \frac{3(0.925) - 4(1.1035) + 1.2}{2(0.25)} = -0.8781 \qquad \varepsilon_t = 3.77\%$$

Richardson Extrapolation

- There are two ways to improve derivative estimates when employing finite divided differences:
  - Decrease the step size, or
  - Use a higher-order formula that employs more points.
- A third approach, based on **Richardson extrapolation**, uses two derivative estimates (with $O(h^2)$ error) to compute a third (with $O(h^4)$ error) , more accurate approximation. We can derive this formula following the same steps used in the case of the integrals:

$$h_2 = h_1/2 \quad \Rightarrow \quad \boxed{D \cong \frac{4}{3} D(h_2) - \frac{1}{3} D(h_1)}$$

<u>**Example**</u>: using the previous example and Richardson's formula, estimate the first derivative at **x=0.5** Using **Centered Difference approx. (with error $O(h^2)$)** with **h=0.5** and **h=0.25** :

$\mathbf{D_{h=0.5}(x=0.5)}$ = (0.2-1.2)/1 = -1 [ε_t=|(-.9125+1)/-.9125| = **9.6%**]

$\mathbf{D_{h=0.25}(x=0.5)}$ = (0.6363-1.103)/0.5=-0.9343 [ε_t=|(-.9125+0.9343)/-.9125| = **2.4%**]

The improved estimate is:

D = 4/3(-0.9343) – 1/3(-1) = -0.9125 [ε_t=(-.9125+.9125)/-.9125 = **0%** ➔ **perfect!**]

Derivatives of Unequally Spaced Data

- Derivation formulas studied so far (especially the ones with $O(h^2)$ error) require multiple points to be spaced evenly.

- Data from experiments or field studies are often collected at unequal intervals.

- Fit a ***Lagrange interpolating polynomial***, and then calculate the 1st derivative.

  As an example, second order *Lagrange interpolating polynomial* is used below*:*

$$f(x) = f(x_{i-1})\frac{(x-x_i)(x-x_{i+1})}{(x_{i-1}-x_i)(x_{i-1}-x_{i+1})} + f(x_i)\frac{(x-x_{i-1})(x-x_{i+1})}{(x_i-x_{i-1})(x_i-x_{i+1})} + f(x_{i+1})\frac{(x-x_{i-1})(x-x_i)}{(x_{i+1}-x_{i-1})(x_{i+1}-x_i)}$$

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

Note that any three points, x_{i-1} x_i and x_{i+1} can be used to calculate the derivative.* ***The points do not need to be spaced equally.*

Example:

The ***heat flux*** at the soil-air interface can be computed with *Fourier's Law*:

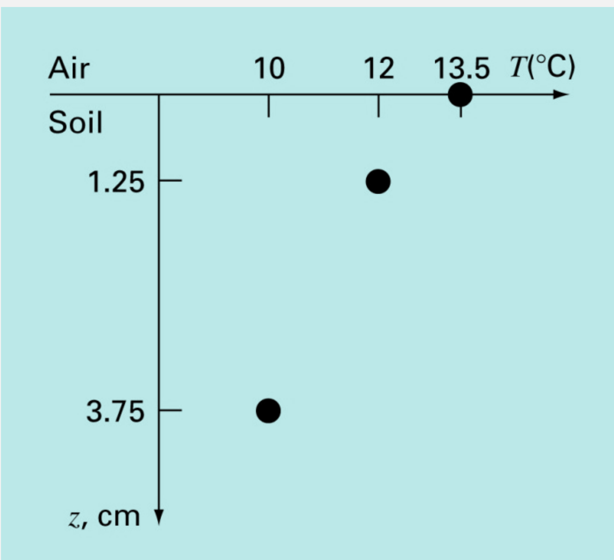
$$q(z=0) = -k\rho C \left.\frac{dT}{dz}\right|_{z=0}$$

q = heat flux
k = coefficient of thermal diffusivity in soil ($\approx 3.5\text{x}10^{-7}$ m^2/s)
ρ = soil density($\approx$ 1800 kg/m^3)
C = soil specific heat($\approx$ 840 J/kg . C^o)
*Positive flux value means heat is transferred from the air to the soil

Calculate ***dT/dz*** (z=0) first and then and determine the heat flux.

A temperature gradient can be measured down into the soil as shown below.

MEASUREMENTS



$$f'(z=0) = 13.5\frac{2(0)-1.25-3.75}{(0-1.25)(0-3.75)}$$
$$+12\frac{2(0)-0-3.75}{(1.25-0)(1.25-3.75)}$$
$$+10\frac{2(0)-0-1.25}{(3.75-0)(3.75-1.25)}$$
$$= -14.4 + 14.4 - 1.333 = -1.333 \quad {}^0C/cm$$

which can be used to compute the *heat flux* at z=0:

q(z=0) = -3.5x10^{-7}(1800)(840)(-133.3 ^{0}C/m)=70.56 W/m^2