1. Check the order of accuracy for the approximation:

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

Solution:

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

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

$$f(x+h) - 2f(x) - f(x-h) = h^2 f''(x) + \frac{h^4}{12}f^{(4)}(x) + \cdots$$

$$\frac{f(x+h) - 2f(x) + f(x-h)}{h^2} = f''(x) + \frac{h^2}{12}f^{(4)}(x) + \cdots$$

$$\left| f''(x) - \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} \right| = \frac{h^2}{12}\left| f^{(4)}(x) + \cdots \right|$$

Therefore this is a second order accurate approximation of $f''(x)$.

2. Construct a 6-th order accurate approximation to $f'(x)$ using the Richardson extrapolation. Write a code to check the result and list a table to report how the error decreases and you decrease the value of h.

Solution: Using Taylor series from above:

$$\Phi(h) = f(x+h) - f(x-h) = 2hf'(x) + \frac{h^3}{3}f''(x) + \frac{h^5}{2^2 \cdot 3 \cdot 5}f^{(5)}(x) + \frac{h^7}{2^2 \cdot 3^2 \cdot 5 \cdot 7}f^{(7)}(x) + \cdots$$

$$\Phi(h/3) = f(x+h/3) - f(x-h/3) = \frac{2h}{3}f'(x) + \frac{h^3}{3^4}f''(x) + \frac{h^5}{2^2 \cdot 3^6 \cdot 5}f^{(5)}(x) + \frac{h^7}{2^3 \cdot 3^9 \cdot 5 \cdot 7}f^{(7)}(x) + \cdots$$

$$\Phi(2h/3) = f(x+2h/3) - f(x-2h/3) = \frac{2^2 h}{3}f'(x) + \frac{2^3 h^3}{3^4}f''(x) + \frac{2^3 h^5}{3^6 \cdot 5}f^{(5)}(x) + \frac{2^4 h^7}{3^9 \cdot 5 \cdot 7}f^{(7)}(x) + \cdots$$

Now we create a linear combination of these three functions and solve the resulting system of equations. $\frac{1}{h}(a\Phi(h) + b\Phi(h/3) + c\Phi(2h/3))$.

$$\begin{cases} 2a + \frac{2b}{3} + \frac{2^2 c}{3} & = 1 \\ \frac{a}{3} + \frac{b}{3^4} + \frac{2^3 c}{3^4} & = 0 \\ \frac{a}{2^2 \cdot 3^6 \cdot 5} + \frac{b}{2^2 \cdot 3^6 \cdot 5} + \frac{2^3 c}{3^6 \cdot 5} & = 0 \end{cases} \implies \left[\begin{array}{ccc|c} 2 & 2/3 & 4/3 & 1 \\ 1/3 & 1/81 & 8/81 & 0 \\ 1/60 & 1/14580 & 8/3645 & 0 \end{array}\right] \implies \begin{cases} a = 1/20 \\ b = 9/4 \\ c = -9/20 \end{cases}$$

The residual term is proportional to $O(h^6)$ which means

$$\frac{1}{h}\left(\frac{1}{20}\Phi(h) + \frac{9}{4}\Phi(h/3) - \frac{9}{20}\Phi(2h/3) \right)$$

is a 6th order accurate approximation to $f'(x)$.

Code: Test function used is $f(x) = e^x$

```
import numpy as np
import pandas as pd

n = 20
f = lambda x: np.exp(x)
h = 0.1
x = 1
fprimeref = np.exp(1)
fprimelist = []
hlist = []
error = []

for i in range(0,n):
    phih = f(x + h) - f(x - h)
    phih3 = f(x + h/3) - f(x - h/3)
    phi2h3 = f(x + 2*h/3) - f(x - 2*h/3)
    fprime = (phih/20 + 9*phih3/4 - 9*phi2h3/20)/h
    fprimelist.append(fprime)
    hlist.append(h)
    error.append(np.abs(fprimeref - fprime))
    h = h/2
    i = i+1

listoftuples = list(zip(error, fprimelist))
df = pd.DataFrame(listoftuples, hlist, columns =
        ['error', 'f prime'])
df.to_csv('fprimedata.csv')
```

Output:

h value	f prime	error
0.1	2.71828182848568	2.66E-11
0.05	2.71828182845945	4.13E-13
0.025	2.71828182845905	1.02E-14
0.0125	2.71828182845905	1.02E-14
0.00625	2.71828182845901	3.24E-14
0.003125	2.71828182845897	6.79E-14
0.001563	2.71828182845854	5.01E-13
0.000781	2.71828182845899	4.71E-14
0.000391	2.71828182846059	1.54E-12
0.000195	2.71828182845786	1.18E-12
9.77E-05	2.71828182845479	4.25E-12
4.88E-05	2.71828182847411	1.51E-11
2.44E-05	2.71828182850003	4.10E-11
1.22E-05	2.71828182839999	5.91E-11
6.10E-06	2.71828182836179	9.72E-11
3.05E-06	2.71828182855097	9.19E-11
1.53E-06	2.71828182881290	3.54E-10
7.63E-07	2.71828182935132	8.92E-10
3.81E-07	2.71828182641183	2.05E-09
1.91E-07	2.71828182751778	9.41E-10

3. Construct a 4-th order accurate approximation to $f''(x)$ using the values of f as $x+2h$, $x+h$, x, $x-h$, $x+2h$. Write a code to check the result and list a table to report how the error decreases as you decrease the value of h.

   Solution: From question 1 above:

$$\Phi(h) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} = f''(x) + \frac{h^2}{2^2 \cdot 3} f^{(4)}(x) + \frac{h^4}{2^3 \cdot 3^2 \cdot 5} f^{(6)}(x) + \cdots$$

$$\Phi(2h) = \frac{f(x+2h) - 2f(x) + f(x-2h)}{h^2} = 2^2 f''(x) + \frac{2^2 h^2}{3} f^{(4)}(x) + \frac{2^3 h^4}{3^2 \cdot 5} f^{(6)}(x) + \cdots$$

   Construct a linear combination of $\Phi(h)$ and $\Phi(2h)$ and solve a system of equations to determine the coefficients that make this a 4-th order approximation to the second derivative.

$$a\Phi(h) + b\Phi(2h) = (a + 2^2 b) f''(x) + \left(\frac{a}{2^2 \cdot 3} + \frac{2^2 b}{3} \right) h^2 f^{(4)}(x) + \left(\frac{a}{2^3 \cdot 3^2 \cdot 5} + \frac{2^3 b}{3^2 \cdot 5} \right) h^4 f^{(6)}(x) + \cdots$$

$$\begin{cases} a + 2^2 b & = 1 \\ \frac{a}{2^2 \cdot 3} + \frac{2^2 b}{3} & = 0 \end{cases} \implies \left[\begin{array}{cc|c} 1 & 4 & 1 \\ 1/12 & 4/3 & 0 \end{array}\right] \implies \begin{cases} a = 4/3 \\ b = -1/12 \end{cases}$$

   Code: Test function used is $f(x) = e^x$

```python
import numpy as np
import pandas as pd

n = 20
f = lambda x: np.exp(x)
h = 0.1
x = 1
fdoubleprimeref = np.exp(1)
fdoubleprimelist = []
hlist = []
error = []

for i in range(0,n):
    phih = (f(x + h) + f(x - h) - 2*f(x))/(h**2)
    phi2h = (f(x + 2*h) + f(x - 2*h) - 2*f(x))/(h**2)
    fdoubleprime = (4*phih/3 - phi2h/12)
    fdoubleprimelist.append(fdoubleprime)
    hlist.append(h)
    error.append(np.abs(fdoubleprimeref - fdoubleprime))
    h = h/2
    i = i+1

listoftuples = list(zip(error, fdoubleprimelist))
df = pd.DataFrame(listoftuples, hlist, columns =
          ['error', 'f  double prime'])
df.to_csv('fdoubleprimedata.csv')
```

Output:

h value	f double prime	error
0.1	2.71827880544809	3.02E-06
0.05	2.71828163964711	1.89E-07
0.025	2.71828181666139	1.18E-08
0.0125	2.71828182772395	7.35E-10
0.00625	2.71828182843023	2.88E-11
0.00313	2.71828182852307	6.40E-11
0.00156	2.71828182840181	5.72E-11
0.00078	2.71828182897782	5.19E-10
0.00039	2.71828183516239	6.70E-09
0.0002	2.71828186038571	3.19E-08
9.77E-05	2.71828183128188	2.82E-09
4.88E-05	2.71828221157193	3.83E-07
2.44E-05	2.71828360855579	1.78E-06
1.22E-05	2.71828919649124	7.37E-06
6.10E-06	2.71827975908915	2.07E-06
3.05E-06	2.71837711334228	9.53E-05
1.53E-06	2.71886189778645	0.00058
7.63E-07	2.71924336751302	0.00096
3.81E-07	2.71504720052083	0.00323
1.91E-07	2.70792643229166	0.01036

4. Derive the approximation

$$f'(x_n) \approx \frac{3f(x_n) - 4f(x_{n-1}) + f(x_{n-2})}{3x_n - 4x_{n-1} + x_{n-2}}$$

and show the error term is $O(h^2)$ as $h \to 0$ if $x_n = x_{n-1} + h = x_{n-2} + 2h$.

Solution: First notice that $x_{n-1} = x_n - h$ and $x_{n-2} = x_n - 2h$

$$f(x_{n-1}) = f(x_n - h) = f(x_n) - hf'(x_n) + \frac{h^2}{2!}f''(x_n) - \frac{h^3}{3!}f'''(x_n) + \frac{h^4}{4!}f^{(4)}(x_n) + \cdots$$

$$f(x_{n-2}) = f(x_n-2h) = f(x_n)-2hf'(x_n)+\frac{2^2h^2}{2!}f''(x_n)-\frac{2^3h^3}{3!}f'''(x_n)+\frac{2^4h^4}{4!}f^{(4)}(x_n)+\cdots$$

Therefore the numerator of the approximation is

$$\begin{aligned}
&3f(x_n)\\
&- 4(f(x_n) - hf'(x_n) + \frac{h^2}{2!}f''(x_n) - \frac{h^3}{3!}f'''(x_n) + \frac{h^4}{4!}f^{(4)}(x_n) + \cdots)\\
&+ f(x_n) - 2hf'(x_n) + \frac{2^2h^2}{2!}f''(x_n) - \frac{2^3h^3}{3!}f'''(x_n) + \frac{2^4h^4}{4!}f^{(4)}(x_n) + \cdots\\
\hline
&2hf'(x_n) - \frac{h^3}{2}f'''(x_n) + \cdots
\end{aligned}$$

The denominator is

$$3x_n - 4x_{n-1} + x_{n-2} = 3x_n - 4(x_n - h) + x_n - 2h = 2h$$

Putting it all together we have

$$\frac{3f(x_n) - 4f(x_{n-1}) + f(x_{n-2})}{3x_n - 4x_{n-1} + x_{n-2}} = f'(x_n) - \frac{h^2}{2}f'''(x_n) + \cdots$$

$$\left| f'(x_n) - \frac{3f(x_n) - 4f(x_{n-1}) + f(x_{n-2})}{3x_n - 4x_{n-1} + x_{n-2}} \right| = \left| \frac{h^2}{2} f'''(x_n) + \cdots \right|$$

Since the residual term is of order two this implies that the formula is a second order accurate approximation to the first derivative at x_n.

5. Derive the Newton-Cotes formula for$\int_0^1 f(x)dx$ based on nodes 0, 1/3, 2/3, 1.

Solution: This can be derived very quickly using test functions or we can use Lagrangian Interpolation techniques to arrive at the formula.

$$\int_0^1 f(x)dx = \sum_{i=0}^{n} f(x_i) \int_0^1 l_i(x) + \frac{f^{(n+1)}(\xi_x)}{(n+1)!}\omega(x)dx$$

where $\omega(x) = \prod_{i=0}^{n}(x-x_i)$. Let $A_i = \int_0^1 l_i(x)dx$. The A_i's can be specifically calculated for each i up to n. Now we have

$$\int_0^1 f(x)dx = \sum_{i=0}^{n} f(x_i)A_i + \frac{f^{(n+1)}(\xi_x)}{(n+1)!} \int_0^1 \prod_{i=0}^{n}(x - x_i)dx$$

Calculate the A_i's:

$$A_0 = \int_0^1 \frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)}dx$$

$$= \frac{\left(\frac{1}{4} - \frac{x_1+x_2+x_3}{3} + \frac{x_1x_2+x_1x_3+x_2x_3}{2} - x_1x_2x_3\right)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)} = \frac{1}{8}$$

$$A_1 = \frac{\left(\frac{1}{4} - \frac{x_0+x_2+x_3}{3} + \frac{x_0x_2+x_0x_3+x_2x_3}{2} - x_0x_2x_3\right)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)} = \frac{3}{8}$$

$$A_2 = \frac{\left(\frac{1}{4} - \frac{x_0+x_1+x_3}{3} + \frac{x_0x_1+x_0x_3+x_1x_3}{2} - x_0x_1x_3\right)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)} = \frac{3}{8}$$

$$A_3 = \frac{\left(\frac{1}{4} - \frac{x_0+x_1+x_2}{3} + \frac{x_0x_1+x_0x_2+x_1x_2}{2} - x_0x_1x_2\right)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)} = \frac{1}{8}$$

The Newton-Cote's formula for $\int_0^1 f(x)dx$ based on nodes 0, 1/3, 2/3, 1 is

$$\int_0^1 f(x)dx \approx \frac{f(0)}{8} + \frac{3f(1/3)}{8} + \frac{3f(2/3)}{8} + \frac{f(1)}{8}$$

6. There are two Newton-Cotes formulas for n=2; namely,

$$\int_0^1 f(x)dx \approx af(0) + bf(1/2) + cf(1)$$

$$\int_0^1 f(x)dx \approx af(1/4) + bf(1/2) + cf(3/4)$$

Which is better?

Solution: We will use Lagrangian Interpolation techniques again to derive and solve for the unknown coefficients:

$$\int_0^1 f(x)dx \approx \sum_{i=0}^{n} f(x_i)l_i(x)$$

$$\int_0^1 f(x)dx = \sum_{i=0}^{n} f(x_i)\int_0^1 l_i(x) + \frac{f^{(n+1)}(\xi_x)}{(n+1)!}\omega(x)dx$$

where $\omega(x) = \prod_{i=0}^{n}(x-x_i)$. Let $A_i = \int_0^1 l_i(x)dx$. The A_i's can be specifically calculated for each i up to n. Now we have

$$\int_0^1 f(x)dx = \sum_{i=0}^{n} f(x_i)A_i + \frac{f^{(n+1)}(\xi_x)}{(n+1)!}\int_0^1 \prod_{i=0}^{n}(x-x_i)dx$$

Calculate the A_i's:

$$A_0 = \int_0^1 l_0(x)dx = \int_0^1 \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}dx$$
$$A_0 = \int_0^1 \frac{x^2-(x_1+x_2)x+x_1x_2}{(x_0-x_1)(x_0-x_2)}dx = \frac{\frac{1}{3}-\frac{1}{2}(x_1+x_2)+x_1x_2}{(x_0-x_1)(x_0-x_2)}$$

Similarly we calculate A_1 and A_2,

$$A_1 = \frac{\frac{1}{3}-\frac{1}{2}(x_0+x_2)+x_0x_2}{(x_1-x_0)(x_1-x_2)} \quad A_2 = \frac{\frac{1}{3}-\frac{1}{2}(x_0+x_1)+x_0x_1}{(x_2-x_0)(x_2-x_1)}$$

When nodes are 0, 1/2, and 1 we have $a = 1/6$, $b = 2/3$, and $c = 1/6$.
When nodes are 1/4, 1/2, and 3/4 we have $a = 2/3$, $b = -1/3$, and $c = 2/3$.

The residual term is similar for both formulas:

$$\left|\int_0^1 f(x)dx - \sum_{i=0}^{n} f(x_i)A_i\right| = \left|\frac{f^{(n+1)}(\xi_x)}{(n+1)!}\int_0^1 \prod_{i=0}^{n}(x-x_i)dx\right|$$
$$= \frac{f^{(3)}(\xi_x)}{(3)!}\int_0^1 |(x-x_0)(x-x_1)(x-x_2)|\, dx$$

For nodes 0, 1/2, and 1 we have the residual term as:

$$\frac{f^{(3)}(\xi_x)}{(3)!}\int_0^1 |x(x-1/2)(x-1)|\,dx = \frac{f^{(3)}(\xi_x)}{(3)!}\frac{1}{32}$$

For nodes 1/4, 1/2, and 3/4 we have the residual term as:

$$\frac{f^{(3)}(\xi_x)}{(3)!}\int_0^1 |(x-1/4)(x-1/2)(x-3/4)|\,dx = \frac{f^{(3)}(\xi_x)}{(3)!}\frac{5}{256}$$

Since the error term for the second formula is bounded by a smaller number this one is better.

7. Is there a formula of the form $\int_0^1 f(x)dx \approx \alpha(f(x_0)+f(x_1))$ that correctly integrates all quadratic polynomials?

Solution: Using test functions $f(x) = 1,\ x,\ x^2$ we can determine the value of α

$$\int_0^1 1dx \approx \alpha(1+1) = 1 \implies \alpha = 1/2$$

$$\int_0^1 xdx = \frac{x^2}{2} \approx \alpha(x_0+x_1) = 1/2$$

$$\int_0^1 x^2dx = \frac{x^3}{3} \approx \alpha(x_0^2+x_1^2) = 1/3$$

We have a system of two equations with two unknowns:

$$\begin{cases} x_0+x_1 = 1 \\ x_0^2+x_1^2 = 2/3 \end{cases}$$

This is a circle of radius $\frac{2}{3}$ and a line which intersect at two points, namely $\left(\frac{3-\sqrt{3}}{6}, \frac{3+\sqrt{3}}{6}\right)$ and $\left(\frac{3+\sqrt{3}}{6}, \frac{3-\sqrt{3}}{6}\right)$. Therefore there are two formulas that would correctly integrate all quadratic polynomials:

$$\int_0^1 f(x)dx = \frac{1}{2}\left(f\left(\frac{3-\sqrt{3}}{6}\right)+f\left(\frac{3+\sqrt{3}}{6}\right)\right)$$

and

$$\int_0^1 f(x)dx = \frac{1}{2}\left(f\left(\frac{3+\sqrt{3}}{6}\right)+f\left(\frac{3-\sqrt{3}}{6}\right)\right)$$

Since the two points are symmetric these are actually the same formula.