Example 2
First Column

$$f(x) = x^{\cos(x)} \text{ at } \quad x = 0.6 \text{ with } \quad h = 0.1$$

$$\Phi(h) = \frac{f(x+h) - f(x-h)}{2h}$$

$$\Phi(0.1) = \frac{f(0.7) - f(0.5)}{0.2} = 1.08483$$

$$\Phi(0.05) = \frac{f(0.65) - f(0.55)}{0.1} = 1.08988$$

$$\Phi(0.025) = \frac{f(0.625) - f(0.575)}{0.05} = 1.09115$$

Example 2
Richardson Table

$$D(n,m)=\frac{1}{4^m-1}\left[4^m D(n,m-1)-D(n-1,m-1)\right]$$

$D(0,0)=1.08483$, D(1,0) = 1.08988, D(2,0) = 1.09115

$$D(n,m)=D(n,m\text{-}1)+\frac{1}{4^m-1}\left[D(n,m\text{-}1)-D(n-1,m\text{-}1)\right]$$

$$D(1,1)=D(1,0)+\frac{1}{4-1}\left[D(1,0)-D(0,0)\right]=1.09156$$

$$D(2,1)=D(2,0)+\frac{1}{4-1}\left[D(2,0)-D(1,0)\right]=1.09157$$

$$D(2,2)=D(2,1)+\frac{1}{4^2-1}\left[D(2,1)-D(1,1)\right]=1.09157$$

Example
Richardson Table

1.08483		
1.08988	1.09156	
1.09115	1.09157	1.09157

This is the best estimate of the derivative of the function.

All entries of the Richardson table are estimates of the derivative of the function.

The first column are estimates using the central difference formula with different h.

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. One can derive this formula following the same steps used in the case of the integrals:

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

High Accuracy Differentiation Formulas

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

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

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

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

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

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

- 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

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

O(*h*)

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

O(*h*²)

Second Derivative

Error

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

O(*h*)

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

O(*h*²)

Backward finite-divided-difference formulas

First Derivative

Error

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

O(*h*)

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

O(*h*²)

Second Derivative

Error

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

O(*h*)

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

O(*h*²)

Centered finite-divided-difference formulas

First Derivative

Error

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

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

Error

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

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)

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

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

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

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

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

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

Evaluate y = 1.2 -0 .25x - 0.5x^2 - 0.15x.^3 -0.1x^4 using MATLAB

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

f(0) = 1.2
f(0.25) =1.1035
f(0.5) = 0.925
f(0.75) = 0.6363
f(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 0.5 0.75 1

Backward: x = 0.25 0.5 0.75 1

Example 3 :

Forward : $f'(x_i) = \dfrac{f(x_{i+1}) - f(x_i)}{h}$

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

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

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

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

Backward : $f'(x_i) = \dfrac{f(x_i) - f(x_{i-1})}{h}$

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

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:

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

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.

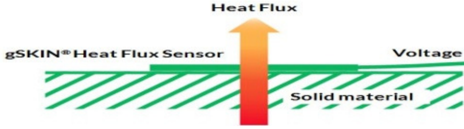
  As an example, second order *Lagrange interpolating polynomial* is used below*:*

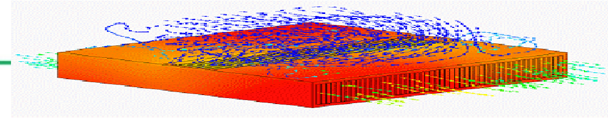
$$f(x) = f(x_{i-1})\frac{(x-x_i)(x-x_{i+1})}{(x_{i-1}-x_i)(x_{i-1}-x_{i+1})} + f(x_i)\frac{(x-x_{i-1})(x-x_{i+1})}{(x_i-x_{i-1})(x_i-x_{i+1})} + f(x_{i+1})\frac{(x-x_{i-1})(x-x_i)}{(x_{i+1}-x_{i-1})(x_{i+1}-x_i)}$$

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

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 4:





*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 (≈3.5×10^{-7} m^2/s)

ρ = soil density(≈ 1800 kg/m^3)

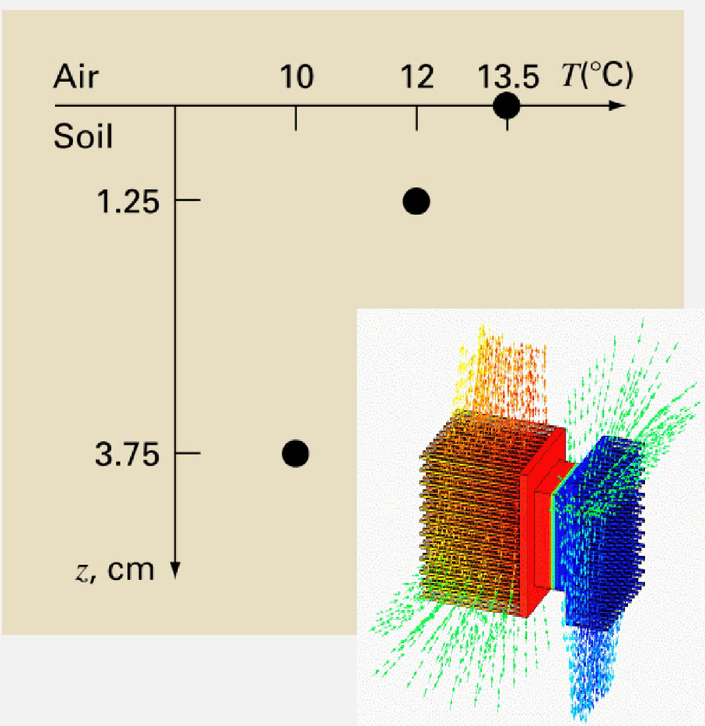
C = soil specific heat(≈ 840 J/kg . C^o)

**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.*

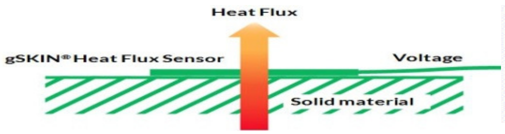
A temperature gradient can be measured down into the soil as shown below.

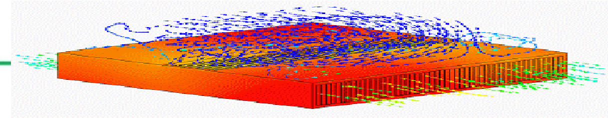
MEASUREMENTS



Z	T
0	13.5
1.25	12
3.75	10

Example 4:





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

*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 (≈3.5x10^{-7} m^2/s)

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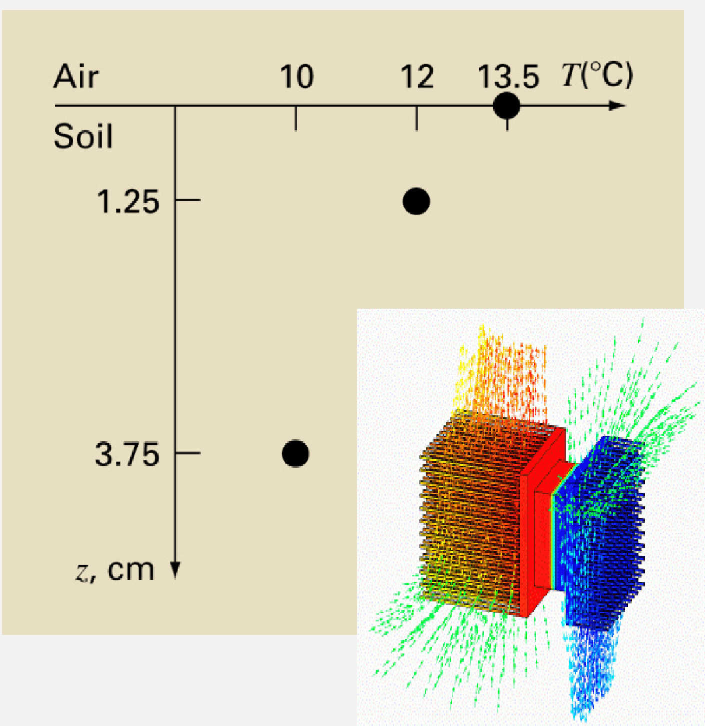
**Positive flux value means heat is transferred from the air to the soil*

*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.

	Z	T
X_o	0	13.5
X_1	1.25	12
X_2	3.75	10

MEASUREMENTS



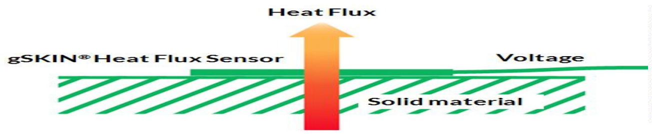
$$f'(z=0) = 13.5\frac{2(0)-1.25-3.75}{(0-1.25)(0-3.75)} + 12\frac{2(0)-0-3.75}{(1.25-0)(1.25-3.75)} + 10\frac{2(0)-0-1.25}{(3.75-0)(3.75-1.25)}$$

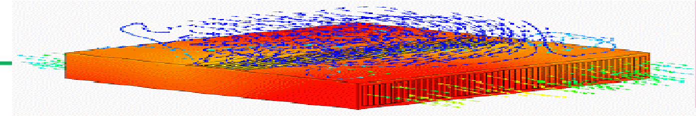
$$= -14.4 + 14.4 - 1.333 = -1.333\ {}^0C/cm$$

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

Example 4:





Method 2

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

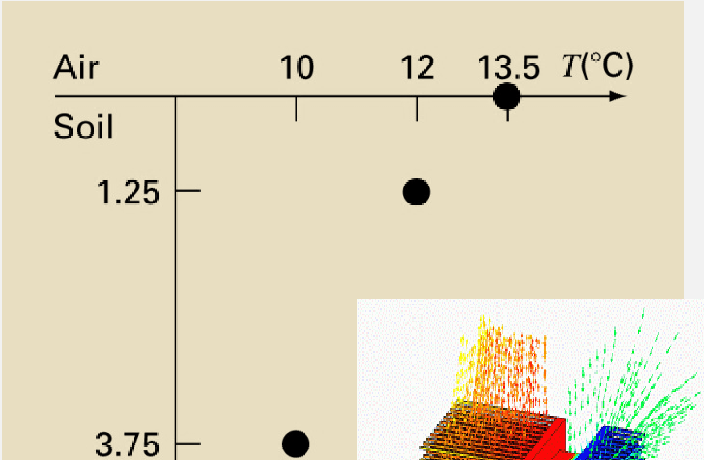
$$q(z=0) = -k\rho C \left.\frac{dT}{dz}\right|_{z=0}$$

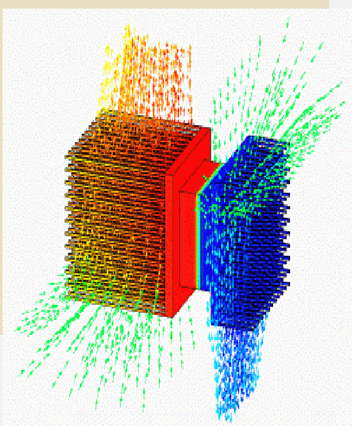
q = heat flux
k = coefficient of thermal diffusivity in soil (≈3.5x10^{-7} m^2/s)
ρ = soil density(≈ 1800 kg/m^3)
C = soil specific heat(≈ 840 J/kg . C^o)
**Positive flux value means heat is transferred from the air to the soil*

*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





$$T_1 = a_1 + a_2 z_1 + a_3 z_1^2$$

$$T_2 = a_1 + a_2 z_2 + a_3 z_2^2$$

$$T_3 = a_1 + a_2 z_3 + a_3 z_3^2$$

$$\overset{\rho}{T} = a_1 + a_2 z + a_3 z^2$$

$$\overset{\rho}{T} \approx a_2 = -1.333 \ {}^0C/cm$$

a_1	13.5
a_2	-1.333
a_3	0.10669

T_1	13.5
T_2	12
T_3	10.0015

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**

Example 5:

Let $f(x) = \ln x$ and $x_0 = 1.8$

Find an approximate value for $f'(1.8)$

h	$f(1.8)$	$f(1.8+h)$	$\frac{f(1.8+h)-f(1.8)}{h}$
0.1	0.5877867	0.6418539	0.5406720
0.01	0.5877867	0.5933268	0.5540100
0.001	0.5877867	0.5883421	0.5554000

The exact value of $f'(1.8) = 0.55\overline{5}$

Assume that a function goes through three points:

$$\left(x_0, f\left(x_0\right)\right), \left(x_1, f\left(x_1\right)\right) \text{ and } \left(x_2, f\left(x_2\right)\right).$$

$$f(x) \approx P(x)$$

$$P\left(x\right) = L_0\left(x\right) f\left(x_0\right) + L_1\left(x\right) f\left(x_1\right) + L_2\left(x\right) f\left(x_2\right)$$

Lagrange Interpolating Polynomial

$$P(x) = L_0(x)f(x_0) + L_1(x)f(x_1) + L_2(x)f(x_2)$$

$$P(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0)$$

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

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

$$f'(x) \approx P'(x)$$

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

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

If the points are equally spaced, i.e.,

$$x_1 = x_0 + h \text{ and } x_2 = x_0 + 2h$$

$$P'(x_0) = \frac{2x_0 - (x_0 + h) - (x_0 + 2h)}{\{x_0 - (x_0 + h)\}\{x_0 - (x_0 + 2h)\}} f(x_0)$$

$$+ \frac{2x_0 - x_0 - (x_0 + 2h)}{\{(x_0 + h) - x_0\}\{(x_0 + h) - (x_0 + 2h)\}} f(x_1)$$

$$+ \frac{2x_0 - x_0 - (x_0 + h)}{\{(x_0 + 2h) - x_0\}\{(x_0 + 2h) - (x_0 + h)\}} f(x_2)$$

$$P'(x_0) = \frac{-3h}{2h^2} f(x_0) + \frac{-2h}{-h^2} f(x_1) + \frac{-h}{2h^2} f(x_2)$$

$$P'(x_0) = \frac{1}{2h}\{-3f(x_0) + 4f(x_1) - f(x_2)\}$$

Three-point formula:

$$f'(x_0) \approx \frac{1}{2h}\{-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)\}$$

If the points are equally spaced with x_0 in the middle:

$$x_1 = x_0 - h \text{ and } x_2 = x_0 + h$$

$$P'(x_0) = \frac{2x_0 - (x_0 - h) - (x_0 + h)}{\{x_0 - (x_0 - h)\}\{(x_0 - (x_0 + h)\}} f(x_0)$$

$$+ \frac{2x_0 - x_0 - (x_0 + h)}{\{(x_0 - h) - x_0\}\{(x_0 - h) - (x_0 + h)\}} f(x_1)$$

$$+ \frac{2x_0 - x_0 - (x_0 - h)}{\{(x_0 + h) - x_0\}\{(x_0 + h) - (x_0 - h)\}} f(x_2)$$

$$P'(x_0) = \frac{0}{-h^2} f(x_0) + \frac{-h}{2h^2} f(x_1) + \frac{h}{2h^2} f(x_2)$$

Another Three-point formula:

$$f'(x_0) \approx \frac{1}{2h}\{f(x_0+h) - f(x_0-h)\}$$

Alternate approach (Error estimate)

Take Taylor series expansion of $f(x+h)$ about x:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f^{(2)}(x) + \frac{h^3}{3!} f^{(3)}(x) + \cdots$$

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

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

$$\frac{f(x+h)-f(x)}{h}=f'(x)+O(h)$$

$$f'(x)=\frac{f(x+h)-f(x)}{h}-O(h)$$

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

Forward Difference Formula

$$O(h)=\frac{h}{2}f^{(2)}(x)+\frac{h^2}{3!}f^{(3)}(x)+\Lambda$$

$$f\left(x+2h\right)=f\left(x\right)+2hf'\left(x\right)+\frac{4h^2}{2}f^{(2)}\left(x\right)+\frac{8h^3}{3!}f^{(3)}\left(x\right)+\Lambda$$

$$f\left(x+2h\right)-f\left(x\right)=2hf'\left(x\right)+\frac{4h^2}{2}f^{(2)}\left(x\right)+\frac{8h^3}{3!}f^{(3)}\left(x\right)+\Lambda$$

$$\frac{f\left(x+2h\right)-f\left(x\right)}{2h}=f'\left(x\right)+\frac{2h}{2}f^{(2)}\left(x\right)+\frac{4h^2}{3!}f^{(3)}\left(x\right)+\Lambda$$

.... (2)

$$\frac{f(x+h)-f(x)}{h}=f'(x)+\frac{h}{2}f^{(2)}(x)+\frac{h^2}{3!}f^{(3)}(x)+\Lambda$$

.... (1)

$$\frac{f(x+2h)-f(x)}{2h}=f'(x)+\frac{2h}{2}f^{(2)}(x)+\frac{4h^2}{3!}f^{(3)}(x)+\Lambda$$

.... (2)

2 X Eqn. (1) – Eqn. (2)

$$2\frac{f(x+h)-f(x)}{h}-\frac{f(x+2h)-f(x)}{2h}$$

$$=f'(x)-\frac{2h^2}{3!}f^{(3)}(x)-\frac{6h^3}{4!}f^{(4)}(x)-\Lambda$$

$$\frac{-f(x+2h)+4f(x+h)-3f(x)}{2h}$$

$$=f'(x)-\frac{2h^2}{3!}f^{(3)}(x)-\frac{6h^3}{4!}f^{(4)}(x)-\Lambda$$

$$=f'(x)+O(h^2)$$

$$\frac{-f(x+2h)+4f(x+h)-3f(x)}{2h}=f'(x)+O(h^2)$$

$$f'(x)=\frac{-f(x+2h)+4f(x+h)-3f(x)}{2h}-O(h^2)$$

$$f'(x)\approx\frac{-f(x+2h)+4f(x+h)-3f(x)}{2h}$$

Three-point Formula

$$O(h^2)=-\frac{2h^2}{3!}f^{(3)}(x)-\frac{6h^3}{4!}f^{(4)}(x)-\Lambda$$

The Second Three-point Formula

Take Taylor series expansion of $f(x+h)$ about x:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f^{(2)}(x) + \frac{h^3}{3!} f^{(3)}(x) + \Lambda$$

Take Taylor series expansion of $f(x-h)$ about x:

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2} f^{(2)}(x) - \frac{h^3}{3!} f^{(3)}(x) + \Lambda$$

Subtract one expression from another

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{2h^3}{3!} f^{(3)}(x) + \frac{2h^6}{6!} f^{(6)}(x) + \Lambda$$

$$f\left(x+h\right)-f\left(x-h\right)=2hf'\left(x\right)+\frac{2h^3}{3!}f^{(3)}\left(x\right)+\frac{2h^6}{6!}f^{(6)}\left(x\right)+\Lambda$$

$$\frac{f\left(x+h\right)-f\left(x-h\right)}{2h}=f'\left(x\right)+\frac{h^2}{3!}f^{(3)}\left(x\right)+\frac{h^5}{6!}f^{(6)}\left(x\right)+\Lambda$$

$$f'\left(x\right)=\frac{f\left(x+h\right)-f\left(x-h\right)}{2h}-\frac{h^2}{3!}f^{(3)}\left(x\right)-\frac{h^5}{6!}f^{(6)}\left(x\right)-\Lambda$$

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + O(h^2)$$

$$O(h^2) = -\frac{h^2}{3!} f^{(3)}(x) - \frac{h^5}{6!} f^{(6)}(x) - \Lambda$$

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

Second Three-point Formula

Summary of Errors

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

Forward Difference Formula

Error term

$$O(h) = \frac{h}{2} f^{(2)}(x) + \frac{h^2}{3!} f^{(3)}(x) + \Lambda$$

Summary of Errors continued

First Three-point Formula

$$f'(x) \approx \frac{-f(x+2h)+4f(x+h)-3f(x)}{2h}$$

Error term $O(h^2) = -\frac{2h^2}{3!} f^{(3)}(x) - \frac{6h^3}{4!} f^{(4)}(x) - \Lambda$

Summary of Errors continued

Second Three-point Formula

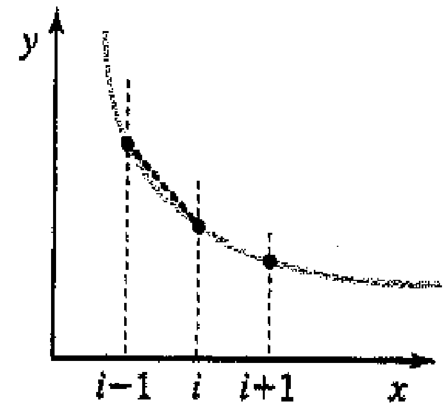
$$f'(x) \approx \frac{f(x+h) - f(x-h)}{2h}$$

Error term $O(h^2) = -\frac{h^2}{3!} f^{(3)}(x) - \frac{h^5}{6!} f^{(6)}(x) - \Lambda$

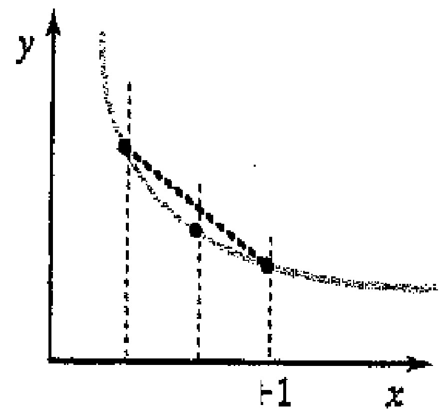
Numerical Differentiation

- First derivatives

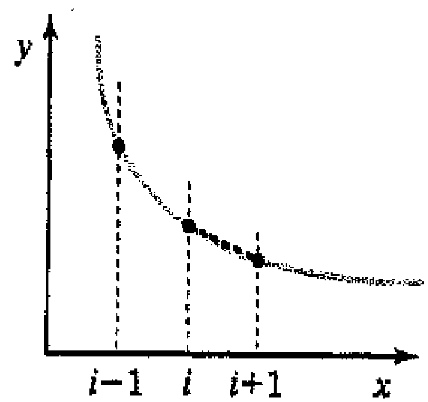
Backward difference $\left.\frac{dy}{dx}\right|_i \approx \frac{y_i - y_{i-1}}{x_i - x_{i-1}}$



Central difference $\left.\frac{dy}{dx}\right|_i \approx \frac{y_{i+1} - y_{i-1}}{x_{i+1} - x_{i-1}}$



Forward difference $\left.\frac{dy}{dx}\right|_i \approx \frac{y_{i+1} - y_i}{x_{i+1} - x_i}$



Numerical Differentiation, cont.

- Second derivatives

SECOND-DERIVATIVE FINITE-DIFFERENCE APPROXIMATIONS	
Backward difference	$$\left.\frac{d^2y}{dx^2}\right\|_i \approx \frac{y_i - 2y_{i-1} + y_{i-2}}{(\Delta x)^2}$$
Central difference	$$\left.\frac{d^2y}{dx^2}\right\|_i \approx \frac{y_{i+1} - 2y_i + y_{i-1}}{(\Delta x)^2}$$
Forward difference	$$\left.\frac{d^2y}{dx^2}\right\|_i \approx \frac{y_{i+2} - 2y_{i+1} + y_i}{(\Delta x)^2}$$

Summary: Forward

Type	Equation	Error
Forward	$f'(x_i) \cong \dfrac{f(x_{i+1}) - f(x_i)}{h}$	$O(h)$
Forward	$f'(x_i) \cong \dfrac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}$	$O(h^2)$
Forward	$f''(x_i) \cong \dfrac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2}$	$O(h)$
Forward	$f''(x_i) \cong \dfrac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2}$	$O(h^2)$
Forward	$f'''(x_i) \cong \dfrac{f(x_{i+3}) - 3f(x_{i+2}) + 3f(x_{i+1}) - f(x_i)}{h^3}$	$O(h)$
Forward	$f'''(x_i) \cong \dfrac{-3f(x_{i+4}) + 14f(x_{i+3}) - 24f(x_{i+2}) + 18f(x_{i+1}) - 5f(x_i)}{h^3}$	$O(h^2)$
Forward	$f^{(4)}(x_i) \cong \dfrac{f(x_{i+4}) - 4f(x_{i+3}) + 6f(x_{i+2}) - 4f(x_{i+1}) + f(x_i)}{h^4}$	$O(h)$
Forward	$f^{(4)}(x_i) \cong \dfrac{-2f(x_{i+5}) + 11f(x_{i+4}) - 24f(x_{i+3}) + 26f(x_{i+2}) - 14f(x_{i+1}) + 3f(x_i)}{h^4}$	$O(h^2)$

Summary: Backward

Backward	$f'(x_i) \cong \dfrac{f(x_i) - f(x_{i-1})}{h}$	$O(h)$
Backward	$f'(x_i) = \dfrac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h}$	$O(h^2)$
Backward	$f''(x_i) \cong \dfrac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2}$	$O(h)$
Backward	$f''(x_i) \cong \dfrac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3})}{h^2}$	$O(h^2)$
Backward	$f'''(x_i) \cong \dfrac{f(x_i) - 3f(x_{i-1}) + 3f(x_{i-2}) - f(x_{i-3})}{h^3}$	$O(h)$
Backward	$f'''(x_i) \cong \dfrac{5f(x_i) - 18f(x_{i-1}) + 24f(x_{i-2}) - 14f(x_{i-3}) + 3f(x_{i-4})}{h^3}$	$O(h^2)$
Backward	$f^{(4)}(x_i) \cong \dfrac{f(x_i) - 4f(x_{i-1}) + 6f(x_{i-2}) - 4f(x_{i-3}) + f(x_{i-4})}{h^4}$	$O(h)$
Backward	$f^{(4)}(x_i) \cong \dfrac{3f(x_i) - 14f(x_{i-1}) + 26f(x_{i-2}) - 24f(x_{i-3}) + 11f(x_{i-4}) - 2f(x_{i-5})}{h^4}$	$O(h^2)$

Higher Order Coefficients

				-1		4		-3				2h
			-2		8		-10		4			$2h^2$
		-3		14		-24		18		-5		$2h^3$
	-4		22		-48		52		-28		6	$2h^4$
-5		32		-76		102		-86		40		$2h^5$ -7
		4,6,8,10, 12.		24,26,28,30, 32.				28,34,40,46		6,8,10,12		

Example 6:

$$f(x) = xe^x$$

Find the approximate value of $f'(2)$ **with** $h = 0.1$

x	$f(x)$
1.9	12.703199
2.0	14.778112
2.1	17.148957
2.2	19.855030

f’ = exp(x) + x*exp(x)

Using the Forward Difference formula:

$$f'(x_0) \approx \frac{1}{h}\left\{ f(x_0+h) - f(x_0) \right\}$$

$$f'(2) \approx \frac{1}{0.1}\left\{ f(2.1) - f(2) \right\}$$

$$= \frac{1}{0.1}\left\{ 17.148957 - 14.778112 \right\}$$

$$= 23.708450$$

x	$f(x)$
1.9	**12.703199**
2.0	**14.778112**
2.1	**17.148957**
2.2	**19.855030**

The exact value of $f'(2)$ **is : 22.167168**

Using the 1st Three-point formula:

$$f'(x_0) \approx \frac{1}{2h}\{-3f(x_0)+4f(x_0+h)-f(x_0+2h)\}$$

$$f'(2) \approx \frac{1}{2\times 0.1}[-3f(2)+4f(2.1)-f(2.2)]$$

$$= \frac{1}{0.2}[-3\times 14.778112 + 4\times 17.148957 - 19.855030]$$

$$= 22.032310$$

x	$f(x)$
1.9	12.703199
2.0	14.778112
2.1	17.148957
2.2	19.855030

The exact value of $f'(2)$ **is : 22.167168**

Using the 2nd Three-point formula:

$$f'(x_0) \approx \frac{1}{2h}\{f(x_0+h) - f(x_0-h)\}$$

$$f'(2) \approx \frac{1}{2 \times 0.1}[f(2.1) - f(1.9)]$$

$$= \frac{1}{0.2}[17.148957 - 12.703199]$$

$$= 22.228790$$

x	$f(x)$
1.9	12.703199
2.0	14.778112
2.1	17.148957
2.2	19.855030

The exact value of $f'(2)$ is : 22.167168

Comparison of the results with $h = 0.1$

The exact value of $f'(2)$ is 22.167168

Formula	$f'(2)$	Error
Forward Difference	23.708450	1.541282
1st Three-point	22.032310	0.134858
2nd Three-point	22.228790	0.061622

x	$f(x)$
1.9	12.703199
2.0	14.778112
2.1	17.148957
2.2	19.855030

Second-order Derivative

$$f\left(x+h\right)=f\left(x\right)+hf'\left(x\right)+\frac{h^2}{2}f^{(2)}\left(x\right)+\frac{h^3}{3!}f^{(3)}\left(x\right)+\Lambda$$

$$f\left(x-h\right)=f\left(x\right)-hf'\left(x\right)+\frac{h^2}{2}f^{(2)}\left(x\right)-\frac{h^3}{3!}f^{(3)}\left(x\right)+\Lambda$$

Add these two equations.

$$f\left(x+h\right)+f\left(x-h\right)=2f\left(x\right)+\frac{2h^2}{2}f^{(2)}\left(x\right)+\frac{2h^4}{4!}f^{(4)}\left(x\right)+\Lambda$$

$$f\left(x+h\right)-2f\left(x\right)+f\left(x-h\right)=\frac{2h^2}{2}f^{(2)}\left(x\right)+\frac{2h^4}{4!}f^{(4)}\left(x\right)+\square$$

$$\frac{f\left(x+h\right)-2f\left(x\right)+f\left(x-h\right)}{h^2}=f^{(2)}\left(x\right)+\frac{2h^2}{4!}f^{(4)}\left(x\right)+\Lambda$$

$$f^{(2)}\left(x\right)=\frac{f\left(x+h\right)-2f\left(x\right)+f\left(x-h\right)}{h^2}-\frac{2h^2}{4!}f^{(4)}\left(x\right)+\Lambda$$

$$f^{(2)}\left(x\right)\approx\frac{f\left(x+h\right)-2f\left(x\right)+f\left(x-h\right)}{h^2}$$

Recall: Numerical Differentiation

1. Forward difference

Taylor series :

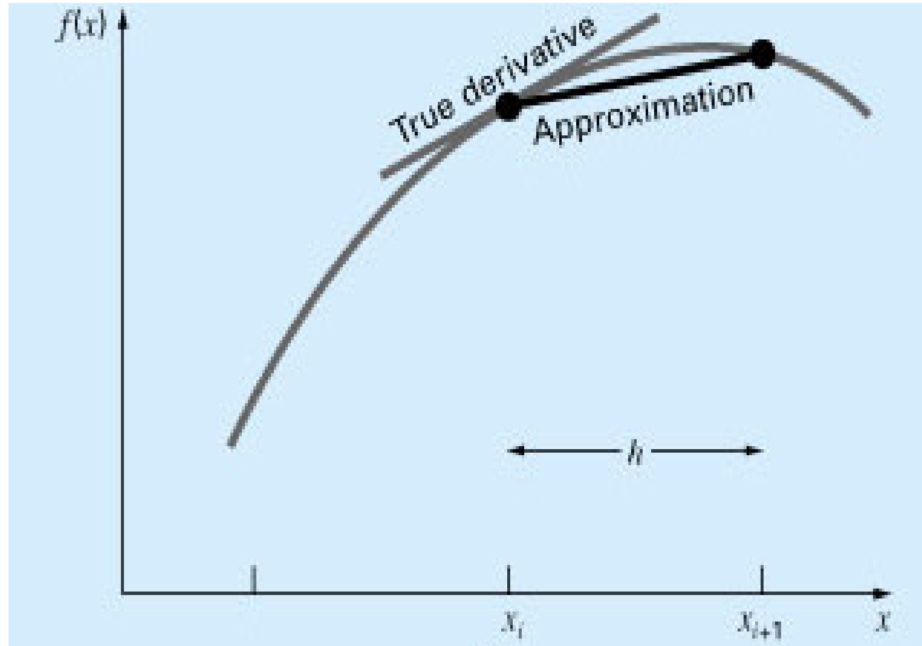
$$f\left(x_{i+1}\right) = f\left(x_i\right) + f'\left(x_i\right)h + \Lambda$$

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

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

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

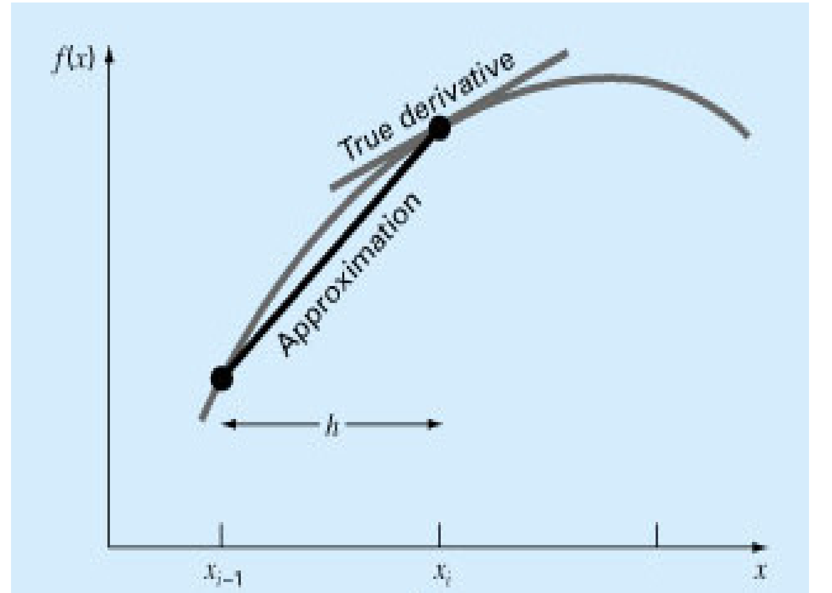
$$f'''(x_i) = \frac{f(x_{i+3}) - 3f(x_{i+2}) + 3f(x_{i+1}) - f(x_i)}{h^3}$$



Numerical Differentiation

2. Backward difference

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



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

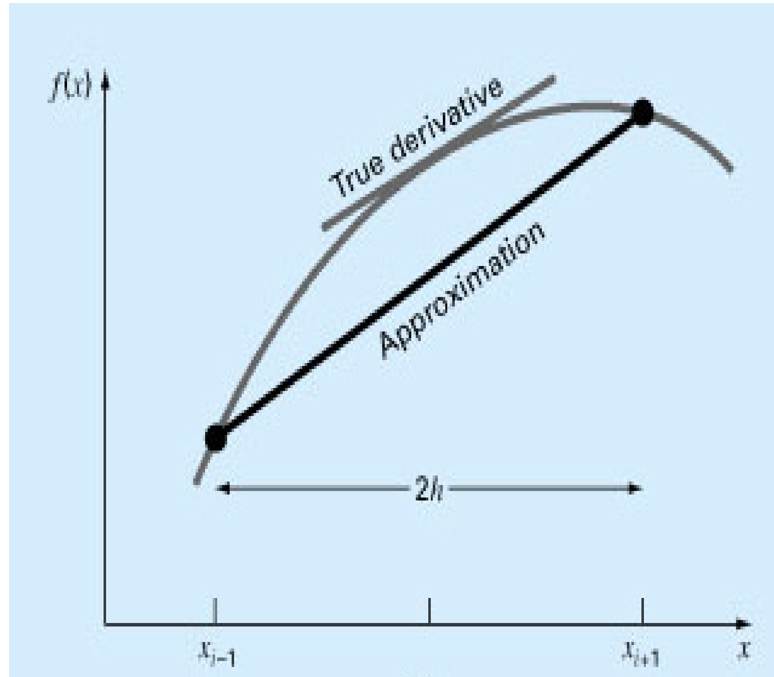
$$= \frac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2}$$

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

Numerical Differentiation

3. Centered difference

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



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

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

Numerical Differentiation

- **Both forward and Backward differentiations have error which is proportional to the order of h. This means that the error decreases linearly with the decrease of h.**

- **Centered differentiation has an error which is proportional to the order of h^2, which means that the error decreases quadratically with the decrease of h.**

- **The notation O(h) and O(h^2) respectively means that the error of order h and h^2.**

High Accuracy Differentiation Formulas

- High-accuracy finite-difference formulas can be generated by including <u>additional terms</u> from the Taylor series expansion.

- <u>An example</u>: High-accuracy forward-difference formula for the first derivative.

Derivation: High-accuracy forward-difference formula for f`(x)

Taylor series expansion

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

Solve for f′(x)

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

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

Substitute the forward-difference approx. of f″(x)

High-accuracy forward-difference formula

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

Derivation: High-accuracy backward-difference formula for f`(x)

Similar improved versions can be developed for the backward and centered formulas as well as for the approximations of the higher derivatives.

Higher Order Forward Divided Difference

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

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

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

Higher Order Backward Divided Difference

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

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

$$f^{///}(x_i)$$

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

Higher Order Central Divided Difference

$$f^{/}(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h}$$

$$f^{//}(x_i)$$
$$= \frac{-f(x_{i=2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2}$$

$$f^{///}(x_i)$$
$$= \frac{-f(x_{i+3}) + 8f(x_{i+2}) - 13f(x_{i+1}) + 13f(x_{i-1}) - 8f(x_{i-2}) + f(x_{i+3})}{8h^3}$$

First Derivatives – Example 7:

- **Use forward, backward and centered difference approximations to estimate the first derivate of:**

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

  at $x = 0.5$ using step size $h = 0.5$ and $h = 0.25$

- **Note that the derivate can be obtained directly:**

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

  The true value of $f'(0.5) = -0.9125$

- **In this example, the function and its derivate are known. However, in general, only tabulated data might be given for ½ & ¼ step size.**

$x_{i-2} = 0.0$	$f(0.0) = 1.2$
$x_{i-1} = 0.25$	$f(0.25) = 1.103516$
$x_i = 0.5$	$f(0.5) = 0.925$
$x_{i+1} = 0.75$	$f(0.75) = 0.63633$
$x = 1.0$	$f(1.0) = 0.2$

Solution with Step Size = 0.5

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

- **f(0.5) = 0.925, f(0) = 1.2, f(1.0) = 0.2**
- **Forward Divided Difference:**

  f'(0.5) ≈ (0.2 – 0.925)/0.5 = -1.45

  $|\varepsilon_t|$ = |(-0.9125+1.45)/-0.9125| = 58.9%

- **Backward Divided Difference:**

  f'(0.5) ≈ (0.925 – 1.2)/0.5 = -0.55

  $|\varepsilon_t|$ = |(-0.9125+0.55)/-0.9125| = 39.7%

- **Centered Divided Difference:**

  f'(0.5) ≈ (0.2 – 1.2)/1.0 = -1.0

  $|\varepsilon_t|$ = |(-0.9125+1.0)/-0.9125| = 9.6%

$x_{i-2} = 0.0$	$f(0.0) = 1.2$
$x_{i-1} = 0.25$	$f(0.25) = 1.$
$x_i = 0.5$	$f(0.5) = 0.9$
$x_{i+1} = 0.75$	$f(0.75) = 0.$
$x_{i+2} = 1.0$	$f(1.0) = 0.2$

Solution with Step Size = 0.25

- $f(0.5)=0.925$, $f(0.25)=1.1035$, $f(0.75)=0.6363$
- **Forward Divided Difference:**

  $f'(0.5) \approx (0.6363 - 0.925)/0.25 = -1.155$

  $|\varepsilon_t| = |(-0.9125+1.155)/-0.9125| = 26.5\%$

$x_{i-2} = 0.0$	$f(0.0) = 1.2$
$x_{i-1} = 0.25$	$f(0.25) = 1.$
$x_i = 0.5$	$f(0.5) = 0.9$
$x_{i+1} = 0.75$	$f(0.75) = 0.$
$x_{i+2} = 1.0$	$f(1.0) = 0.2$

- **Backward Divided Difference:**

  $f'(0.5) \approx (0.925 - 1.1035)/0.25 = -0.714$

  $|\varepsilon_t| = |(-0.9125+0.714)/-0.9125| = 21.7\%$

- **Centered Divided Difference:**

  $f'(0.5) \approx (0.6363 - 1.1035)/0.5 = -0.934$

  $|\varepsilon_t| = |(-0.9125+0.934)/-0.9125| = 2.4\%$

First Derivatives – Example 7a

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 with h = 0.5 and 0.25 (exact sol. = -0.9125)

- **Forward Difference**

$$\begin{cases} h = 0.5,\ f'(0.5) = \dfrac{f(1) - f(0.5)}{1 - 0.5} = \dfrac{0.2 - 0.925}{0.5} = -1.45, \quad |\varepsilon_t| = 58.9\% \\ h = 0.25,\ f'(0.5) = \dfrac{f(0.75) - f(0.5)}{0.75 - 0.5} = \dfrac{0.63632813 - 0.925}{0.25} = -1.155, \ |\varepsilon_t| = 26.5\% \end{cases}$$

- **Backward Difference**

$$\begin{cases} h = 0.5,\ f'(0.5) = \dfrac{f(0.5) - f(0)}{0.5 - 0} = \dfrac{0.925 - 1.2}{0.5} = -0.55, \quad |\varepsilon_t| = 39.7\% \\ h = 0.25,\ f'(0.5) = \dfrac{f(0.5) - f(0.25)}{0.5 - 0.25} = \dfrac{0.925 - 1.10351563}{0.25} = -0.714, \ |\varepsilon_t| = 21.7\% \end{cases}$$

First Derivatives – Example 7:

- **Central Difference**

$x_{i-2} = 0.0$ $f(0.0) = 1.2$
$x_{i-1} = 0.25$ $f(0.25) = 1.103516$
$x_i = 0.5$ $f(0.5) = 0.925$
$x_{i+1} = 0.75$ $f(0.75) = 0.63633$
$x_{i+2} = 1.0$ $f(1.0) = 0.2$

$$h = 0.5,\ \ f'(0.5) = \frac{f(1) - f(0)}{1 - 0} = \frac{0.2 - 1.2}{1} = -1.0, \quad \left|\varepsilon_{\mathrm{t}}\right| = 9.6\%$$

$$h = 0.25,\ \ f'(0.5) = \frac{f(0.75) - f(0.25)}{0.75 - 0.25} =$$

$$\frac{0.63632813 - 1.10351563}{0.5} = -0.934,\ \left|\varepsilon_{\mathrm{t}}\right| = 2.4\%$$

First Derivatives – Example 7:

Employing the high-accuracy formulas (h=0.25):

$x_{i-2} = 0.0$ $\quad f(0.0) = 1.2$

$x_{i-1} = 0.25$ $\quad f(0.25) = 1.103516$

$x_i = 0.5$ $\quad f(0.5) = 0.925$

$x_{i+1} = 0.75$ $\quad f(0.75) = 0.63633$

$x_{i+2} = 1.0$ $\quad f(1.0) = 0.2$

<u>Forward Difference</u>

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

$$f'(0.5) = \frac{-0.2 + 4(0.6363281) - 3(0.925)}{2(0.25)} = -0.8594$$

First Derivatives – Example 7:

- **Backward Difference**

$$f'(0.5) = \frac{3(0.925) - 4(1.035156) + 1.2}{2(0.25)} = -0.8781$$

- **Central Difference**

$$f'(0.5) = \frac{-0.2 + 8(0.636328) - 8(1.035156)}{12(0.25)} = -0.9125$$

$x_{i-2} = 0.0$	$f(0.0) = 1.2$
$x_{i-1} = 0.25$	$f(0.25) = 1.103516$
$x_i = 0.5$	$f(0.5) = 0.925$
$x_{i+1} = 0.75$	$f(0.75) = 0.63633$
$x_{i+2} = 1.0$	$f(1.0) = 0.2$

Summary

True value: f`(0.5) = -0.9125

Basic formulas

h = 0.25	Forward $O(h)$	Backward $O(h)$	Centered $O(h^2)$
Estimate	-1.155	-0.714	-0.934
$\lvert\varepsilon_t\rvert$	26.5%	21.7%	2.4%

High-Accuracy formulas

h = 0.25	Forward $O(h^2)$	Backward $O(h^2)$	Centered $O(h^4)$
Estimate	-0.859375	-0.878125	-0.9125
$\lvert\varepsilon_t\rvert$	5.82%	3.77%	0%

Example8

$$f(x) = x^3$$

x	f(x)
0.9	0.729
0.95	0.857
1	1
1.05	1.158
1.1	1.331

Calculate f'(1) using FD, BD, CD.

$(\therefore f'(x) = 3x^2$, $f'(1) = 3)$

FD:

h=0.1

$$f'(1) = \frac{f(1.1) - f(1)}{0.1} = 3.31 \qquad error = 0.31$$

$\Theta\ error \propto h$

h=0.05

$$f'(1) = \frac{f(1.05) - f(1)}{0.05} = 3.1525 \qquad error = 0.1525$$

BD:

h=0.1

$$f'(1) = \frac{f(1) - f(0.9)}{0.1} = 2.71 \qquad error = 0.29$$

h=0.05

$$f'(1) = \frac{f(1) - f(0.95)}{0.05} = 2.8453 \qquad error = 0.1547$$

CD:

h=0.1

$$f'(1) = \frac{f(1.1) - f(0.9)}{0.2} = 3.01 \qquad error = 0.01$$

$\Theta\ error \propto h^2$

h=0.05

$$f'(1) = \frac{f(1.05) - f(0.95)}{0.1} = 3.00250 \qquad error = 0.00250$$

h=0.1 $$f'(1) = \frac{f(1.1) - f(1)}{0.1} = 3.31 \qquad error = 0.31$$

h=0.05 $$f'(1) = \frac{f(1.05) - f(1)}{0.05} = 3.1525 \qquad error = 0.1525$$

h=0.1 $$f'(1) = \frac{f(1) - f(0.9)}{0.1} = 2.71 \qquad error = 0.29$$

h=0.05 $$f'(1) = \frac{f(1) - f(0.95)}{0.05} = 2.8453 \qquad error = 0.1547$$

h=0.1 $$f'(1) = \frac{f(1.1) - f(0.9)}{0.2} = 3.01 \qquad error = 0.01$$

h=0.05 $$f'(1) = \frac{f(1.05) - f(0.95)}{0.1} = 3.00250 \qquad error = 0.00250$$

- Remarks:
  - FD, BD, CD each involves 2 function calls, 1 subtraction, and 1 division: same computation time
  - **CD is the most accurate (hence, the most recommended method)**
  - ***However*, sometimes, CD cannot be applied**

*More Accurate **FD** Formula (cont)*

- Better accuracy can be achieved using this formula
- But, it involves more computations:
  - 3 function calls, two +/–, one division
- Trade-off:
  - More computation is the price you paid for better accuracy
- Similar idea applies to *more accurate **BD** formula*

Richardson Extrapolation

Idea:

- exact

  = computed+ error

- **The truncation error is of the form: ch^k**
  - **where *c* is some constant**

- Use different *h* to estimate the truncation error
- **Use extrapolation to get more accurate result**

Richardson Extrapolation (cont)

- Example: CD for $f'(x)$

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + O(h^2)$$

- Using Different h (h_1, h_2) :

$$\begin{aligned} exact &= R_1 + c_1 h_1^2 \\ &= R_2 + c_2 h_2^2 \end{aligned}$$

- c_1 and c_2 could be different

Richardson Extrapolation (cont)

- If $c_1 \approx c_2 \equiv c$

$$R_1 + ch_1^2 = R_2 + ch_2^2 = exact$$

$$c\left(h_1^2 - h_2^2\right) = R_2 - R_1 \qquad \Rightarrow c = \frac{R_2 - R_1}{h_1^2 - h_2^2}$$

$$exact = R_2 + \frac{R_2 - R_1}{h_1^2 - h_2^2} \cdot h_2^2 = R_2 + \frac{R_2 - R_1}{h_2^2\left(\frac{h_1^2}{h_2^2} - 1\right)} \cdot h_2^2$$

$$\Rightarrow exact \approx R_2 + \frac{R_2 - R_1}{\left(\frac{h_1}{h_2}\right)^2 - 1}$$

Example 8a

- $f(\mathrm{x}) = x^3$. Use CD with Richardson extrapolation to compute $f'(1)$

$$exact \approx R_2 + \frac{R_2 - R_1}{\left(\frac{h_1}{h_2}\right)^2 - 1}$$

$$h_1 = 0.1$$
$$h_2 = 0.05$$

$$f'(1) = 3.01 \rightarrow R_1$$
$$f'(1) = 3.0025 \rightarrow R_2$$

$$exact \approx 3.0025 + \frac{3.0025 - 3.01}{\left(\frac{0.1}{0.05}\right)^2 - 1} = 3.0000$$

Magic? Coincidence ?

Revisit CD Formula for $f'(x)$

$$f(x+h) = f(x) + f'(x)h + \frac{1}{2}f''(x)h^2 + \frac{1}{3!}f'''(x)h^3 + \frac{1}{4!}f^{(4)}(x)h^4 + \frac{1}{5!}f^{(5)}(x)h^5 + \cdots$$

$$-)\quad f(x-h) = f(x) - f'(x)h + \frac{1}{2}f''(x)h^2 - \frac{1}{3!}f'''(x)h^3 + \frac{1}{4!}f^{(4)}(x)h^4 - \frac{1}{5!}f^{(5)}(x)h^5 + \cdots$$

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{2}{3!}f''(x)h^3 + \frac{2}{5!}f^{(5)}(x)h^5 + \cdots$$

$$\Rightarrow f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{2}{3!}f'''(x)h^2 - \frac{2}{5!}f^{(5)}(x)h^4 - \mathrm{K}$$

Change notation:

$$f'(x) = F(h) + a_1 h^2 + a_2 h^4 + O(h^6)$$

Error Analysis

$$F(h) = f'(x) - a_1 h^2 - a_2 h^4 + O(h^6)$$

$$F(\frac{h}{2}) = f'(x) - \tilde{a}_1 \left(\frac{h}{2}\right)^2 - \tilde{a}_2 \left(\frac{h}{2}\right)^4 - O\left(\frac{h}{2}\right)^6$$

Assuming $a_1 \approx \tilde{a}_1$ and $a_2 \approx \tilde{a}_2$

Eliminate a_1 to get better accuracy

Error Analysis (cont)

$$4\times \quad F(\frac{h}{2}) = f'(x) - a_1\left(\frac{h}{2}\right)^2 - a_2\left(\frac{h}{2}\right)^4 - O\left(\frac{h}{2}\right)^6$$

$$-) \qquad F(h) = f'(x) - a_1 h^2 - a_2 h^4 + O(h^6)$$

$$4F(\frac{h}{2}) - F(h) = 3f'(x) + \left[1 - 4\cdot\frac{1}{16}\right]a_2 h^4 + O(h^6)$$

$$f'(x) = \frac{1}{3}\left[4F(\frac{h}{2}) - F(h)\right] - \frac{1}{4}a_2 h^4 + O(h^6)$$

$$O(h^4)$$

Revisit Previous Example

- $f(\mathrm{x}) = x^3$. Use CD with Richardson extrapolation to compute $f'(1)$
- **a_2 involves $\mathbf{f^{(5)}(x)}$, hence, the exact solution is no surprise.**

Remark

- How much effort did we use to get this level of accuracy?
  - F(h): f(x+h), f(x-h); one –, one ÷
  - F(h/2): f(x+h/2), f(x-h/2); one –, one ÷
  - R.E.: two ×, one –

Example: Evaporation Rates

Table: Saturation Vapor Pressure (e_s) in mm Hg as a Function of Temperature (T) in °C

T(°C)	e_s(mm Hg)
20	17.53
21	18.65
22	19.82
23	21.05
24	22.37
25	23.75

T(°C)	e_s(mm Hg)
20	17.53
21	18.65
22	19.82
23	21.05
24	22.37
25	23.75

The slope of the saturation vapor pressure curve at 22°C (3 methods) :

Forward $$\frac{de_s}{dT} = \frac{e_s(23) - e_s(22)}{23 - 22} = \frac{21.05 - 19.82}{1} = 1.23 \text{ mm Hg/°C}$$

Backward $$\frac{de_s}{dT} = \frac{e_s(22) - e_s(21)}{22 - 21} = \frac{19.82 - 18.65}{1} = 1.17 \text{ mm Hg/°C}$$

Central $$\frac{de_s}{dT} = \frac{e_s(23) - e_s(21)}{23 - 21} = \frac{21.05 - 18.65}{2} = 1.20 \text{ mm Hg/°C}$$

The true value is 1.20 mm Hg/°C, so the central (two-step) method provides the most accurate estimate.

Differentiation :Finite-difference Table

Example: Finite-difference Table for Specific Enthalpy (h) in Btu/lb and Temperature (T) in ºF

T	h	Δh	$\Delta^2 h$	$\Delta^3 h$	$\Delta^4 h$
800	1305				
		155			
1000	1460		-30		
		125		25	
1200	1585		-5		-20
		120		5	
1400	1705		0		
		120			
1600	1825				

- For example, at a temperature of 1200 ºF, the forward, backward, and two-step methods yield:

$$c_p = \frac{\Delta h}{\Delta T} = \frac{1705-1585}{1400-1200} = \frac{120}{200} = 0.6 \text{ Btu/lb/°F}$$

$$c_p = \frac{\Delta h}{\Delta T} = \frac{1585-1460}{1200-1000} = \frac{125}{200} = 0.625 \text{ Btu/lb/°F}$$

$$c_p = \frac{\Delta h}{\Delta T} = \frac{1705-1460}{1400-1000} = \frac{245}{400} = 0.6125 \text{ Btu/lb/°}$$

- The rate of change of c_p at T= 1200 ºF

$$\frac{\Delta^2 h}{\Delta T^2} = \frac{-5}{200} = -0.025 \text{ Btu/lb/(°F)}^2$$

T	h	Δh	Δ^2h	Δ^3h	Δ^4
800	1305				
		155			
1000	1460		-30		
		125		25	
1200	1585		-5		-2
		120		5	
1400	1705		0		
		120			
1600	1825				

Summary

Formulas for the first derivative:

$$f'(x_0) = \frac{f_1 - f_0}{h} + O(h)$$

$$f'(x_0) = \frac{f_1 - f_{-1}}{2h} + O(h^2) \qquad \text{Central difference}$$

$$f'(x_0) = \frac{-f_2 + 4f_1 - 3f_0}{2h} + O(h^2)$$

$$f'(x_0) = \frac{-f_2 + 8f_1 - 8f_{-1} + f_{-2}}{12h} + O(h^4) \qquad \text{Central difference}$$

Formulas for the second derivative:

$$f''(x_0) = \frac{f_2 - 2f_1 + f_0}{h^2} + O(h)$$

$$f''(x_0) = \frac{f_1 - 2f_0 + f_{-1}}{h^2} + O(h^2) \qquad \text{Central difference}$$

$$f''(x_0) = \frac{-f_3 + 4f_2 - 5f_1 + 2f_0}{h^2} + O(h^2)$$

$$f''(x_0) = \frac{-f_2 + 16f_1 - 30f_0 + 16f_{-1} - f_{-2}}{12h^2} + O(h^4) \qquad \text{Central difference}$$

Formulas for the third derivative:

$$f'''(x_0) = \frac{f_3 - 3f_2 + 3f_1 - f_0}{h^3} + O(h)$$

$$f'''(x_0) = \frac{f_2 - 2f_1 + 2f_{-1} - f_{-2}}{2h^3} + O(h^2) \quad \text{Averaged difference}$$

Formulas for the fourth derivative:

$$f^{iv}(x_0) = \frac{f_4 - 4f_3 + 6f_2 - 4f_1 + f_0}{h^4} + O(h)$$

$$f^{iv}(x_0) = \frac{f_2 - 4f_1 + 6f_0 - 4f_{-1} + f_{-2}}{h^4} + O(h^2) \quad \text{Central difference}$$

Forward Finite-divided differences

First Derivative | Error

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

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

Second Derivative

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

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

Third Derivative

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

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

Fourth Derivative

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

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

Backward finite-divided differences

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

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

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

Centered Finite-Divided Differences

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	
$f''''(x_i) = \dfrac{f(x_{i+2}) - 4f(x_{i+1}) + 6f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{h^4}$	$O(h^2)$
$f''''(x_i) = \dfrac{-f(x_{i+3}) + 12f(x_{i+2}) + 39f(x_{i+1}) + 56f(x_i) - 39f(x_{i-1}) + 12f(x_{i-2}) + f(x_{i-3})}{6h^4}$	$O(h^4)$


Thank You!