Definition 5. *A matrix $A_{x\times n}$ is said to be diagonally dominant iff, for each $i = 1, 2, \cdots, n$*

$$|a_{ii}| > \sum_{j=1; j\neq i}^{n} |a_{ij}|$$

For **Jacobi method** we can use the following Matlab code:

Matlab Code 3.12. *Jacobi method*

```
% ******************************************
% ****  Solve a system of linear equation ****
% **       AX=b  by Jaccobi method         **
% ******************************************
clc
clear
close all
A=[4 1 2;1 3 1;1 2 5]; % input the matrix A
b=[16;10;12];          % input the vector b
x0=[0;0;0];            % input the vector X0
n = length(b);
fprintf(' k     x1          x2        x3    \n')
for j = 1 : n
x(j)=((b(j)-A(j,[1:j-1,j+1:n])*x0([1:j-1,j+1:n]))/A(j,j));
end
fprintf('%2.0f  %2.8f %2.8f %2.8f \n',1,x(1),x(2),x(3))
x1 = x';
k = 1;
while abs(x1-x0) > 0.0001
for j = 1 : n
xnew(j)=((b(j)-A(j,[1:j-1,j+1:n])*x1([1:j-1,j+1:n]))/ A(j,j));
```

```
end
 x0 = x1;
 x1 = xnew';
fprintf('%2.0f     %2.8f    %2.8f    %2.8f \n', k+1
    ,xnew(1),xnew(2), xnew(3))
k = k + 1;
end
```

The result as the following:

```
 k       x1           x2          x3
 1    4.00000000   3.33333333   2.40000000
 2    1.96666667   1.20000000   0.26666667
 3    3.56666667   2.58888889   1.52666667
 4    2.58944444   1.63555556   0.65111111
         ....         ....         ....
27    3.00003358   2.00003137   1.00002897
>>
```

Now for 3.3 if we suggests an iterative method by

$$x_1^{k+1} = \frac{1}{a_{11}}\left(b_1 - \sum_{j=2}^{n} a_{1j}x_1^k\right)$$

$$\cdots \quad \cdots \quad \cdots \quad \cdots$$

$$x_i^{k+1} = \frac{1}{a_{ii}}\left(b_i - \sum_{j=1}^{i-1} a_{ij}x_j^{k+1} - \sum_{j=i+1}^{n} a_{ij}x_j^k\right)$$

$$\cdots \quad \cdots \quad \cdots \quad \cdots$$

$$x_n^{k+1} = \frac{1}{a_{11}}\left(b_n - \sum_{j=1}^{n-1} a_{nj}x_j^{k+1}\right)$$

This called **Gauss-Seidel** method.

In the Jacobi method the updated vector x is used for the computations only after all the variables (i.e. all components of the vector x) have been updated. On the other hand in the Gauss-Seidel method, the updated variables are used in the computations as soon as they are updated. Thus in the Jacobi method, during the computations for a particular iteration, the "known" values are all from the previous iteration. However in the Gauss-Seidel method, the "known" values are a mix of variable values from the previous iteration (whose values have not yet been evaluated in the current iteration), as well as variable values that have already been updated in the current iteration.

Example 3.13. *Apply the Gauss-Seidel method to solve*

$$\begin{aligned} 5x_1 - 2x_2 + 3x_3 &= 12 \\ -3x_1 + 9x_2 + x_3 &= 14 \\ 2x_1 - x_2 - 7x_3 &= -12 \end{aligned}$$

Choose the initial guess $\boldsymbol{x}^{(0)} = (0, 0, 0)$.
Solution: *To begin, rewrite the system*

$$\begin{aligned} x_1^{k+1} &= \frac{1}{5}(12 + 2x_2^k - 3x_3^k) \\ x_2^{k+1} &= \frac{1}{9}(14 + 3x_1^{k+1} - x_3^k) \\ x_3^{k+1} &= \frac{-1}{7}(-12 - 2x_1^{k+1} + x_2^{k+1}) \end{aligned}$$

the approximation is

k	x_1	x_2	x_3
0	*0*	*0*	*0*
1	*2.40000000*	*2.35555556*	*2.06349206*
2	*2.10412698*	*2.02765432*	*2.02579995*
3	*1.99558176*	*1.99566059*	*1.99935756*
4	*1.99864970*	*1.99962128*	*1.99966830*
6	...	...	...

For **Gauss-Seidel method** we can use the following Matlab code:

Matlab Code 3.14. *Gauss-Seidel method*

```
% ****************************************
% ****   Solve a system of linear equation ****
% **     Ax=b by Gauss-Seidel method          **
% ****************************************
 clc
 clear
 close all
A=[4 1 2;1 3 1;1 2 5]; % input the matrix A
b=[16;10;12];          % input the vector b
x0=[0;0;0];            % input the vector X0
xnew=x0;
n = length(b);
fprintf(' k     x1      x2        x3    \n')
fprintf('%2.0f %2.0f  %2.0f %2.0f \n', 0 ,x0(1),
    x0(2),x0(3))
flag=1;
w=0;
while flag > 0
w=w+1;
      for k=1:n
            sum=0;
            for i=1:n
                if k~=i
                      sum=sum+A(k,i)*xnew(i);
                end
            end
            xnew(k)=(b(k)-sum)/A(k,k);
      end
fprintf('%2.0f %2.8f %2.8f %2.8f \n',w,xnew(1),
```

```
    xnew(2),xnew(3))
    for k=1:n
        if abs(xnew(k)-x0(k)) > 0.0001
            x0=xnew;
            break
        else
            flag=0;
        end
    end
end
```

The result as the following:

```
k        x1            x2            x3
0         0             0              0
1    4.00000000    2.00000000    0.80000000
2    3.10000000    2.03333333    0.96666667
3    3.00833333    2.00833333    0.99500000
4    3.00041667    2.00152778    0.99930556
5    2.99996528    2.00024306    0.99990972
6    2.99998437    2.00003530    0.99998900
>>
```

3.9 EXERCISE

1. Will Jacobi's or Gauss-Seidel iteration iterative method converge for the linear system $AX = b$, if

$$A = \begin{pmatrix} -10 & 2 & 3 \\ 4 & -50 & 6 \\ 7 & 8 & -90 \end{pmatrix}.$$

Solve the system in both methods if $b = [5, 40, 75]^t$ with initial gauss $X = (0, 0, 0)$.

2. Solve the system

$$\begin{pmatrix} -2 & 1 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & 0 \\ 0 & 1 & -2 & 1 & 0 \\ 0 & 0 & 1 & -2 & 1 \\ 0 & 0 & 0 & 1 & -2 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

using both the Jacobi and the Gauss-Seidel iterations.

3. Solve the system linear of equations

$$\begin{aligned} 2x_1 + 7x_2 + x_3 &= 19 \\ 4x_1 + x_2 - x_3 &= 3 \\ x_1 - 3x_2 + 12x_3 &= 31 \end{aligned}$$

by the Jacobi method and by the Gauss-Seidel method (stop after three iterations).

Chapter 4

Interpolation and Curve Fitting

Suppose one has a set of data pairs:

x_i	x_1	x_2	$\cdots$	x_n
y_i	y_1	y_2	$\cdots$	y_n

and we need to find a function $f(x)$ such that

$$y_i = f(x_i), \quad i = 1, \ldots n \tag{4.1}$$

The equation (4.1) is called the **interpolation equation** or **interpolation condition**. It says that the function $f(x)$ passes through the data points. A function $f(x)$ satisfying the interpolation condition is called an **interpolating function** for the data.
Some of the applications for interpolating function are:

1. Plotting a smooth curve through discrete data points.

2. Reading between lines of a table.

3. in some numerical methods we need an approximation function of tabular data.

4.1 General Interpolation

The general interpolation is to assume the function $f(x)$ is a linear combination of **basis functions** $f_1(x), \ldots, f_n(x)$

$$f(x) = a_1 f_1(x) + a_2 f_2(x) + \cdots + a_n f_n(x)$$

The problem then is to find the values of a_i, $i = 1, \ldots, n$ so that the interpolation conditions

$$y_i = f(x_i) = a_1 f_1(x_i) + a_2 f_2(x_i) + \cdots + a_n f_n(x_i) \quad i = 1, \ldots, n$$

are satisfied. We are assuming that we have the same number of basis functions as we have data points, so that the interpolation conditions are a system of n linear equations for the n unknowns a_i.

Writing out the interpolation conditions in full gives

$$\begin{aligned}
y_1 &= f_1(x_1)a_1 + f_2(x_1)a_2 + \cdots + f_n(x_1)a_n \\
y_2 &= f_1(x_2)a_1 + f_2(x_2)a_2 + \cdots + f_n(x_2)a_n \\
&\vdots \\
y_n &= f_1(x_n)a_1 + f_2(x_n)a_2 + \cdots + f_n(x_n)a_n
\end{aligned}$$

or, in matrix form

$$\begin{bmatrix} f_1(x_1) & f_2(x_1) & \cdots & f_n(x_1) \\ f_1(x_2) & f_2(x_2) & \cdots & f_n(x_2) \\ \vdots & \vdots & \vdots & \vdots \\ f_1(x_n) & f_2(x_n) & \cdots & f_n(x_n) \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

This shows that the general interpolation problem can be reduced to solving a system of linear equations. The matrix in these equations is called the **basis matrix**. Each column of the basis matrix consists of one of the basis functions evaluated at all the x data values. The right-hand-side of

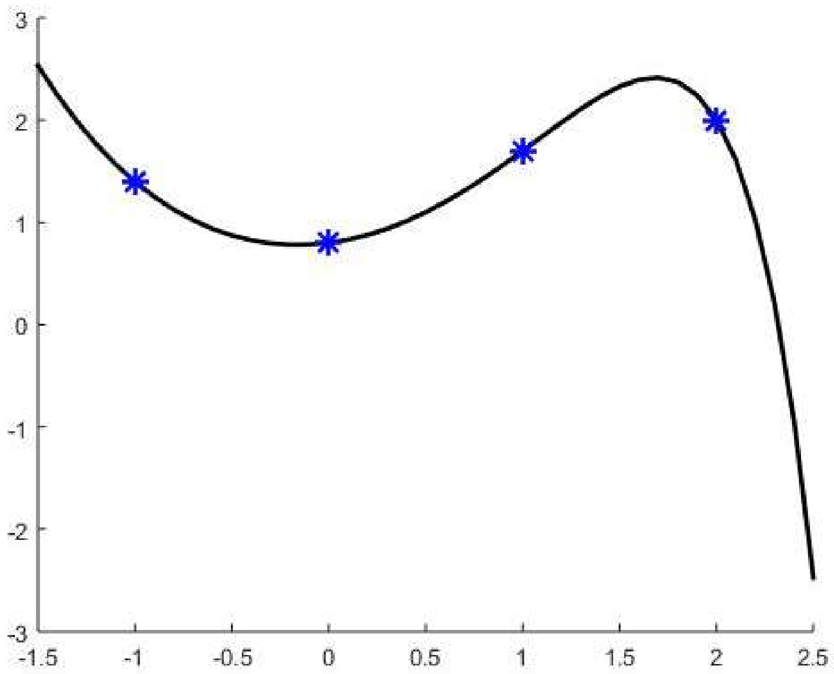

Figure 4.1: digram of function $f(x)$ of example 4.1, the given points are blue stars

the system of equations is the vector of y data values. The solution of the linear system gives the coefficients of the basis functions. We can use the general formalism above to solve many interpolation problems.

Example 4.1. *We will interpolate the data*

x	-1	0	1	2
y	1.4	0.8	1.7	2

by a function of the form

$$f(x) = a_1 e^{-x} + a_2 + a_3 e^{x} + a_4 e^{2x}$$

In this case the basis functions are

$$f_1(x) = e^{-x}, \quad f_2(x) = 1, \quad f_3(x) = e^{x}, \quad f_4(x) = e^{2x}$$

Now the problem is to determine the coefficients a_1, a_2, a_3 *and* a_4. *The basis matrix is*

$$\begin{bmatrix} e^{-x_1} & 1 & e^{x_1} & e^{2x_1} \\ e^{-x_2} & 1 & e^{x_2} & e^{2x_2} \\ e^{-x_3} & 1 & e^{x_3} & e^{2x_3} \\ e^{-x_4} & 1 & e^{x_4} & e^{2x_4} \end{bmatrix} = \begin{bmatrix} e^{1} & 1 & e^{-1} & e^{-2} \\ e^{0} & 1 & e^{0} & e^{0} \\ e^{-1} & 1 & e^{1} & e^{2} \\ e^{-2} & 1 & e^{2} & e^{4} \end{bmatrix}$$

and the right-hand-side vector is $b = [1.4, 0.8, 1.7, 2]^t$ *and the coefficients of the basis functions are* $[a_1, a_2, a_3, a_4] = [0.7352, -1.0245, 1.1978, -$
So our interpolating function is (see figure 4.1):

$$f(x) = 0.7352e^{-x} - 1.0245 + 1.1978e^{x} - 0.1085e^{2x}$$

Example 4.2. *We will again interpolate the same data in example 4.1 but by a cubic polynomial*

$$f(x) = a_1 + a_2x + a_3x^2 + a_4x^3.$$

In this case the basis functions are

$$f_1(x) = 1, \quad f_2(x) = x, \quad f_3(x) = x^2, \quad f_3(x) = x^3$$

Then the basis matrix is

$$\begin{bmatrix} 1 & x_1 & x_1^2 & x_1^3 \\ 1 & x_2 & x_2^2 & x_2^3 \\ 1 & x_3 & x_3^2 & x_3^3 \\ 1 & x_4 & x_4^2 & x_4^3 \end{bmatrix} = \begin{bmatrix} 1 & -1 & 1 & -1 \\ 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 \\ 1 & 2 & 4 & 8 \end{bmatrix}$$

and we need to solve

$$\begin{bmatrix} 1 & -1 & 1 & -1 \\ 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 \\ 1 & 2 & 4 & 8 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \\ a_4 \end{bmatrix} = \begin{bmatrix} 1.4 \\ 0.8 \\ 1.7 \\ 2 \end{bmatrix}$$

Solving the problem gives $[a1, a2, a3, a_4] = [0.8, 0.5, 0.75, -0.35]$ *and we have the interpolating polynomial (see figure 4.2):*

$$f(x) = 0.8 + 0.5x + 0.75x^2 - 0.35x^3$$

.

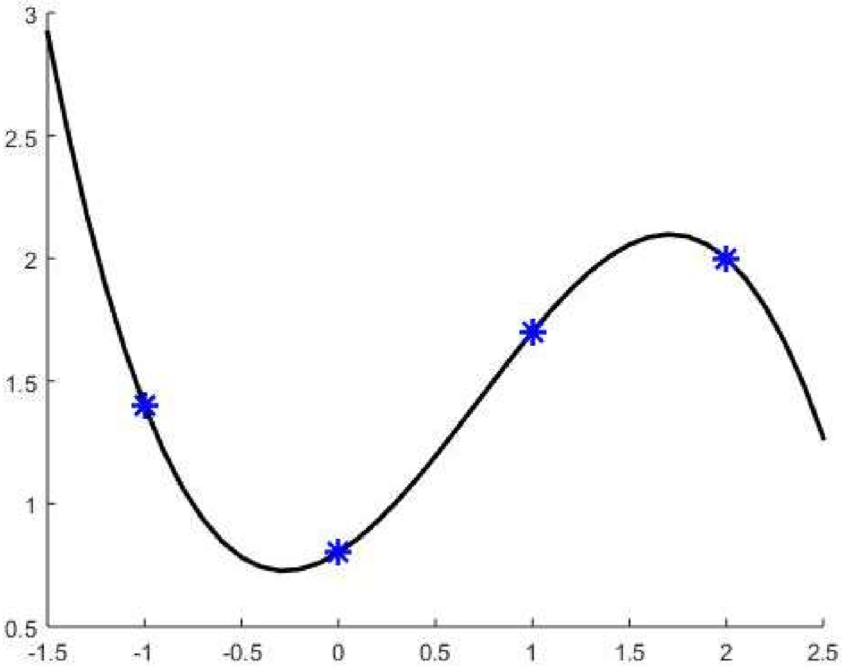

Figure 4.2: digram of function $f(x)$ of example 4.2, the given points are blue stars

4.2 Polynomial Interpolation

We have from the Fundamental theorem of Algebra:
Given any set of data

$$(x_i, y_i), \quad i = 1, \dots n,$$

there is a *unique* polynomial of degree *at most* $n-1$ which interpolates the data. Note that a polynomial of degree $n-1$ has n coefficients, the same as the number of data points. Writing the interpolating polynomial as

$$p(x) = a_1 + a_2 x + a_3 x^2 + \cdots + a_n x^{n-1}.$$

the basis functions are

$$f_1(x) = 1, \quad f_2(x) = x, \quad f_3(x) = x^2, \quad \dots, \quad f_n(x) = x^{n-1}$$

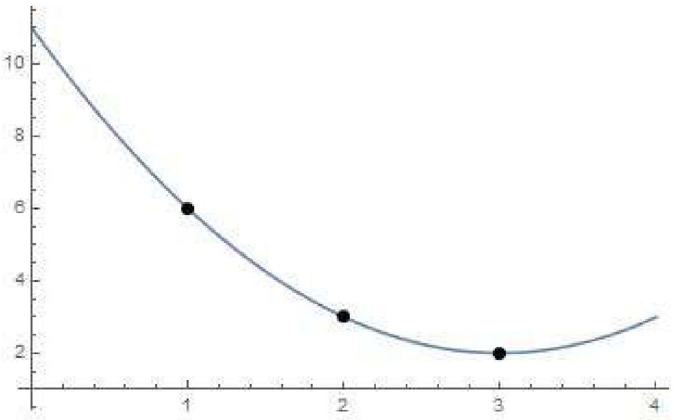

Figure 4.3: digram of function $f(x)$ of example 4.3

For data $x_1, \ldots, x_n$ the basis matrix is

$$\begin{bmatrix} 1 & x_1 & x_1^2 & \ldots & x_1^{n-1} \\ 1 & x_2 & x_2^2 & \ldots & x_2^{n-1} \\ \vdots & \vdots & \ddots & \vdots & \\ 1 & x_n & x_n^2 & \ldots & x_n^{n-1} \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} \tag{4.2}$$

Example 4.3. *Determine the equation of the polynomial of degree two whose graph passes through the points* $(1, 6)$*,* $(2, 3)$ *and* $(3, 2)$.

Solution:

Suppose the polynomial of degree Two is $y = a_1 + a_2x + a_3x^2$. Then, the corresponding system of linear equations is

$$\begin{aligned} a_1 + a_2 + a_3 &= 6 \\ a_1 + 2a_2 + 2^2a_3 &= 3 \\ a_1 + 3a_2 + 3^2a_3 &= 2 \end{aligned}$$

Or by matrix notation

$$\begin{bmatrix} 1 & 1 & 1 \\ 1 & 2 & 2^2 \\ 1 & 3 & 3^2 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ a_3 \end{bmatrix} = \begin{bmatrix} 6 \\ 3 \\ 2 \end{bmatrix} \tag{4.3}$$

and the solution of the above system is: $a_1 = 11$, $a_1 = -6$ and $a_3 = 1$ which gives $y = x^2 - 6x + 11$. (see figure 4.4)

Example 4.4. *Determine the equation of the polynomial whose graph passes through the points:*

x	*0*	*0.5*	*1.0*	*1.5*	*2.0*	*3.0*
y	*0.0*	*-1.40625*	*0.0*	*1.40625*	*0.0*	*0.0*

The Solution is Homework

which giving the interpolating polynomial

$$p(x) = -6x + 5x^2 + 5x^3 - 5x^4 + x^5.$$

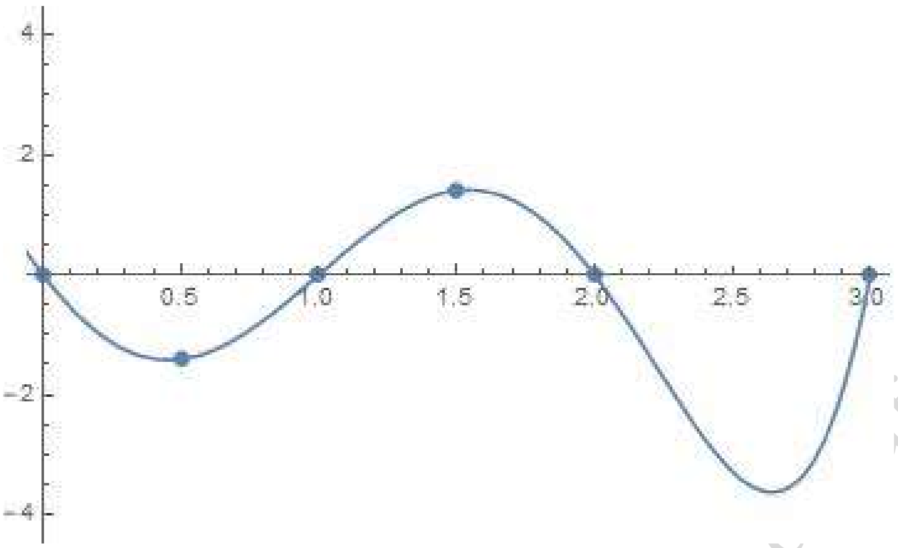

Figure 4.4: digram of function $f(x)$ of example 4.4

4.3 Lagrange Interpolation

Another way to construct the interpolating polynomial is through the Lagrange interpolation formula. Suppose one has a set of data pairs $(x_i, y_i); i = 0, 1, 2, \cdots, n$, then the interpolation polynomial $p_n(x)$ is expressed in terms of the $L_k(x)$ as

$$p_n(x) = \sum_{k=0}^{n} y_k \; L_k(x) \tag{4.4}$$

$$= y_0 \; L_0(x) + y_1 \; L_1(x) + \cdots + y_n \; L_n(x) \tag{4.5}$$

where

$$L_k(x) = \prod_{i=0, i \neq k}^{n} \frac{x - x_i}{x_k - x_i} \tag{4.6}$$

or

$$L_k(x) = \frac{(x - x_0)(x - x_1) \cdots (x - x_{k-1})(x - x_{k+1}) \cdots (x - x_n)}{(x_k - x_0)(x_k - x_1) \cdots (x_k - x_{k-1})(x_k - x_{k+1}) \cdots (x_k - x_n)}$$

Note that

$$L_k(x_i) = \delta_{ik} = \begin{cases} 1 & i = k \\ 0 & i \neq k \end{cases} \tag{4.7}$$

this lead to

$$\begin{aligned} p_n(x_i) &= y_0\ L_0(x_i) + \cdots + y_{i-1}\ L_{i-1}(x_i) + y_i\ L_i(x_i) + y_{i+1}\ L_{i+1}(x_i) + \cdots + y_n\ L_n(x_i) \\ &= y_0\ 0 + \cdots + y_{i-1}\ 0 + y_i\ 1 + y_{i+1}\ 0 + \cdots + y_n\ 0 \\ &= y_i \end{aligned}$$

Theorem 4.5. *Let $x_0, x_1, \cdots, x_n$, be $n+1$ distinct numbers, and let $f(x)$ be a function defined on a domain containing these numbers. Then the polynomial defined by*

$$p_n(x) = \sum_{k=0}^{n} f(x_k)\ L_k(x) \tag{4.8}$$

is the unique polynomial of degree n that satisfies

$$p_n(x_i) = f(x_i); \ i = 0, 1, 2, \cdots, n \tag{4.9}$$

Example 4.6. *We will use Lagrange interpolation to find the polynomial $p_n(x)$, of degree 3 or less, that agrees with the following data*

i	0	1	2	3
x_i	-1	0	1	2
y_i	3	-4	5	-6

In other words, we must have a polynomial $p(x)$ satisfy $p(-1) = 3$, $p(0) = -4$, $p(1) = 5$ and $p(2) = -6$. First, we construct the Lagrange polynomials $\{L_j(x)\}_{j=0}^{3}$ using the formula (4.6). *This* *yields*

$$
\begin{aligned}
L_0(x) &= \frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)} \\
&= \frac{(x-0)(x-1)(x-2)}{(-1-0)(-1-1)(-1-2)} \\
&= \frac{x(x^2-3x+2)}{(-1)(-2)(-3)} \\
&= \frac{-1}{6}(x^3-3x^2+2x)
\end{aligned}
$$

$$
\begin{aligned}
L_1(x) &= \frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)} \\
&= \frac{(x+1)(x-1)(x-2)}{(0+1)(0-1)(0-2)} \\
&= \frac{(x^2-1)(x-2)}{(1)(-1)(-2)} \\
&= \frac{1}{2}(x^3-2x^2-x+2)
\end{aligned}
$$

$$
\begin{aligned}
L_2(x) &= \frac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)} \\
&= \frac{(x+1)(x-0)(x-2)}{(1+1)(1-0)(1-2)} \\
&= \frac{x(x^2-x-2)}{(2)(1)(-1)} \\
&= \frac{-1}{2}(x^3-x^2-2x)
\end{aligned}
$$

$$\begin{aligned} L_3(x) &= \frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)} \\ &= \frac{(x+1)(x-0)(x-1)}{(2+1)(2-0)(2-1)} \\ &= \frac{x(x^2-1)}{(3)(2)(1)} \\ &= \frac{1}{6}(x^3-x) \end{aligned}$$

By substituting x_i for x in each Lagrange polynomial $L_j(x)$, for $j = 0, 1, 2, 3$, it can be verified that

$$L_j(x_i) = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases} \tag{4.10}$$

It follows that the Lagrange interpolating polynomial $p(x)$ is given by

$$p_3(x) = \sum_{k=0}^{3} f(x_k)\; L_k(x) \tag{4.11}$$

$$\begin{aligned} p_3(x) &= \sum_{j=0}^{3} f(x_j)\; L_j(x) \\ &= y_0\; L_0(x) + y_1\; L_1(x) + y_2\; L_2(x) + y_3\; L_3(x) \\ &= (3)\left(\frac{-1}{6}\right)(x^3-3x^2+2x) + (-4)\left(\frac{1}{2}\right)(x^3-2x^2-x+2) \\ &+ (5)\left(\frac{-1}{2}\right)(x^3-x^2-2x) + (-6)\left(\frac{1}{6}\right)(x^3-x) \\ &= -6x^3+8x^2+7x-4 \end{aligned}$$

Substituting each x_i, for $i = 0, 1, 2, 3$, into $p_3(x)$, we can verify that we obtain $p_3(x_i) = y_i$ in each case. [see figure 4.5]

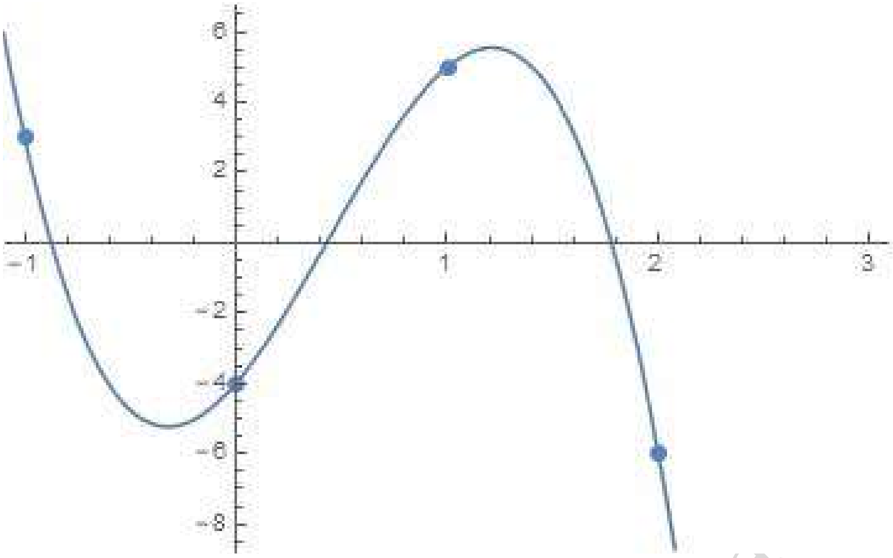

Figure 4.5: digram of function $p_3(x)$ of example 4.6

Using Lagrange Interpolation method with the Matlab code to plot the interpolation polynomial.

Matlab Code 4.7. *Lagrange Interpolation method*

```
% ****************************************************
% ****                interpolation                ****
% **   Plot using Lagrange Polynomial Interpolation   **
% ****************************************************
clc
clear
close all

% xi=[-1.000, -0.960, -0.860, -0.790, 0.220,
```

```
0.500, 0.930]; % x_i data
% yi=[-1.000, -0.151, 0.894, 0.986, 0.895, 0.500, -0.306];  % y_i data

xi=[-2, -1,0,1,2,3];
yi=[4 , 3, 5,5,-7, -2];

m=length(xi);       % m= n+1 i.e degree of the polynomial
% we plotting the lagrang polynomial use x values
% from x_1 to x_n with 1000 divisions
dx=(xi(m)- xi(1))/1000;
x=(xi(1):dx:xi(m));

xlabel('x');
ylabel('y');

L=ones(m,length(x));

for k=1:m     %the rows, i.e L1,L2, L3, L4....
    for i=1:m  %the columns L11, L12, L13....L17
        if (k~=i)       % if k not equal to i
            L(k,:)=L(k,:).*((x-xi(i))/(xi(k)-xi(i)));
        end
    end
end

y=0;
for k=1:m
    f=yi(k).*L(k,:);
    y=y+f;
```

```
 end

plot(x,y,'-b','linewidth',3)          % the
   interpolation polynomial
hold on
plot(xi,yi,'*r','linewidth',4)
xlabel('x');
ylabel('y');
title('Plot using Lagrange Polynomial
   Interpolation')
```

The result as the figure 4.6.

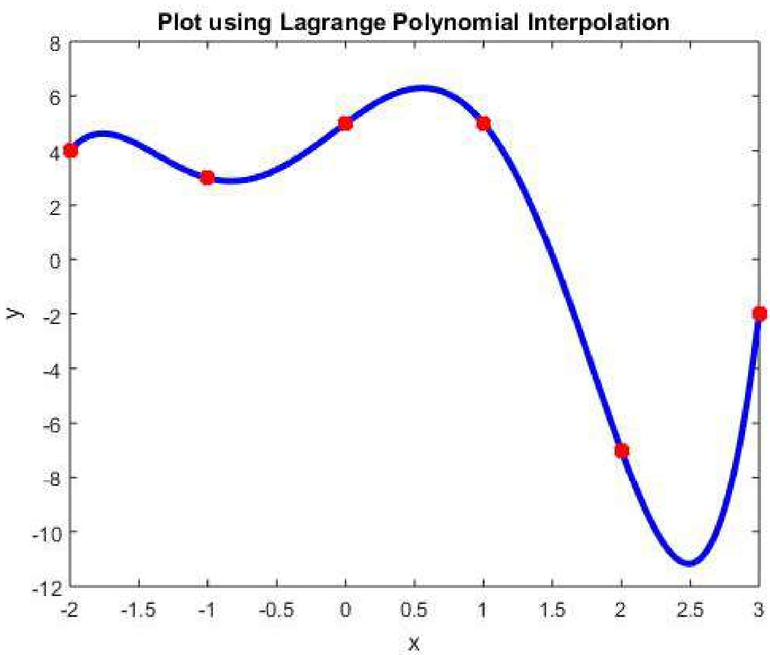

Figure 4.6: digram of Matlab code example 4.7

4.4 EXERCISE

1. Solve example 4.6 using polynomial interpolation method and compare with the Lagrange interpolation method. Estimate the value of $f(1.5)$ and $f(2.5)$.

2. Solve examples 4.1, 4.2, 4.3, 4.4 using Lagrange interpolation method and compare with polynomial interpolation method. Find the approximation value of $f(1.25)$ and $f(2.75)$.

3. Construct the cubic interpolating polynomial to the following data and hence estimate f(1):

x_i	-2	0	3	4
$f(x_i)$	5	1	55	209

4. Use each of the methods described before to construct a polynomial that interpolates the points

$$\{(-2,4),(-1,3),(0,5),(1,5),(2,-7),(3,-2)\}$$

.

4.5 Divided Differences Method

It's also called **Newton's Divided Difference**. Suppose that $P_n(x)$ is the nth Lagrange polynomial that agrees with the function f at the distinct numbers $x_0, x_1, \cdots, x_n$. Although this polynomial is unique, **(Why ?)**, there are alternate algebraic representations that are useful in certain situations. The divided differences of f with respect to $x_0, x_1, \cdots, x_n$ are used to express $P_n(x)$ in the form

$$P_n(x) = a_0+a_1(x-x_0)+a_2(x-x_0)(x-x_1)+\cdots+a_n(x-x_0)\cdots(x-x_{n-1}) \tag{4.12}$$

for appropriate constants $a_0, a_1, \cdots, a_n$. To determine the first of these constants, a_0, note that if $P_n(x)$ is written in the form of Eq. (4.12), then evaluating $P_n(x)$ at x_0 leaves only the constant term a_0; that is

$$a_0 = P_n(x_0) = f(x_0)$$

Similarly, when $P(x)$ is evaluated at x_1, the only nonzero terms in the evaluation of $P_n(x_1)$ are the constant and linear terms

$$f(x_0) + a_1(x_1 - x_0) = P_n(x_1) = f(x_1)$$

so

$$a_1 = \frac{f(x_1) - f(x_0)}{x_1 - x_0} \tag{4.13}$$

We now introduce the divided difference notation, The zeroth divided difference of the function f with respect to x_i, denoted $f[x_i]$, is simply the value of f at x_i

$$f[x_i] = f(x_i) \tag{4.14}$$

The remaining divided differences are defined recursively; the first divided difference of f with respect to x_i and x_{i+1} is denoted $f[x_i, x_{i+1}]$ and defined as

$$f[x_i, x_{i+1}] = \frac{f[x_{i+1}] - f[x_i]}{x_{i+1} - x_i} \tag{4.15}$$

The second divided difference, $f[x_i, x_{i+1}, f_{i+2}]$ is defined as

$$f[x_i, x_{i+1}, x_{i+2}] = \frac{f[x_{i+1}, x_{i+2}] - f[x_i, x_{i+1}]}{x_{i+2} - x_i} \tag{4.16}$$

Similarly, after the $(k-1)$st divided differences $f[x_i, x_{i+1}, \cdots, x_{i+k-1}]$ and $f[x_{i+1}, x_{i+2}, \cdots, x_{i+k-1}, x_{i+k}]$ have been determined, **the** k**th divided difference** relative to $x_i, x_{i+1}, x_{i+2}, \cdots, x_{i+k}$ is

$$f[x_i, x_{i+1}, \cdots, x_{i+k}] = \frac{f[x_{i+1}, x_{i+2}, \cdots, x_{i+k}] - f[x_i, x_{i+1}, \cdots, x_{i+k-1}]}{x_{i+k} - x_i} \tag{4.17}$$

The process ends with the single nth divided difference

$$f[x_0, x_1, \cdots, x_n] = \frac{f[x_1, x_2, \cdots, x_n] - f[x_0, x_1, \cdots, x_{n-1}]}{x_n - x_0} \tag{4.18}$$

Because of Eq. (4.13) we can write $a_1 = f[x_0, x_1]$ just as a_0 can be expressed as $a_0 = f[x_0] = f(x_0)$. Hence the interpolating polynomial in Eq. (4.12) is

$$P_n(x) = f[x_0] + f[x_0, x_1](x-x_0) + a_2(x-x_0)(x-x_1) + \cdots + a_n(x-x_0)\cdots(x-x_{n-1})$$

As might be expected from the evaluation of a_0 and a_1, the required constants are

$$a_k = f[x_0, x_1, \cdots, x_k]$$

for each $k = 0, 1, ..., n$. So $P_n(x)$ can be rewritten in a form of Newton's Divided Difference

$$P_n(x) = f[x_0] + \sum_{k=1}^{n} f[x_0, x_1, \cdots, x_k](x - x_0)(x - x_1)\cdots(x - x_{k-1})$$

x	$f(x)$	1st Divided Difference	2nd Divided Difference	3rd Divided Difference
x_0	$f[x_0]$			
		$f[x_0,x_1]=\frac{f[x_1]-f[x_0]}{x_1-x_0}$		
x_1	$f[x_1]$		$f[x_0,x_1,x_2]=\frac{f[x_1,x_2]-f[x_0,x_1]}{x_2-x_0}$	
		$f[x_1,x_2]=\frac{f[x_2]-f[x_1]}{x_2-x_1}$		$f[x_0,x_1,x_2,x_3]=\frac{f[x_1,x_2,x_3]-f[x_0,x_1,x_2]}{x_3-x_0}$
x_2	$f[x_2]$		$f[x_1,x_2,x_3]=\frac{f[x_2,x_3]-f[x_1,x_2]}{x_3-x_1}$	
		$f[x_2,x_3]=\frac{f[x_3]-f[x_2]}{x_3-x_2}$		$f[x_1,x_2,x_3,x_4]=\frac{f[x_2,x_3,x_4]-f[x_1,x_2,x_3]}{x_4-x_1}$
x_3	$f[x_3]$		$f[x_2,x_3,x_4]=\frac{f[x_3,x_4]-f[x_2,x_3]}{x_4-x_2}$	
		$f[x_3,x_4]=\frac{f[x_4]-f[x_3]}{x_4-x_3}$		$f[x_2,x_3,x_4,x_5]=\frac{f[x_3,x_4,x_5]-f[x_2,x_3,x_4]}{x_5-x_2}$
x_4	$f[x_4]$		$f[x_3,x_4,x_5]=\frac{f[x_4,x_5]-f[x_3,x_4]}{x_5-x_3}$	
		$f[x_4,x_5]=\frac{f[x_5]-f[x_4]}{x_5-x_4}$		
x_5	$f[x_5]$			

Table 4.1: General Newton's Divided-Difference Table

The value of $f[x_0, x_1, \cdots, x_k]$ is independent of the order of the numbers x_0, x_1, $\cdots$, x_k, as shown later. The generation of the divided differences is outlined in Table 4.1.

Example 4.8. *Complete the divided difference table for the set of data pairs:*

x	1.0	1.3	1.6	1.9	2.2
$f(x)$	0.7651977	0.6200860	0.4554022	0.2818186	0.1103623

and find the interpolating value of $x = 1.5$*.*

Solution:

The first divided difference involving x_0 *and* x_1 *is*

$$\begin{aligned} f[x_0, x_1] &= \frac{f[x_1] - f[x_0]}{x_1 - x_0} \\ &= \frac{0.6200860 - 0.7651977}{1.3 - 1.0} \\ &= -0.4837057 \end{aligned}$$

The remaining first divided differences are found in a similar manner and are shown in the fourth column in Table 4.2. The second divided difference involving x_0, x_1 *and* x_2 *is*

$$\begin{aligned} f[x_0, x_1, x_2] &= \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_1} \\ &= \frac{0.5489460 - (-0.4837057)}{1.6 - 1.0} \\ &= -0.1087339 \end{aligned}$$

The remaining second divided differences are shown in the $5th$ *column of Table 4.2. The third divided difference involving* x_0, x_1, x_2 *and* x_3 *and the fourth divided difference involving all*

i	x_i	$f[x_i]$	$f[x_{i-1}, x_i]$	$f[x_{i-2}, x_{i-1}, x_i]$	$f[x_{i-3}, \cdots, x_i]$	$f[x_{i-4}, \cdots, x_i]$
0	1.0	0.7651977				
			-0.4837057			
1	1.3	0.6200860		-0.1087339		
			-0.5489460		0.0658784	
2	1.6	0.4554022		-0.0494433		0.0018251
			-0.5786120		0.0680685	
3	1.9	0.2818186		0.0118183		
			-0.5715210			
4	2.2	0.1103623				

Table 4.2: Newton's Divided-Difference Table of example 4.8

the data points are, respectively,

$$
\begin{aligned}
f[x_0, x_1, x_2, x_3] &= \frac{f[x_1, x_2, x_3] - f[x_0, x_1, x_2]}{x_3 - x_0} \\
&= \frac{-0.0494433 - (-0.1087339)}{1.9 - 1.0} \\
&= 0.0658784
\end{aligned}
$$

and

$$
\begin{aligned}
f[x_0, x_1, x_2, x_3, x_4] &= \frac{f[x_1, x_2, x_3, x_4] - f[x_0, x_1, x_2, x_3]}{x_4 - x_0} \\
&= \frac{0.0680685 - 0.0658784}{2.2 - 1.0} \\
&= 0.0018251
\end{aligned}
$$

All the entries are given in Table 4.2.
The coefficients of the Newton divided difference of the interpolating polynomial are along the diagonal in the table. This polynomial is

$$
\begin{aligned}
P_4(x) = 0.7651977 &- 0.4837057(x - 1.0) - 0.1087339(x - 1.0)(x - 1.3) \\
&+ 0.0658784(x - 1.0)(x - 1.3)(x - 1.6) \\
&+ 0.0018251(x - 1.0)(x - 1.3)(x - 1.6)(x - 1.9)
\end{aligned}
$$

we can now find the value of $P(1.5) = 0.5118200$.

4.6 EXERCISE

1. Solve example 4.8 using polynomial interpolation method and Lagrange interpolation method, then compare with the Newton's Divided Difference method. Estimate the value of $f(1.1)$ and $f(2.0)$.
2. Solve all Exercise 4.4 using Newton's Divided Difference method and compare with all previous methods.

4.7 Curve Fitting

Curve fitting is the process of finding equations to approximate straight lines and curves that best fit given sets of data. For example, for the data of Figure 4.7, we can use the equation of a straight line, that is:

$$y = mx + b$$

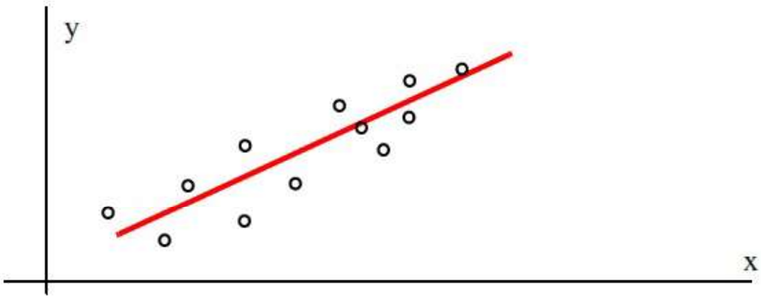

Figure 4.7: Straight line approximation

For Figure 4.8, we can use the equation for the quadratic or parabolic curve of the form

$$y = ax^2 + bx + c$$

In finding the best line, we normally assume that the data, shown by the small circles in Figures 4.7 and 4.8, represent the independent variable , and our task is to find the dependent variable. This process is called regression.
Regression can be linear (straight line) or curved (quadratic, cubic, etc.). Obviously, we can find more than one straight line or curve to fit a set of given data, but we interested in finding the most suitable.
Let the distance of data point x_1 from the line be denoted as d_1, the distance of data point x_2 from the same line as d_2, and so on. The best fitting straight line or curve has the

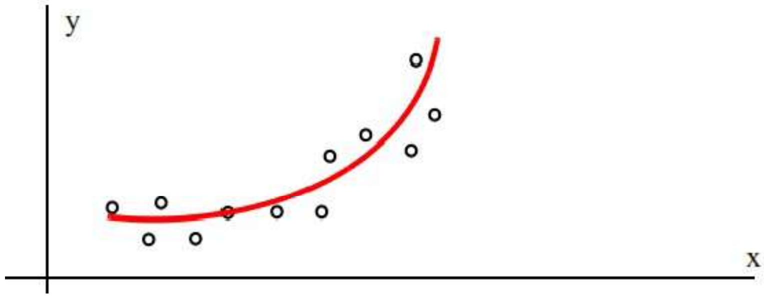

Figure 4.8: Parabolic line approximation

property that

$$d_1^2 + d_2^2 + \cdots + d_n^2 = minimum \tag{4.19}$$

and it is referred to as the least squares curve. Thus, a straight line that satisfies equation (4.19) is called a least squares line. If it is a parabola, we call it a least squares parabola.

4.8 Linear Regression

With this method, we compute the coefficients m (slope) and b (y-intercept) of the straight line equation

$$y = mx + b \tag{4.20}$$

such that the sum of the squares of the errors will be minimum. We derive the values of m and b, that will make the equation of the straight line to best fit the observed data, as follows:
Let x and y be two related variables, and assume that corresponding to the values $x_1, x_2, \cdots, x_n$, we have observed the values $y_1, y_2, \cdots, y_n$. Now, let us suppose that we have plotted the values of y versus the corresponding values of x, and we have observed that the points (x_1, y_1), (x_2, y_2), (x_3, y_3), $\cdots$,

(x_n, y_n) approximate a straight line. We denote the straight line equations passing through these points as

$$\begin{aligned} y_1 &= mx_1 + b \\ y_2 &= mx_2 + b \\ y_3 &= mx_3 + b \\ &\cdots \cdots \\ y_n &= mx_n + b \end{aligned} \tag{4.21}$$

In equations (4.21), the slope m and y-intercept b are the same in all equations since we have assumed that all points lie close to one straight line. However, we need to determine the values of the unknowns m and b from all n equations.
The error (difference) between the observed value y_1, and the value that lies on the straight line, is $y_1 - (mx_1 + b)$. This difference could be positive or negative, depending on the position of the observed value, and the value at the point on the straight line. Likewise, the error between the observed value y_2 and the value that lies on the straight line is $y_2-(mx_2+b)$ and so on. The straight line that we choose must be a straight line such that the distances between the observed values, and the corresponding values on the straight line, will be minimum. This will be achieved if we use the magnitudes (absolute values) of the distances; if we were to combine positive and negative values, some may cancel each other and give us a wrong sum of the distances. Accordingly, we find the sum of the squared distances between observed points and the points on the straight line. For this reason, this method is referred to as the method of least squares.

Let the sum of the squares of the errors be

$$\sum squares = [y_1 - (mx_1 + b)]^2 + [y_2 - (mx_2 + b)]^2 + \cdots + [y_n - (mx_n + b)]^2 \quad (4.22)$$

Since $(\sum squares)$ is a function of two variables m and b, to minimize (4.22) we must equate to zero its two partial derivatives with respect to m and b. Then

$$\frac{\partial}{\partial m}\sum squares = -2x_1[y_1 - (mx_1 + b)] - 2x_2[y_2 - (mx_2 + b)] - \cdots - 2x_n[y_n - (mx_n + b)] = 0 \quad (4.23)$$

and

$$\frac{\partial}{\partial b}\sum squares = -2[y_1 - (mx_1 + b)] - 2[y_2 - (mx_2 + b)] - \cdots - 2[y_n - (mx_n + b)] = 0 \quad (4.24)$$

The second derivatives of (4.23) and (4.24) are positive and thus $(\sum squares)$ will have its minimum value.
Collecting like terms, and simplifying (4.23) and (4.24) to obtain

$$\begin{aligned}(\sum_{i=1}^{i=n} x_i^2)m + (\sum_{i=1}^{i=n} x_i)b &= \sum_{i=1}^{i=n} x_i y_i \\ (\sum_{i=1}^{i=n} x_i)m + nb &= \sum_{i=1}^{i=n} y_i\end{aligned} \quad (4.25)$$

or by matrix notation

$$\begin{bmatrix}\sum_{i=1}^{i=n} x_i^2 & \sum_{i=1}^{i=n} x_i \\ \sum_{i=1}^{i=n} x_i & n\end{bmatrix}\begin{bmatrix}m \\ b\end{bmatrix} = \begin{bmatrix}\sum_{i=1}^{i=n} x_i y_i \\ \sum_{i=1}^{i=n} y_i\end{bmatrix} \quad (4.26)$$

We can solve the equations of (4.26) simultaneously by any method from previous chapter, like Cramer's rule, m and n

are computed as: (for simplicity we right $\sum$ as $\sum_{i=1}^{i=n}$, x as x_i and y as y_i)

$$m = \frac{D_1}{\Delta}$$
$$b = \frac{D_2}{\Delta} \tag{4.27}$$

where

$$\Delta = det \begin{bmatrix} \sum x^2 & \sum x \\ \sum x & n \end{bmatrix} \tag{4.28}$$

$$D_1 = det \begin{bmatrix} \sum xy & \sum x \\ \sum y & n \end{bmatrix} \tag{4.29}$$

$$D_2 = det \begin{bmatrix} \sum x^2 & \sum xy \\ \sum x & \sum y \end{bmatrix} \tag{4.30}$$

Example 4.9. *Compute the straight line equation that best fits the following data*

x	0	10	20	30	40	50	60	70	80	90	100
y	*27.6*	*31.0*	*34.0*	*37*	*40*	*42.6*	*45.5*	*48.3*	*51.1*	*54*	*56.7*

Solution:

There are 11 *sets of data and thus* $n = 11$*. We need to compute the values of* $\sum x$, $\sum x^2$, $\sum y$ *and* $\sum xy$:

x	y	x^2	xy
0	27.6		
10	31		
20	34		
30	37		
40	40		
50	42.6		
60	45.5		
70	48.3		
80	51.1		
90	54		
100	56.7		
$\sum x = 550$	$\sum y = 467.8$	$\sum x^2 = 38500$	$\sum xy = 26559$

Now we can compute the values of equations (4.28), (4.29) and (4.30):

$$\Delta = det \begin{bmatrix} \sum x^2 & \sum x \\ \sum x & n \end{bmatrix} = det \begin{bmatrix} 38500 & 550 \\ 550 & 11 \end{bmatrix} = 121000$$

$$D_1 = det \begin{bmatrix} \sum xy & \sum x \\ \sum y & n \end{bmatrix} = det \begin{bmatrix} 26559 & 550 \\ 467.8 & 11 \end{bmatrix} = 34859$$

$$D_2 = det \begin{bmatrix} \sum x^2 & \sum xy \\ \sum x & \sum y \end{bmatrix} = det \begin{bmatrix} 38500 & 26559 \\ 550 & 467.8 \end{bmatrix} = 3402850$$

this lead to

$$m = \frac{D_1}{\Delta} = 0.288$$
$$b = \frac{D_2}{\Delta} = 28.123$$

then the linear approximation of the data is:

$$y = mx + b = 0.288x + 28.123$$

see figure 4.9.

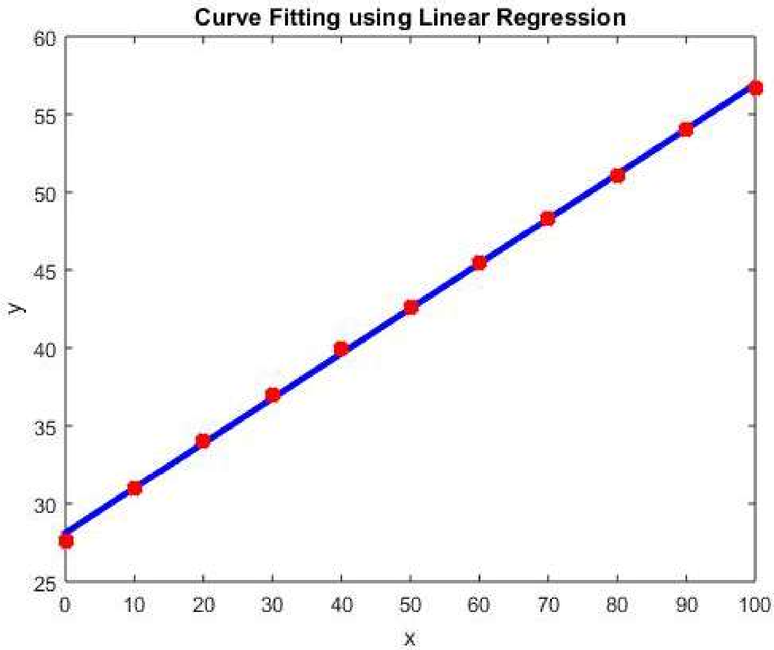

Figure 4.9: Plot of the straight line for Example 4.9

Example 4.10. *Compute the straight line equation that best fits the following data*

x	770	677	428	410	371	504	1136	695	551	550
y	54	47	28	38	29	38	80	52	45	40
x	568	504	560	512	448	538	410	409	504	777
y	49	33	50	40	31	40	27	31	35	57
x	496	386	530	360	355	1250	802	741	739	650
y	31	26	39	25	23	102	72	57	54	56
x	592	577	500	469	320	441	845	435	435	375
y	45	42	36	30	22	31	52	29	34	20
x	364	340	375	450	529	412	722	574	498	493
y	33	18	23	30	38	31	62	48	29	40
x	379	579	458	454	952	784	476	453	440	428
y	30	42	36	33	72	57	34	46	30	21

Solution:

There are 60 *sets of data and thus* $n = 60$*. by the same procedure in example 4.9 we find:*

$$\Delta = det\begin{bmatrix} \sum x^2 & \sum x \\ \sum x & n \end{bmatrix} = det\begin{bmatrix} 19954638 & 32780 \\ 32780 & 60 \end{bmatrix}$$

$$D_1 = det\begin{bmatrix} \sum xy & \sum x \\ \sum y & n \end{bmatrix} = det\begin{bmatrix} 1487462 & 32780 \\ 2423 & 60 \end{bmatrix}$$

$$D_2 = det\begin{bmatrix} \sum x^2 & \sum xy \\ \sum x & \sum y \end{bmatrix} = det\begin{bmatrix} 19954638 & 1487462 \\ 32780 & 2423 \end{bmatrix}$$

this lead to

$$m = \frac{D_1}{\Delta} = 0.08$$
$$b = \frac{D_2}{\Delta} = -3.3313$$

then the linear approximation of the data is:

$$y = mx + b = 0.08x - 3.3313$$

see figure 4.10.

the Matlab code for Linear regression is:

Matlab Code 4.11. *Linear regression curve fitting*

```
% ***********************************************
% ****              Linear  Fitting              ****
% ***********************************************
```

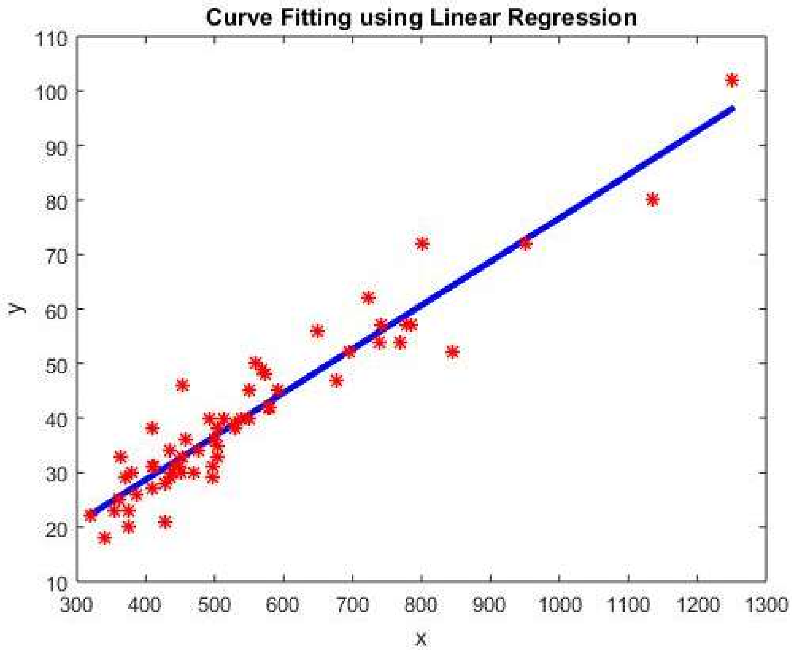

Figure 4.10: Plot of the straight line for Example 4.10

```
clc
clear
close all
% inter the dasta points
x
  =[770,677,428,410,371,504,1136,695,551,550,568,504,560,5

y
  =[54,47,28,38,29,38,80,52,45,40,49,33,50,40,31,40,27,31,3


% x=[0,10,20,30,40,50,60,70,80,90,100];
% y
  =[27.6,31.0,34.0,37,40,42.6,45.5,48.3,51.1,54,56.7];

```

```
% x =  1:5;
% y = [1  2  1.3  3.75  2.25];

% the number of data is n
n = length(x);
% we need to comput the quantities
sumxi = sum(x);
sumyi = sum(y);
sumxiyi = sum(x.*y);
sumxi2 = sum(x.^2);
% comput m and b
m=(sumxi*sumyi-n*sumxiyi)/(sumxi^2-n*sumxi2)
b=(sumxiyi*sumxi-sumyi*sumxi2)/(sumxi^2-n*sumxi2)
%          y=mx+b
xmin=min(x); xmax=max(x);
dx=(xmax-xmin)/100;
w=xmin:dx:xmax;
fw=m*w+b;
plot(w,fw, '-b', 'linewidth',3)          % the interpolation polynomial
hold on
plot(x,y, '*r', 'linewidth',1)
xlabel('x');
ylabel('y');
title('Curve Fitting using Linear Regression')
```

4.9 Parabolic Regression

The least squares parabola that fits a set of sample points with

$$y = ax^2 + bx + c \tag{4.31}$$

where the coefficients a, b and c are found from

$$\begin{aligned}(\sum x^2)a + (\sum x)b + nc &= \sum y \\ (\sum x^3)a + (\sum x^2)b + (\sum x)c &= \sum xy \\ (\sum x^4)a + (\sum x^3)b + (\sum x^2)c &= \sum x^2 y\end{aligned} \tag{4.32}$$

where n is number of data points.

Example 4.12. *Compute the straight line equation that best fits the following data*

x	*1.2*	*1.5*	*1.8*	*2.6*	*3.1*	*4.3*	*4.9*	*5.3*
y	*4.5*	*5.1*	*5.8*	*6.7*	*7.0*	*7.3*	*7.6*	*7.4*
x	*5.7*	*6.4*	*7.1*	*7.6*	*8.6*	*9.2*	*9.8*	
y	*7.2*	*6.9*	*6.6*	*5.1*	*4.5*	*3.4*	*2.7*	

Solution:

We compute the coefficient of equations (4.32) *from the data of the table and get:*

$$\begin{aligned} n &= 15 \\ \sum x &= 79.1 \\ \sum x^2 &= 530.15 \\ \sum x^3 &= 4004.50 \\ \sum x^4 &= 32331.49 \\ \sum y &= 87.8 \\ \sum xy &= 437.72 \\ \sum x^2 y &= 2698.37 \end{aligned}$$

By substitution into equations (4.32) to get

$$(\sum x^2)a + (\sum x)b + nc = \sum y$$
$$530.15a + 79.1b + 15c = 87.8$$
$$(\sum x^3)a + (\sum x^2)b + (\sum x)c = \sum xy$$
$$4004.50a + 530.15b + 79.1c = 437.72$$
$$(\sum x^4)a + (\sum x^3)b + (\sum x^2)c = \sum x^2y$$
$$32331.49a + 4004.50b + 530.15c = 2698.37$$

Solve these equations with any method from previous chapter to get $a = -0.2$, $b = 1.94$, *and* $c = 2.78$. *Therefore, the least squares parabola is*

$$y = -0.2x^2 + 1.9x + 2.78$$

The plot for this parabola is shown in Figure 4.11.

the Matlab code for parabola regression is:

Matlab Code 4.13. *parabola regression curve fitting*

```
%
    ***********************************************
% ****   least squares parabola Fitting
    ****
%
    ***********************************************
clc
clear
close all
% inter the dasta points
x
    =[1.2,1.5,1.8,2.6,3.1,4.3,4.9,5.3,5.7,6.4,7.1,7.6,8.6,9.
```

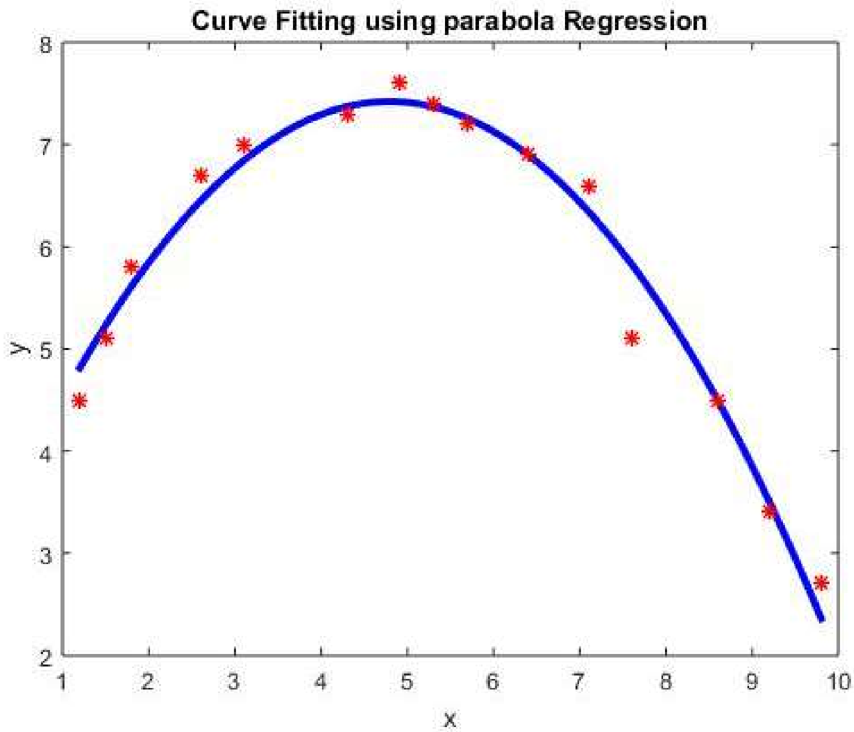

Figure 4.11: Plot of the least squares parabola for Example 4.12

```
y
  =[4.5,5.1,5.8,6.7,7.0,7.3,7.6,7.4,7.2,6.9,6.6,5.1,4.5,3.


% x
  =[770,677,428,410,371,504,1136,695,551,550,568,504,560,5

% y
  =[54,47,28,38,29,38,80,52,45,40,49,33,50,40,31,40,27,31,3

% x=[0,10,20,30,40,50,60,70,80,90,100];
% y
```

```
    =[27.6,31.0,34.0,37,40,42.6,45.5,48.3,51.1,54,56.7];

% x =  1:5;
% y = [1  2  1.3  3.75  2.25];

% the number of data is n
n = length(x);
% we need to comput the quantities
sumxi = sum(x);
sumyi = sum(y);
sumxi2 = sum(x.^2);
sumxi3 = sum(x.^3);
sumxi4 = sum(x.^4);
sumxiyi = sum(x.*y);
sumxi2yi = sum(x.*x.*y)
% comput a0,a1,a2 from the linear system      AX=
    B
A=[sumxi2,sumxi,n
        sumxi3,sumxi2,sumxi
        sumxi4,sumxi3,sumxi2];
B=[sumyi,sumxiyi,sumxi2yi]';
% S=[a0,a1,a2]
S=inv(A)*B;
xmin=min(x);  xmax=max(x);
dx=(xmax-xmin)/100;
w=xmin:dx:xmax;
fw=S(1)*w.^2+S(2)*w+S(3);
plot(w,fw,'-b','linewidth',3)           % the
    interpolation polynomial
hold on
plot(x,y,'*r','linewidth',1)
xlabel('x');
```

```
ylabel('y');
title('Curve Fitting using parabola Regression')
```

Chapter 5

Numerical Differentiation and Integration

5.1 Numerical Differentiation: Finite Differences

The first questions that comes up to mind is: why do we need to approximate derivatives at all? After all, we do know how to analytically differentiate every function. Nevertheless, there are several reasons as of why we still need to approximate derivatives:

- Even if there exists an underlying function that we need to differentiate, we might know its values only at a sampled data set without knowing the function itself.

- There are some cases where it may not be obvious that an underlying function exists and all that we have is a discrete data set. We may still be interested in studying changes in the data, which are related, of course, to derivatives.

- There are times in which exact formulas are available but they are very complicated to the point that an exact computation of the derivative requires a lot of function evaluations. It might be significantly simpler to approximate the derivative instead of computing its exact value.

- When approximating solutions to ordinary (or partial) differential equations, we typically represent the solution as a discrete approximation that is defined on a grid. Since we then have to evaluate derivatives at the grid points, we need to be able to come up with methods for approximating the derivatives at these points, and again, this will typically be done using only values that are defined on a lattice. The underlying function itself (which in this cased is the solution of the equation) is unknown.

Suppose that a variable $f(x)$ depends on another variable x but we only know the values of f at a finite set of points, e.g., as data from an experiment or a simulation:

$$(x_1, f(x_1)), (x_2, f(x_2)), \cdots, (x_n, f(x_n))$$

with equal mesh spacing $h = x_{i+1} - x_i$ for $i = 1, 2, \cdots, n-1$, we have the Taylor series Suppose then that we need information about the derivative of $f(x)$. We begin by writing the Taylor expansion of $f(x+h)$ and $f(x-h)$ about x:

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(x) + \cdots \quad (5.1)$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(x) + \cdots \quad (5.2)$$

$$f(x+2h) = f(x) + 2hf'(x) + 4\frac{h^2}{2}f''(x) + 8\frac{h^3}{6}f'''(x) + 16\frac{h^4}{24}f^{(4)}(x) + \cdots \quad (5.3)$$

$$f(x-2h) = f(x) - 2hf'(x) + 4\frac{h^2}{2}f''(x) - 8\frac{h^3}{6}f'''(x) + 16\frac{h^4}{24}f^{(4)}(x) - \cdots \quad (5.4)$$

and so on.

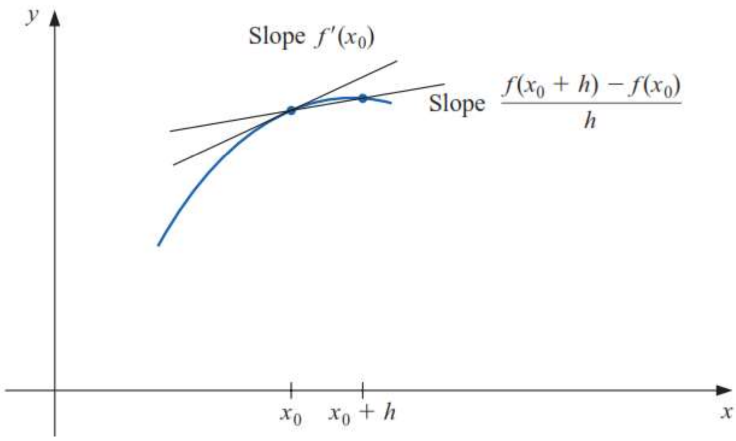

Figure 5.1: digram of the forward-difference approximation of the function $f(x)$

5.1.1 Finite Difference Formulas for $f'(x)$:

To derive a formula for $f'(x)$ there are many formulas, as example: from equation (5.1):

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2} f''(\xi_+) \tag{5.5}$$

Note that we have replaced terms in h^2 by corresponding remainder terms. Dividing by h, we obtain the formula

$$f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{h}{2} f''(\xi_+); \qquad \xi_+ \in [x, x+h]$$

or

$$f'(x) = \frac{f(x+h) - f(x)}{h} \tag{5.6}$$

This formula have error of $O(h)$ and called a **forward-difference approximation** to the derivative because it looks forward along the $x-$axis to get an approximation to $f'(x)$, see figure 5.1.

By the same procedure we can get from (5.2):

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2} f''(\xi_-) \tag{5.7}$$

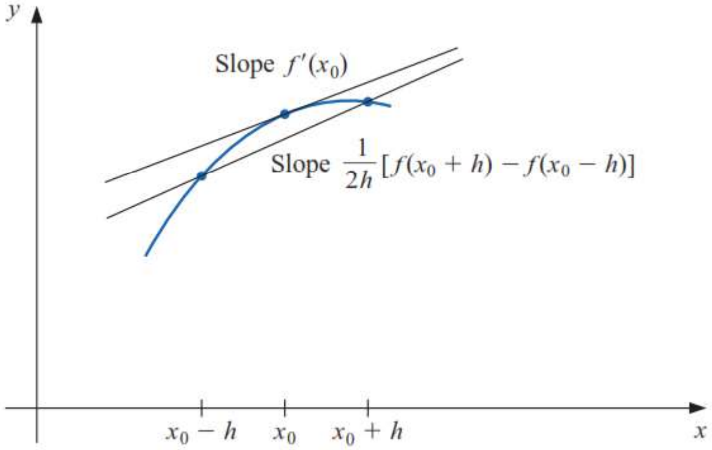

Figure 5.2: digram of the central-difference approximation of the function $f(x)$

and

$$f'(x) = \frac{f(x) - f(x-h)}{h} \tag{5.8}$$

This formula have error of $O(h)$ and called a **backward-difference** approximation $f'(x)$.
Subtract (5.7) from (5.5) to get:

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

Note that the error term consists of two evaluations of f''', one at $\xi_+ \in [x, x+h]$ from truncating the series for $f(x+h)$ and the other at $\xi_- \in [x-h, x]$ from truncating the series for $f(x-h)$. If f''' is continuous, the average of these two values can be written as $f'''(\xi)$, where $\xi \in [x-h, x+h]$. Hence we have the **central-difference** formula, see figure 5.2:

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6}f'''(\xi); \qquad \xi_+ \in [x-h, x+h] \tag{5.9}$$

or

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} \tag{5.10}$$

The error in the central-difference formula is of $O(h^2)$, it is ultimately more accurate than a forward difference scheme. By the same procedure we can get (**Homework**):

$$f'(x) = \frac{-3f(x) + 4f(x+h) - f(x+2h)}{2h} + O(h^2) \tag{5.11}$$

this is forward difference approximation, and

$$f'(x) = \frac{3f(x) - 4f(x-h) + f(x-2h)}{2h} + O(h^2) \tag{5.12}$$

this is backward difference approximation, and

$$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} + O(h^4) \tag{5.13}$$

this a central finite difference formula. There are many other formulas for the finite difference approximation and every formula has it is properties.

Example 5.1. *Consider the values given in the following Table and use all the applicable formulas to approximate $f'(2.0)$:*

x	*1.6*	*1.7*	*1.8*	*1.9*	
$f(x)$	*7.924851879*	*9.305710566*	*10.88936544*	*12.70319944*	*14.77*
x	*2.1*	*2.2*	*2.3*	*2.4*	
$f(x)$	*17.14895682*	*19.8550297*	*22.94061965*	*26.45562331*	

in fact these values from $f(x) = xe^x$. Compare the approximate values with the value of $f'(x) = xe^x + e^x$ and $f'(2) = 22.1672$, see the tangent line m in figure 5.3.

Solution:

$$x = 2.0, \qquad h = 0.1$$

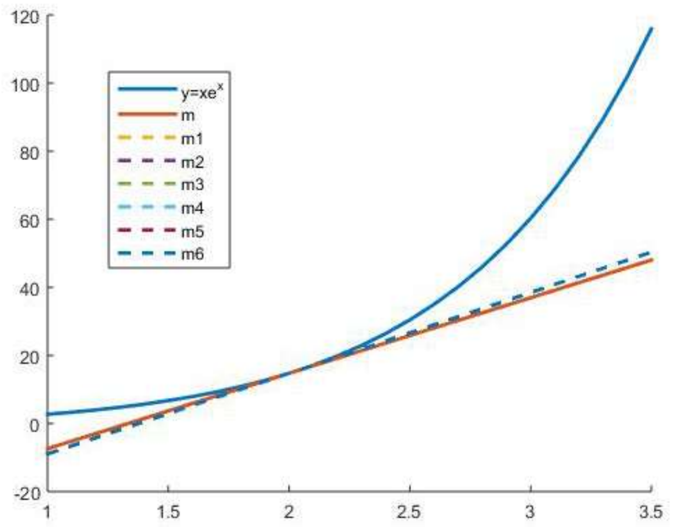

Figure 5.3: digram of the solution of example 5.1, m is the tangent line and the others are the approximated tangent lines

then from formula (5.6)*:*

$$f'(x) = \frac{f(x+h) - f(x)}{h}$$
$$f'(2) = \frac{f(2.1) - f(2)}{0.1}$$
$$= \frac{17.14895682 - 14.7781122}{0.1}$$
$$= 23.70844619$$

the absolute error is $|22.1672 - 23.70844619| = 1.54124619$*.*
the relative error is $|\frac{22.1672 - 23.70844619}{23.70844619}| = 0.065008317$*.*
see the tangent line $m1$ *in figure 5.3.*

from formula (5.8)*:*

$$\begin{aligned} f'(2) &= \frac{f(x)-f(x-h)}{h} \\ &= \frac{f(2)-f(1.9)}{0.1} \\ &= \frac{14.7781122-12.70319944}{0.1} \\ &= 20.74912758 \end{aligned}$$

the absolute error is $|22.1672-20.74912758| = 1.41807242$*.*
the relative error is $|\frac{22.1672-20.74912758}{23.70844619}| = 0.068343713$*.*
see the tangent line $m2$ *in figure 5.3.*

from formula (5.10)*:*

$$\begin{aligned} f'(2) &= \frac{f(x+h)-f(x-h)}{2h} \\ &= \frac{f(2.1)-f(1.9)}{0.2} \\ &= \frac{17.14895682-12.70319944}{0.2} \\ &= 22.22878688 \end{aligned}$$

the absolute error is $|22.1672-22.22878688| = 0.06158688$*.*
the relative error is $|\frac{22.1672-22.22878688}{22.22878688}| = 0.002770591$*.*
see the tangent line $m3$ *in figure 5.3.*

from formula (5.11)*:*

$$\begin{aligned} f'(2) &= \frac{-3f(x)+4f(x+h)-f(x+2h)}{2h} \\ &= \frac{-3f(2)+4f(2.1)-f(2.2)}{0.2} \\ &= \frac{-3(14.7781122)+4(17.14895682)-(19.8550297)}{0.2} \\ &= 22.03230487 \end{aligned}$$

the absolute error is $|22.1672 - 22.03230487| = 0.13489513$.
the relative error is $|\frac{22.1672-22.03230487}{22.03230487}| = 0.006122606$.
see the tangent line $m4$ *in figure 5.3.*

from formula (5.12)*:*

$$\begin{aligned} f'(2) &= \frac{3f(x) - 4f(x-h) + f(x-2h)}{2h} \\ &= \frac{3f(2) - 4f(1.9) + f(1.8)}{0.2} \\ &= \frac{3(14.7781122) - 4(12.70319944) + (10.88936544)}{0.2} \\ &= 22.05452134 \end{aligned}$$

the absolute error is $|22.1672 - 22.05452134| = 0.11267866$.
the relative error is $|\frac{22.1672-22.05452134}{22.05452134}| = 0.005109096$.
see the tangent line $m5$ *in figure 5.3.*

from formula (5.13)*:*

$$\begin{aligned} f'(2) &= \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} \\ &= \frac{-f(2.2) + 8f(2.1) - 8f(1.9) + f(1.8)}{1.2} \\ &= \frac{-3(14.7781122) + 4(17.14895682) - (19.8550297)}{0.2} \\ &= 22.16699562 \end{aligned}$$

the absolute error is $|22.1672 - 22.16699562| = 0.00020438$.
the relative error is $|\frac{22.1672-22.16699562}{22.16699562}| = 9.22001 \times 10^{-6}$.
see the tangent line $m6$ *in figure 5.3.*

5.1.2 Finite Difference Formulas for $f''(x)$:

To get a formula for the second derivative, we choose the coefficients to pick off the first two terms of the Taylor expansion (5.1) and (5.2):

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(\xi_+)$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2}f''(x) - \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(\xi_-)$$

then

$$f(x+h) - 2f(x) + f(x-h) = h^2 f''(x) + \frac{h^4}{6}\frac{f^{(4)}(\xi_+) + f^{(4)}(\xi_-)}{2}$$

where $\xi_+ \in [x, x+h]$ and $\xi_- \in [x-h, x]$. It follows that

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} - \frac{h^2}{6}f^{(4)}(\xi) \qquad \xi_+ \in [x-h, x+h]$$

or

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

This is the **central difference formula** for $f''(x)$.
We can notice that the technique is quite flexible and can be used to derive formulas for special cases. By the same procedure we can find (**Homework**):
forward difference approximations:

$$f''(x) = \frac{2f(x) - 5f(x+h) + 4f(x+2h) - f(x+3h)}{h^3} + O(h^2)$$

The **backward difference approximations**:

$$f''(x) = \frac{2f(x) - 5f(x-h) + 4f(x-2h) - f(x-3h)}{h^3} + O(h^2)$$

and **centered difference approximations**:

$$f''(x) = \frac{-f(x+2h) + 16f(x+h) - 30f(x) + 16f(x-h) - f(x-2h)}{12h^2} + O(h^4)$$

Example 5.2. *Consider the same values given in Example 5.1 and use all the applicable formulas to approximate* $f''(2.0)$.

The solution is Homework

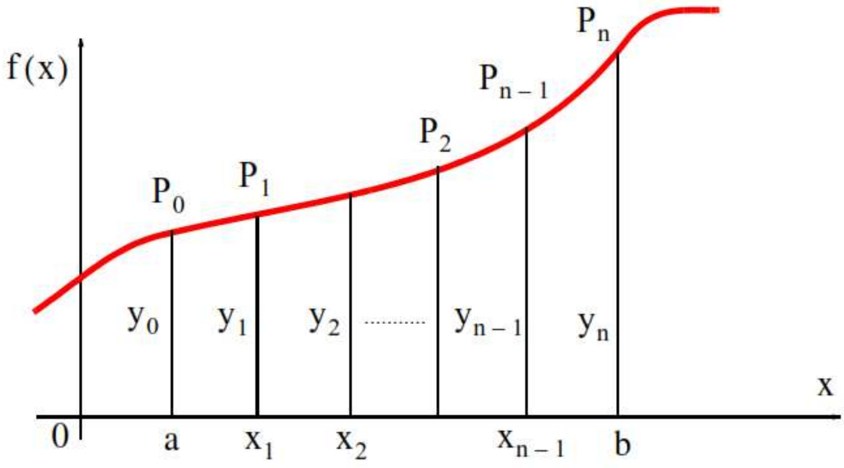

Figure 5.4: Integration by the trapezoidal rule

5.2 Numerical Integration

The need often arises for evaluating the definite integral of a function that has no explicit antiderivative or whose antiderivative is not easy to obtain. The basic method involved in approximating $\int_a^b f(x)dx$. It uses a sum $\sum_{i=0}^{n} a_i f(x_i)$ to approximate $\int_a^b f(x)dx$.

5.2.1 The Trapezoidal Rule

Consider the function $y = f(x)$ for the interval $a \leq x \leq b$, shown in Figure 5.4. To evaluate the definite integral $\int_a^b f(x)dx$, we divide the interval $a \leq x \leq b$ into n subintervals each of length $\Delta x = \frac{b-a}{n}$. Then, the number of points between $x_0 = a$ and $x_n = b$ is $x_1 = a + \Delta x$, $x_2 = a + 2\Delta x$, $\cdots$, $x_{n-1} = a + (n-1)\Delta x$. Therefore, the integral from a to b is the sum of the integrals from a to x_1, from x_1 to x_2, and so on, and finally from x_{n-1} to b. The total area is

$$\int_a^b f(x)dx = \int_a^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \cdots + \int_{x_{n-1}}^{b} f(x)dx$$
$$= \sum_{k=1}^{n} \int_{x_{k-1}}^{k} f(x)dx$$

The integral over the first subinterval, can now be approximated by the area of the trapezoid $a\ P_0\ P_1\ x_1$ that is equal to $\frac{1}{2}(y_0 + y_1)\Delta x$ plus the area of the trapezoid $x_1\ P_1\ P_2\ x_2$ that is equal to $\frac{1}{2}(y_1 + y_2)\Delta x$, and so on. Then, the trapezoidal approximation becomes

$$T = \frac{1}{2}(y_0 + y_1)\Delta x + \frac{1}{2}(y_1 + y_2)\Delta x + \cdots + \frac{1}{2}(y_{n-1} + y_n)\Delta x$$

Or

$$T = \left(\frac{1}{2}y_0 + y_1 + y_2 + \cdots + y_{n-1} + \frac{1}{2}y_n\right)\Delta x \tag{5.14}$$

Example 5.3. *Using the trapezoidal rule with $n = 4$, estimate the value of the definite integral*

$$\int_1^2 x^2 dx$$

Compare with the exact value, and compute the Absolute Error and Relative Error.

Solution:

The exact value of this integral is

$$\int_1^2 x^2 dx = \left[\frac{x^3}{3}\right]_1^2 = \frac{7}{3} = 2.3333333 \tag{5.15}$$

For the trapezoidal rule approximation we have

$$x_0 = a = 1; \quad x_n = b = 2; \quad n = 4$$
$$\Delta x = \frac{b-a}{n} = \frac{2-1}{4} = 0.25$$
$$y = f(x) = x^2$$

Then,

$$x_0 = a = 1; \qquad y_0 = f(x_0) = 1^2 = 1$$
$$x_1 = a + \Delta x = \frac{5}{4}; \quad y_1 = f(x_1) = \left(\frac{5}{4}\right)^2 = \frac{25}{16}$$
$$x_2 = a + 2\Delta x = \frac{6}{4}; \quad y_2 = f(x_2) = \left(\frac{6}{4}\right)^2 = \frac{36}{16}$$
$$x_3 = a + 3\Delta x = \frac{7}{4}; \quad y_3 = f(x_3) = \left(\frac{7}{4}\right)^2 = \frac{49}{16}$$
$$x_4 = b = 2; \qquad y_4 = f(x_4) = \left(\frac{8}{4}\right)^2 = \frac{64}{16}$$

and by substitution into equation (5.14)

$$\begin{aligned} T &= \left(\frac{1}{2}y_0 + y_1 + y_2 + y_3 + \frac{1}{2}y_4\right)\Delta x \\ &= \left(\frac{1}{2}\times 1 + \frac{25}{16} + \frac{36}{16} + \frac{49}{16} + \frac{1}{2}\times\frac{64}{16}\right)\times\frac{1}{4} \\ &= \frac{75}{32} = 2.34375 \end{aligned} \tag{5.16}$$

From (5.14) *and* (5.16), *we find that the absolute and relative error are: Absolute Error*$= |2.34375 - 2.33333| \simeq 0.01042$.
Relative Error$= |\frac{2.34375-2.33333}{2.33333}| \simeq 0.0045$.

Example 5.4. *Using the trapezoidal rule with* $n = 5$, *and* $n = 10$ *to estimate the value of the definite integral*

$$\int_1^2 \frac{1}{x}\, dx$$

Compare with the exact value, and compute the Absolute Error and Relative Error.

Solution:

Homework *(The analytical value of this definite integral is* $\ln 2 = 0.6931$*).*

For **Trapezoidal Rule** we can use the following Matlab code:

Matlab Code 5.5. *Trapezoidal Rule*

```
% ***********   Trapzodal Rule *************
%  estimates the value of the integral of y=f(x)
%     from a to b by using trapezoidal rule
clc
clear
close all
a=1; % the start of integral interval
b=2;  % the end of integral interval
n=4; % the number of subintervals
h = (b-a)/n;
Area=0;
x = a:h:b; % to comput the x_i values
% this Example of f(x)=x^2
y=x.^2;     % to comput the y_i values
for  i = 2:n,
Area = Area + 2*y(i);
end
Area = Area + y(1) + y(n+1);
Area = Area*h/2
```

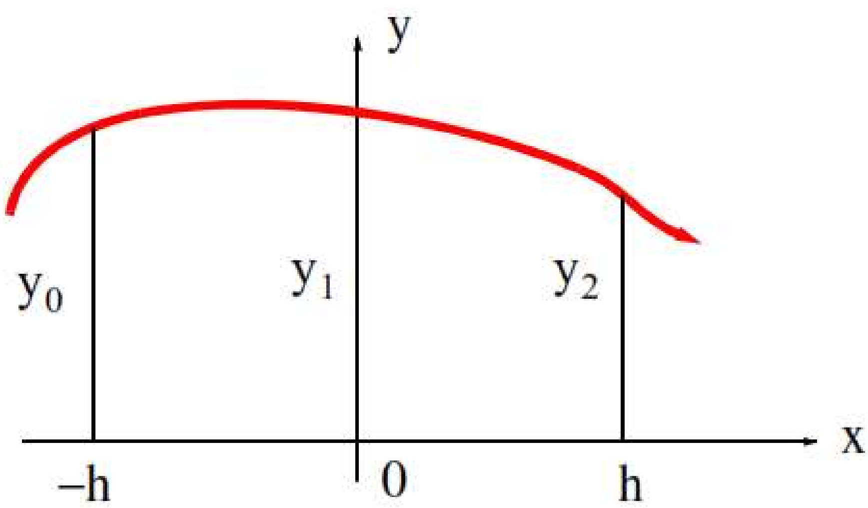

Figure 5.5: Simpson's rule of integration

5.2.2 Simpson's Rule

For numerical integration, let the curve of Figure 5.5 be represented by the parabola

$$y = \alpha x^2 + \beta x + \gamma \tag{5.17}$$

The area under this curve for the interval $-h \le x \le h$ is

$$\begin{aligned} Area|_{-h}^{h} &= \int_{-h}^{h} (\alpha x^2 + \beta x + \gamma)\, dx \\ &= \left(\frac{\alpha x^3}{3} + \frac{\beta x^2}{2} + \gamma x\right)|_{-h}^{h} \\ &= \left(\frac{\alpha h^3}{3} + \frac{\beta h^2}{2} + \gamma h\right) - \left(-\frac{\alpha h^3}{3} + \frac{\beta h^2}{2} - \gamma h\right) \\ &= \frac{2\alpha h^3}{3} + 2\gamma h \qquad (5.18) \\ &= \frac{1}{3} h \left(2\alpha h^2 + 6\gamma\right) \end{aligned}$$

The curve passes through the three points $(-h, y_0)$, $(0, y_1)$, and (h, y_2). Then, by equation (5.17) we have:

$$y_0 = \alpha h^2 - \beta h + \gamma \tag{5.19}$$

$$y_1 = \gamma \tag{5.20}$$

$$y_2 = \alpha h^2 + \beta h + \gamma \tag{5.21}$$

We can now evaluate the coefficients α, β and γ express (5.18) in terms of y_0, y_1 and y_2. This is done with the following procedure.
By substitution of (5.20) into (5.19) and (5.21) and rearranging we obtain

$$\alpha h^2 - \beta h = y_0 - y_1 \tag{5.22}$$

$$\alpha h^2 + \beta h = y_2 - y_1 \tag{5.23}$$

Addition of (5.22) with (5.23) yields

$$2\alpha h^2 = y_0 - 2y_1 + y_2 \tag{5.24}$$

and by substitution into (5.18) we obtain

$$\begin{aligned} Area|_{-h}^{h} &= \frac{1}{3}h\left(2\alpha h^2 + 6\gamma\right) \\ &= \frac{1}{3}h\left[(y_0 - 2y_1 + y_2) + 6y_1\right] \end{aligned} \tag{5.25}$$

or

$$Area|_{-h}^{h} = \frac{1}{3}h\left(y_0 + 4y_1 + y_2\right) \tag{5.26}$$

Now, we can apply (5.26) to successive segments of any curve y=f(x) in the interval $a \leq x \leq b$ as shown on the curve of Figure 5.6. From Figure 5.6, we observe that each segment of width $2h$ of the curve can be approximated by a parabola through its ends and its midpoint. Thus, the area under segment AB is

$$Area|_{AB} = \frac{1}{3}h\left(y_0 + 4y_1 + y_2\right) \tag{5.27}$$

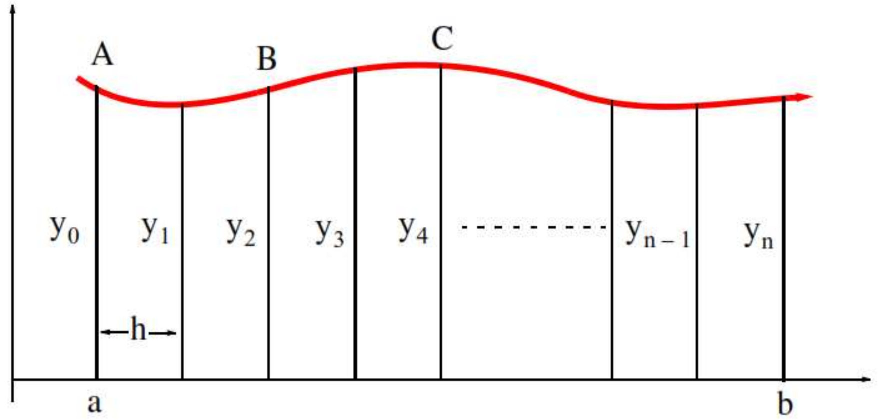

Figure 5.6: Simpson's rule of integration by successive segments

Likewise, the area under segment BC is

$$Area|_{BC} = \frac{1}{3}h\,(y_2 + 4y_3 + y_4) \tag{5.28}$$

and so on. When the areas under each segment are added, we obtain

$$Area = \frac{h}{3}\left[y_0 + 4y_1 + 2y_2 + 4y_3 + 2y_4 + \cdots + 2y_{n-2} + 4y_{n-1} + y_n\right] \tag{5.29}$$

This is the **Simpson's Rule of Numerical Integration**. Since each segment has width $2h$, to apply Simpson's rule of numerical integration, the number of subdivisions **must be even**. This restriction does not apply to the trapezoidal rule of numerical integration. The value of h for (5.29) is found from

$$h = \frac{b-a}{n}; \qquad n = even \tag{5.30}$$

Example 5.6. *Using Simpson's rule with* 4 *subdivisions* $(n = 4)$*, compute the approximate value of*

$$\int_1^2 \frac{1}{x}dx \tag{5.31}$$

and compute the Absolute Error and Relative Error.

5.2.3 Solution:

$a = x_0 = 1; \qquad b = x_4 = 2; \qquad n = 4; \qquad Then\ h = \dfrac{b-a}{n} = 0.25$

$x_0 = 1$	$x_1 = a + h = 1.25$	$x_2 = a + 2h = 1.5$	$x_3 = a + 3h = 1.75$	$x_4 = 2.0$
$y_0 = 1$	$y_1 = 0.8$	$y_2 = 0.66667$	$y_3 = 0.57143$	$y_4 = 0.5$

From equation 5.29 we have

$$\begin{aligned} Area &= \frac{h}{3}\left[y_0 + 4y_1 + 2y_2 + 4y_3 + y_4\right] \\ &= \frac{0.25}{3}\left[1 + 4(0.8) + 2(0.66667) + 4(0.57143) + 0.5\right] \\ &= 0.69325 \end{aligned}$$

The Absolute Error $= |0.6931 - 0.69325| = 0.00015$
and Relative Error $= |\frac{0.6931-0.69325}{0.69325}| = 0.00021637216$.

For **Simpson's Rule** we can use the following Matlab code:

Matlab Code 5.7. *Simpson's Rule*

```
% ***********   Simpson Rule **************
%  estimates the value of the integral of y=f(x)
%      from a to b by using Simpson rule
clc
clear
close all
a=1; % the start of integral interval
b=2;  % the end of integral interval
n=4; % the number of subintervals
h = (b-a)/n;
Area=0;
x = a:h:b; % to comput the x_i values
% this Example of f(x)=x^2
y=x.^2;       % to comput the y_i values
```

```
for i = 2:2:n,
Area = Area + 4*y(i);
end
for i = 3:2:n-1,
Area = Area +2*y(i);
end
Area = Area + y(1) + y(n+1);
Area = Area*h/3
```

5.2.4 EXERCISE

Use the trapezoidal approximation and Simpson's rule to compute the values the following definite integrals with $n = 4;\ n = 8$ and compare your results with the analytical values.

1. $y = \int_0^2 e^{-x^2} dx.$
2. $y = \int_2^4 \sqrt{x} dx.$
3. $y = \int_2^4 \sqrt{x} dx.$
4. $y = \int_0^2 x^2 dx.$
5. $y = \int_0^{\pi} \sin(x) dx.$
6. $y = \int_0^1 \frac{1}{x^2+1} dx.$

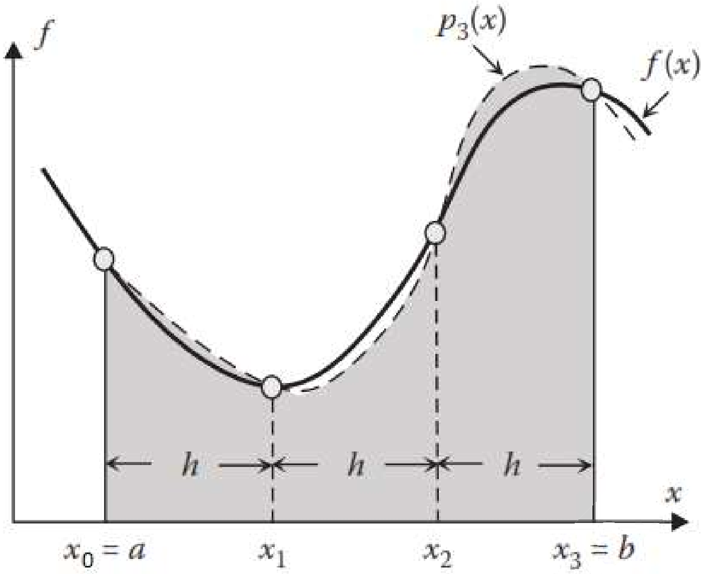

Figure 5.7: Simpson's 3/8 rule.

5.3 Simpson's $3/8$ Rule

The Simpson's $3/8$ rule also called **four points Simpson rule**, uses a third-degree polynomial to approximate the integrand f(x), so we need four points to form this polynomial. see figure 5.7 The definite integral will be evaluated with this polynomial replacing the integrand

$$\int_a^b f(x)dx \approx \int_a^b p_3(x)dx$$

by the same procedure we can find

$$\int_a^b p_3(x)dx = \frac{3h}{8}[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)] + O(h^4), \; h = \frac{b-a}{3}$$

The method is known as the $3/8$ rule because h is multiplied by $3/8$. **To apply Simpson's** $3/8$ **rule the interval** $[a, b]$ **must be divided into a number** n **of subintervals must be a**

multiple of 3 and the Composite Simpson's $3/8$ Rule will be

$$\begin{aligned}\int_a^b p_3(x)dx = &\frac{3h}{8}[y_0+3y_1+3y_2+y_3] \\ &+\frac{3h}{8}[y_3+3y_4+3y_5+y_6] \\ &+\frac{3h}{8}[y_6+3y_7+3y_8+y_9] \\ &+\cdots \\ &+\frac{3h}{8}[y_{n-3}+3y_{n-2}+3y_{n-1}+y_n]\end{aligned}$$

$$= \frac{3h}{8}[y_0+3y_1+3y_2+2y_3+3y_4+3y_5+2y_6+\cdots+3y_{n-2}+3y_{n-1}+y_n]$$

5.3.1 Boole's Rule

Boole's Rule is **five points rule** uses a four degree polynomial to approximate the integrand f(x), so we need five points to form this polynomial. The definite integral will be approximated with the integrand

$$\int_a^b f(x)dx \cong \int_a^b p_4(x)dx$$

by the same procedure we can find

$$\int_a^b p_4(x)dx = \frac{2h}{45}[7f(x_0)+32f(x_1)+12f(x_2)+32f(x_3)+7f(x_4)]+O(h^7)$$

To apply Boole's rule the interval $[a,b]$ **must be divided into a number** n **of subintervals must be a multiple of** 4 **.**

5.3.2 Weddle's Rule

Weddle's Rule is **seven points rule**, so we need seven points to form this rule. Weddle's rule is given by

$$\int_a^b p_4(x)dx = \frac{3h}{10}\left[f(x_0) + 5f(x_1) + f(x_2) + 6f(x_3) + f(x_4) + 5f(x_5) + f(x_6)\right] + O(h^7)$$

To apply Weddle's rule the interval $[a, b]$ must be divided into a number n of subintervals must be a multiple of 6 .

5.3.3 EXERCISE

Use the trapezoidal approximation and Simpson's rule to compute the values the following definite integrals with $n = 4;\ n = 8$ and compare your results with the analytical values.

1. $y = \int_0^2 e^{-x^2} dx$.
2. $y = \int_2^4 \sqrt{x}dx$.
3. $y = \int_2^4 \sqrt{x}dx$.
4. $y = \int_0^2 x^2 dx$.
5. $y = \int_0^{\pi} \sin(x)dx$.
6. $y = \int_0^1 \frac{1}{x^2+1}dx$.

Chapter 6

Numerical Solution of Ordinary Differential Equations

This chapter is an introduction to several methods that can be used to obtain approximate solutions of differential equations. Such approximations are necessary when no exact solution can be found. The Taylor Series, Euler's and Runge Kutta methods are discussed.

6.1 Taylor Series Method

The Taylor series expansion about point x is

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2}f''(x) + \frac{h^3}{6}f'''(x) + \frac{h^4}{24}f^{(4)}(x) + \cdots$$

For a value $x_1 > x_0$, close to x_0, we replace $f(x+h)$ by y_1 and $f(x)$ by y_0 to get

$$y_1 = y_0 + hy_0' + \frac{h^2}{2}y_0'' + \frac{h^3}{6}y_0''' + \frac{h^4}{24}y_0^{(4)} + \cdots$$

For another value $x_2 > x_1$, close to x_1, we repeat the procedure then

$$y_2 = y_1 + hy_1' + \frac{h^2}{2}y_1'' + \frac{h^3}{6}y_1''' + \frac{h^4}{24}y_1^{(4)} + \cdots$$

In general,

$$y_{i+1} = y_i + hy'_i + \frac{h^2}{2}y''_i + \frac{h^3}{6}y'''_i + \frac{h^4}{24}y_i^{(4)} + \cdots \tag{6.1}$$

Example 6.1. *Use the Taylor series method to obtain a solution of*

$$y' = -xy \tag{6.2}$$

for values $x_0 = 0.0$, $x_1 = 0.1$, $x_2 = 0.2$, $x_3 = 0.3$, $x_4 = 0.4$, *and* $x_5 = 0.5$ *with the initial condition* $y(0) = 1$*. (use the Taylor series up to* $y^{(4)}$*).*

Solution:

For this example, $h = x_1 - x_0 = 0.1$, and by substitution into equation 6.1 we have:

$$y_{i+1} = y_i + 0.1y'_i + \frac{0.01}{2}y''_i + \frac{0.001}{6}y'''_i + \frac{0.0001}{24}y_i^{(4)} + \cdots \tag{6.3}$$

for $i = 1, 2, 3$ and 4. The first through the fourth derivatives of 6.2:

$$\begin{aligned}
y' &= -xy \\
y'' &= -xy' - y = -x(-xy) - y = (x^2 - 1)y \\
y''' &= (x^2 - 1)y' + 2xy = (x^2 - 1)(-xy) + 2xy = (-x^3 + 3x)y \\
y^{(4)} &= (-x^3 + 3x)y' + (-3x^2 + 3)y = (x^4 - 6x^2 + 3)y
\end{aligned}$$

We use the subscript i to express them as

$$\begin{aligned}
y'_i &= -x_i y_i \\
y''_i &= (x_i^2 - 1)y_i \\
y'''_i &= (-x_i^3 + 3x_i)y_i \\
y_i^{(4)} &= (x_i^4 - 6x_i^2 + 3)y_i
\end{aligned} \tag{6.4}$$

where x_i represents $x_0 = 0.0$, $x_1 = 0.1$, $x_2 = 0.2$, $x_3 = 0.3$, and $x_4 = 0.4$. Substitution these the values of the coefficients of y_i in 6.4 we obtain the following relations:

$$\begin{aligned}
y_0' &= -x_0 y_0 = -0y_0 = 0 \\
y_1' &= -x_1 y_1 = -0.1y_1 \\
y_2' &= -x_2 y_2 = 0.2y_2 \\
y_3' &= -x_3 y_3 = 0.3y_3 \\
y_4' &= -x_4 y_4 = 0.4y_4
\end{aligned} \tag{6.5}$$

$$\begin{aligned}
y_0'' &= (x_0^2 - 1)y_0 = -y_0 \\
y_1'' &= (x_1^2 - 1)y_1 = -0.99y_1 \\
y_2'' &= (x_2^2 - 1)y_2 = -0.96y_2 \\
y_3'' &= (x_3^2 - 1)y_3 = -0.91y_3 \\
y_4'' &= (x_4^2 - 1)y_4 = -0.84y_4
\end{aligned} \tag{6.6}$$

$$\begin{aligned}
y_0''' &= (-x_0^3 + 3x_0)y_0 = 0 \\
y_1''' &= (-x_1^3 + 3x_1)y_1 = 0.299y_1 \\
y_2''' &= (-x_2^3 + 3x_2)y_2 = 0.592y_2 \\
y_3''' &= (-x_3^3 + 3x_3)y_3 = 0.873y_3 \\
y_4''' &= (-x_4^3 + 3x_4)y_4 = 1.136y_4
\end{aligned} \tag{6.7}$$

$$\begin{aligned}
y_0^{(4)} &= (x_0^4 - 6x_0^2 + 3)y_0 = 3y_0 \\
y_1^{(4)} &= (x_1^4 - 6x_1^2 + 3)y_1 = 2.9401y_1 \\
y_2^{(4)} &= (x_2^4 - 6x_i^2 2 + 3)y_i 2 = 2.7616y_2 \\
y_3^{(4)} &= (x_3^4 - 6x_3^2 + 3)y_3 = 2.4681y_3 \\
y_4^{(4)} &= (x_4^4 - 6x_4^2 + 3)y_4 = 2.0656y_4
\end{aligned} \tag{6.8}$$

By substitution of 6.5 through 6.8 into 6.3, and using the given initial condition $y_0 = 1$, we obtain:

$$\begin{aligned} y_1 &= y_0 + 0.1y_0' + \frac{0.01}{2}y_0'' + \frac{0.001}{6}y_0''' + \frac{0.0001}{24}y_0^{(4)} \\ &= 1 + 0.1(0) + \frac{0.01}{2}(-1) + \frac{0.001}{6}(0) + \frac{0.0001}{24}(3) \\ &= 0.99501 \end{aligned}$$

Similarly

$$\begin{aligned} y_2 &= y_1 + 0.1y_1' + \frac{0.01}{2}y_1'' + \frac{0.001}{6}y_1''' + \frac{0.0001}{24}y_1^{(4)} \\ &= (1 - 0.01 – 0.00495 – 0.00005 + 0.00001)y_1 \\ &= 0.98511(0.99501) \\ &= 0.980194 \end{aligned}$$

$$\begin{aligned} y_3 &= y_2 + 0.1y_2' + \frac{0.01}{2}y_2'' + \frac{0.001}{6}y_2''' + \frac{0.0001}{24}y_2^{(4)} \\ &= (1 - 0.02 – 0.0048 – 0.0001 + 0.00001)y_2 \\ &= (0.97531)0.980194 \\ &= 0.955993 \end{aligned}$$

$$\begin{aligned} y_4 &= y_3 + 0.1y_3' + \frac{0.01}{2}y_3'' + \frac{0.001}{6}y_3''' + \frac{0.0001}{24}y_3^{(4)} \\ &= (1 - 0.03 – 0.00455 + 0.00015 + 0.00001)y_3 \\ &= (0.9656)0.955993 \\ &= 0.923107 \end{aligned}$$

$$\begin{aligned} y_5 &= y_4 + 0.1y_4' + \frac{0.01}{2}y_4'' + \frac{0.001}{6}y_4''' + \frac{0.0001}{24}y_4^{(4)} \\ &= (1 - 0.04 – 0.0042 + 0.00019 + 0.00001)y_4 \\ &= (0.95600)0.923107 \\ &= 0.88249 \end{aligned}$$

We can compare between the approximated and the analytical solution $\left[y = e^{\frac{-x}{2}}\right]$ for the differential equation $\frac{dy}{dx} = -xy$.
Homework

6.2 Euler's Method

Taylor expansion from equation 6.1 is

$$y_{i+1} = y_i + hy_i' + \frac{h^2}{2}y_i'' + \frac{h^3}{6}y_i''' + \frac{h^4}{24}y_i^{(4)} + \cdots$$

Retaining the linear terms only of Taylor expansion gives

$$y(x_1) = y(x_0) + hy'(x_0) + \frac{h^2}{2}y''(\xi_0) \tag{6.9}$$

for some ξ_0 between x_0 and x_{i+1}. In general, expanding $y(x_{i+1}$ about x_i yields

$$y(x_{i+1}) = y(x_i) + hy'(x_i) + \frac{h^2}{2}y''(\xi_i)$$

for some ξ_i between x_i and x_{i+1}. Note that $y'(x_i) = f(x_i, y_i)$. the estimated solution y_{i+1} can be found via

$$y(x_{i+1}) = y(x_i) + hf(x_i, y_i); \quad i = 0, 1, 2, 3, \cdots, n-1 \tag{6.10}$$

known as Euler's method.

Example 6.2. *Consider the Initial Value Problem (IVP):*

$$y' + y = 2x, \qquad 0 \le x \le 1 \tag{6.11}$$

with initial condition $y(0) = 1$ *and* $h = 0.1$.

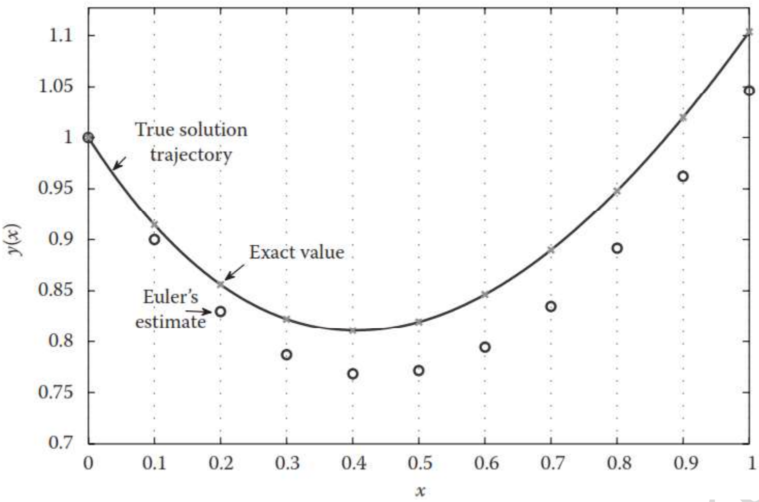

Figure 6.1: Comparison of Euler's and exact solutions in Example 6.2

Solution:

we have $f(x, y) = -y + 2x$. *Starting with* $x = 0$, $y = 1$, *as*

$$\begin{aligned} y_1 = y(0.1) &= y_0 + hf(x_0, y_0) \\ &= 1 + 0.1f(0, 1) \\ &= 1 + 0.1(-1) = 0.9 \end{aligned}$$

Now with $x = 0.1$, $y = 0.9$, *calculate* $y_2 = y(0.2)$ *as*

$$\begin{aligned} y_2 &= y_1 + hf(x_1, y_1) \\ &= 0.9 + 0.1f(0.1, 0.9) \\ &= 0.9 + 0.1(-0.9 + 2(0.1)) = 0.83 \end{aligned}$$

and so on $\cdots$.
The exact solution is $y(x) = 2x + 3e^{-x} - 2$.
so the exact $y(0.1) = 0.914512$ *and* $y(0.2) = 0.856192$. *see figure 6.1*

6.3 Runge Kutta Method

The Runge Kutta method is the most widely used method of solving differential equations with numerical methods. It differs from the Taylor series method in that we use values of the first derivative of $f(x, y)$ at several points instead of the values of successive derivatives at a single point.
For a Runge Kutta method of order 2, the following formulas are applicable

Runge-Kutta Method of Order 2:

$$\begin{aligned} k_1 &= hf(x_n, y_n) \\ k_2 &= hf(x_n + h, y_n + h) \\ y_{n+1} &= y_n + \frac{1}{2}(k_1 + k_2) \end{aligned} \tag{6.12}$$

When higher accuracy is desired, we can use order 3 or order 4. The applicable formulas are as follows

Runge-Kutta Method of Order 3:

$$\begin{aligned} I_1 &= hf(x_n, y_n) \\ I_2 &= hf(x_n + \frac{h}{2}, y_n + \frac{I_1}{2}) \\ I_3 &= hf(x_n + h, y_n + 2(I_2 - I_1) \\ y_{n+1} &= y_n + \frac{1}{6}(I_1 + 4I_2 + I_3) \end{aligned} \tag{6.13}$$

Runge-Kutta Method of Order 4:

$$\begin{aligned} m_1 &= hf(x_n, y_n) \\ m_2 &= hf(x_n + \frac{h}{2}, y_n + \frac{m_1}{2}) \\ m_3 &= hf(x_n + \frac{h}{2}, y_n + \frac{m_2}{2}) \\ m_4 &= hf(x_n + h, y_n + m_3) \\ y_{n+1} &= y_n + \frac{1}{6}(m_1 + 2m_2 + 2m_3 + m_4) \end{aligned} \tag{6.14}$$

Example 6.3. *Compute the approximate value of y at $x = 0.2$ from the solution $y(x)$ of the differential equation*

$$y' = x + y^2 \tag{6.15}$$

given the initial condition $y(0) = 1$. Use order 2, 3, and 4 Runge Kutta methods with $h = 0.2$.

Solution:

For order 2, we use 6.12. Since we are given that $y(0) = 1$, we begin with $x = 0$, and $y = 1$. Then

$$\begin{aligned}
k_1 &= hf(x_n, y_n) = hf(0, 1) \\
&= 0.2(0 + 1^2) = 0.2 \\
k_2 &= hf(x_n + h, y_n + h) = hf(0.2, 1.2) \\
&= 0.2\left[0.2 + (1.2)^2\right] = 0.328 \\
y_1 &= y_0 + \frac{1}{2}(k_1 + k_2) \\
&= 1 + \frac{1}{2}(0.2 + 0.328) = 1.264
\end{aligned}$$

For order 3, we use 6.13. Then

$$\begin{aligned}
I_1 &= hf(x_n, y_n) = 0.2 \\
I_2 &= hf(x_n + \frac{h}{2}, y_n + \frac{I_1}{2}) = hf(0 + \frac{0.2}{2}, 1 + \frac{0.2}{2}) \\
&= 0.262 \\
I_3 &= hf(x_n + h, y_n + 2(I_2 - I_1)) \\
&= 0.2f(0 + 0.2, 1 + 2(0.262 - 0.2)) \\
&= 0.2\left[0.2 + (1 + 0.124)^2\right] \\
&= 0.391 \\
y_1 &= y_0 + \frac{1}{6}(I_1 + 4I_2 + I_3) \\
&= 1 + \frac{1}{6}(0.2 + 4(0.262 + 0.391) \\
&= 1.273
\end{aligned}$$

For Order 4: we use 6.14. Then

$$\begin{aligned}
m_1 &= hf(x_n, y_n) = 0.2 \\
m_2 &= hf(x_n + \frac{h}{2}, y_n + \frac{m_1}{2}) = 0.2f(0 + \frac{0.2}{2}, 1 + \frac{0.2}{2}) \\
&= 0.262 \\
m_3 &= hf(x_n + \frac{h}{2}, y_n + \frac{m_2}{2}) \\
&= 0.2f(0 + \frac{0.2}{2}, 1 + \frac{0.262}{2}) \\
&= 0.276 \\
m_4 &= hf(x_n + h, y_n + m_3) \\
&= 0.2f(0 + 0.2, 1 + 0.276) = 0.366 \\
y_1 &= y_0 + \frac{1}{6}(m_1 + 2m_2 + 2m_3 + m_4) \\
&= 1 + \frac{1}{6}(0.2 + 2(0.262) + 2(0.276) + 0.366) \\
&= 1.274
\end{aligned}$$

6.3.1 EXERCISE

Compute the approximate value of $y(x)$ of the following differential equations using Taylor series, Euler's, and Runge Kutta Method of Order 2, 3, and 4.

1. $y' = 3x^2$. with h=0.1 and the initial condition $y(2) = 0.5$
2. $y' = -y^3 + 0.2\sin(x)$. with h=0.1 and the initial condition $y(0) = 0.707$
3. $y' = x^2 - y$. with h=0.1 and the initial condition $y(0) = 1$