

# Interpolation and Curve Fitting

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# Motivating Ideas

## Motivating Ideas

## Curve Fitting

Curve fitting is the process of constructing a curve (or mathematical function) that has a best fit to a series of data points.

### **Benefits of Curve Fitting:**

- Provides a means to observe and quantify general trends.
  - Removes noise from a function.
  - Can extract meaningful parameters when measured data is fitted to an analytical equation.
  - Can derive finite difference approximations.

# Motivating Ideas

## Categories of Curve Fitting

### Exact Curve Fitting (Interpolation)

Exact fit (interpolation) occurs when we want to **learn a curve** that **passes through** the data points exactly.

### Best Curve Fitting (Least Squares Analysis)

**Best fit curves** make sense when we know that the data contains noise – rather than fit the data exactly, we aim to **learn a function** that **minimizes** some **predefined error function** on the data points.

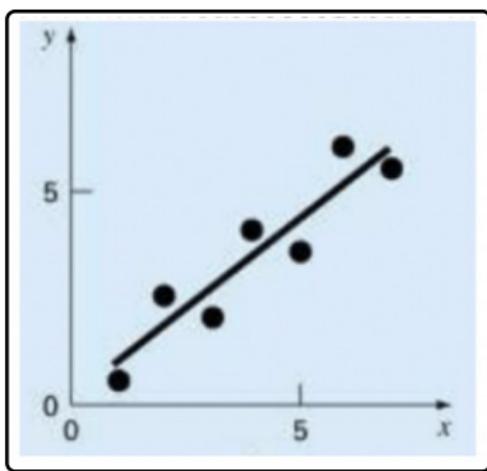
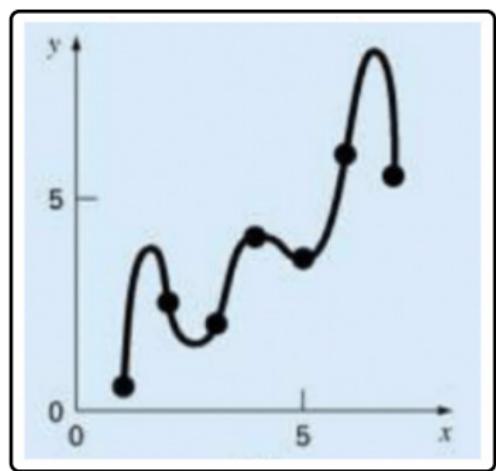
# Motivating Ideas

## Categories of Curve Fitting

Curve Fitting

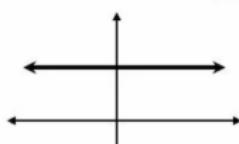
Exact Fit

Best Fit

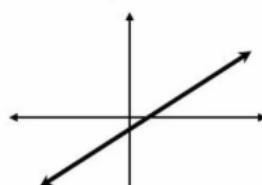


# Motivating Ideas

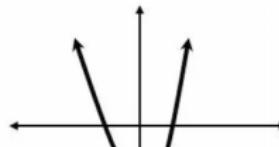
## Graphs of Polynomial Functions:



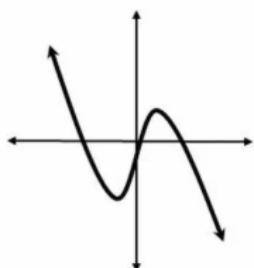
Constant Function  
(degree = 0)



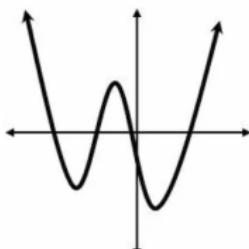
Linear Function  
(degree = 1)



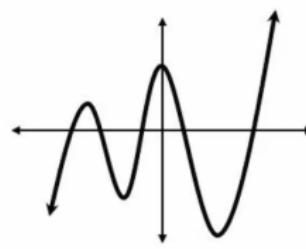
Quadratic Function  
(degree = 2)



Cubic Function  
(deg. = 3)



Quartic Function  
(deg. = 4)



Quintic Function  
(deg. = 5)

# Motivating Ideas

## Real-World Data

Data relating to (or collected from) a real-world application.

### Real-World Data:

- Data collected from mobile systems (e.g., smart watches, automobiles, Google Street View).

### Opportunities and Challenges:

- Provides real-world evidence needed for the **design** and **operation** of modern systems.
- Pathway to **system-specific** decision making procedures.
- Real-world data can be noisy.
- Easy to collect too much data.

# Motivating Ideas

## Model Fidelity Assessment:

### Underfitting

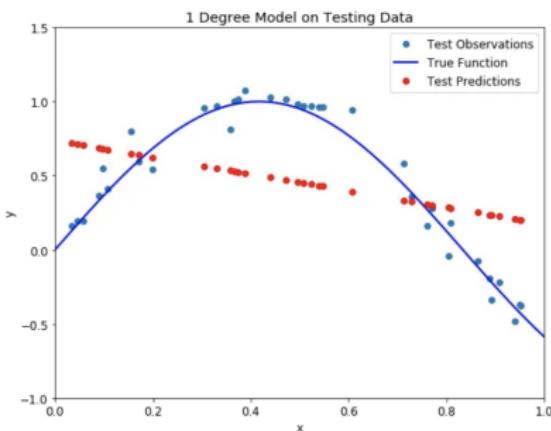
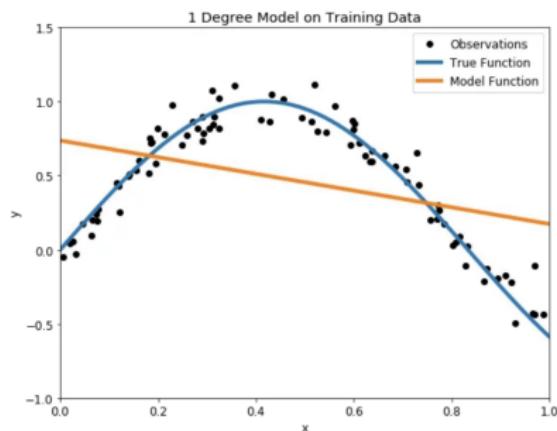
A condition where a **curve fitting model** is incapable of capturing the **general trend** in the data; this, in turn, affects the accuracy of a model.

### Overfitting

A condition where a **curve fitting model** begins to describe the **random error (fluctuations)** in the data rather than the **underlying relationships among variables**.

# Motivating Ideas

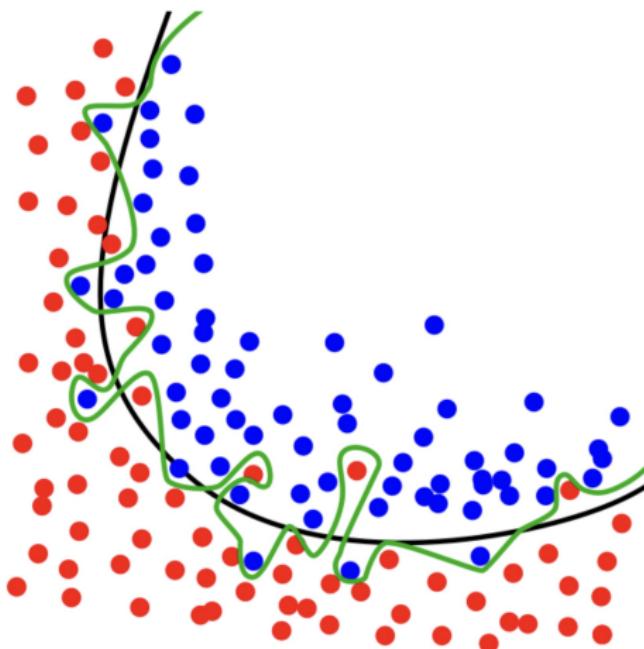
**Example. Underfitting in Data Science:** We wish to predict the relationship between input  $x$  and output  $y$ .



Clearly, the **linear function approximation underfits** the **true relationship** between  $x$  and  $y$ .

# Motivating Ideas

**Example. Overfitting in Data Science:** We wish to find a low-order function that separates the red and blue data points.



# Method of Divided Differences

# Method of Divided Differences

## Divided Differences

Given a set of **distinct points**  $x_0, x_1, \dots, x_n$ , and known function values  $f_0 = f(x_0), f_1 = f(x_1), \dots, f_n = f(x_n)$ , the method of divided differences is a **numerical procedure** for **interpolating the data** with a **polynomial fit**.

**Polynomial Fit.** Let:

$$f(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + \dots + a_n(x - x_0) \cdots (x - x_{(n-1)}). \quad (1)$$

The **method of divided differences** provides systematic way to determine the **polynomial coefficients**  $a_0$  through  $a_{(n-1)}$ .

# Method of Divided Differences

**Divided Difference Table and Formulae.** For  $f(x)$  based on  $x_0, x_1, x_2, x_3$ .

$x_i$	$f[x_i] = f(x_i)$	$f[,]$	$f[,,]$	$f[,,,]$
$x_0$	$f(x_0)$	$f[x_0, x_1]$	$f[x_0, x_1, x_2]$	$f[x_0, x_1, x_2, x_3]$
$x_1$	$f(x_1)$	$f[x_1, x_2]$	$f[x_1, x_2, x_3]$	
$x_2$	$f(x_2)$	$f[x_2, x_3]$		
$x_3$	$f(x_3)$			

Here,

$$\begin{aligned}
 f[x_i] &= f(x_i) \\
 f[x_i, x_{i+1}] &= \frac{f[x_{i+1}] - f[x_i]}{x_{i+1} - x_i}. \tag{2}
 \end{aligned}$$

# Method of Divided Differences

Generally,

$$f[x_i, \dots, x_{i+k}] = \frac{f[x_{i+1}, \dots, x_{i+k}] - f[x_i, \dots, x_{i+k-1}]}{x_{i+k} - x_i}. \quad (3)$$

The interpolated polynomial is:

$$\begin{aligned} f(x) = & f[x_0] + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1) + \\ & f[x_0, x_1, x_2, x_3](x - x_0)(x - x_1)(x - x_2). \end{aligned}$$

**Note:** The algorithm depends only on the values  $x_i, \dots, x_{i+k}$ , and not their order.

# Method of Divided Differences

**Example 1.** Find a polynomial that interpolates the data set:

x		0	1	3
<hr/>				
f(x)		1	0	10

**Solution:** We seek:

$x_i$	$f[x_i] = f(x_i)$	$f[,]$	$f[,,]$
0	1	$f[x_0, x_1]$	$f[x_0, x_1, x_2]$
1	0	$f[x_1, x_2]$	
3	10		

where

$$f[x_0, x_1] = \left[ \frac{f(x_1) - f(x_0)}{x_1 - x_0} \right] = \left[ \frac{0 - 1}{1 - 0} \right] = -1. \quad (4)$$

# Method of Divided Differences

$$f[x_1, x_2] = \left[ \frac{f(x_2) - f(x_1)}{x_2 - x_1} \right] = \left[ \frac{10 - 0}{3 - 1} \right] = 5. \quad (5)$$

$$f[x_0, x_1, x_2] = \left[ \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0} \right] = \left[ \frac{5 + 1}{3 - 0} \right] = 2. \quad (6)$$

## Interpolated Polynomial:

$$\begin{aligned} f(x) &= f[x_0] + f[x_0, x_1](x - x_0) + f[x_0, x_1, x_2](x - x_0)(x - x_1) \\ &= 1 + -1(x - 0) + 2(x - 0)(x - 1) \\ &= 1 - 3x + 2x^2 \end{aligned}$$

**Validate:**  $f(0) = 1$ ;  $f(1) = 0$ ;  $f(3) = 1 - 9 + 18 = 10$ .

# Method of Divided Differences

## Python Code: Divided difference test program

```
1 # =====
2 # TestInterpolationDividedDifferences01.py: Compute divided differences polynomial.
3 #
4 # Written By: Mark Austin
5 # =====
6
7 import math;
8 import numpy as np
9 import matplotlib.pyplot as plt
10
11 import Interpolation;
12
13 # main method ...
14
15 def main():
16     print(" --- Case Study 1: Small test problem ... ");
17
18     x = np.array( [ 0, 1, 3 ] )
19     y = np.array( [ 1, 0, 10 ] )
20
21     print(" --- Compute divided difference table ... ");
22
23     dTable= Interpolation.divideddifference(x, y)[0, :]
24
25     print(" --- Evaluate on new data points ... ");
26
27     x_new = np.arange( -1.0, 4.0, .2 )
28     y_new = Interpolation.newtonpolynomial(dTable, x, x_new)
```

# Method of Divided Differences

## Python Code: Divided difference test program

```
29
30     print("---- Plot divided difference polynomial ... ");
31
32     plt.figure(figsize = (12, 8))
33     plt.plot(x_new, y_new, 'b', x, y, 'ro')
34     plt.title('Divided Difference Polynomial')
35     plt.xlabel('x')
36     plt.ylabel('f(x)')
37     plt.grid()
38     plt.show()
39
40 # call the main method ...
41
42 main()
```

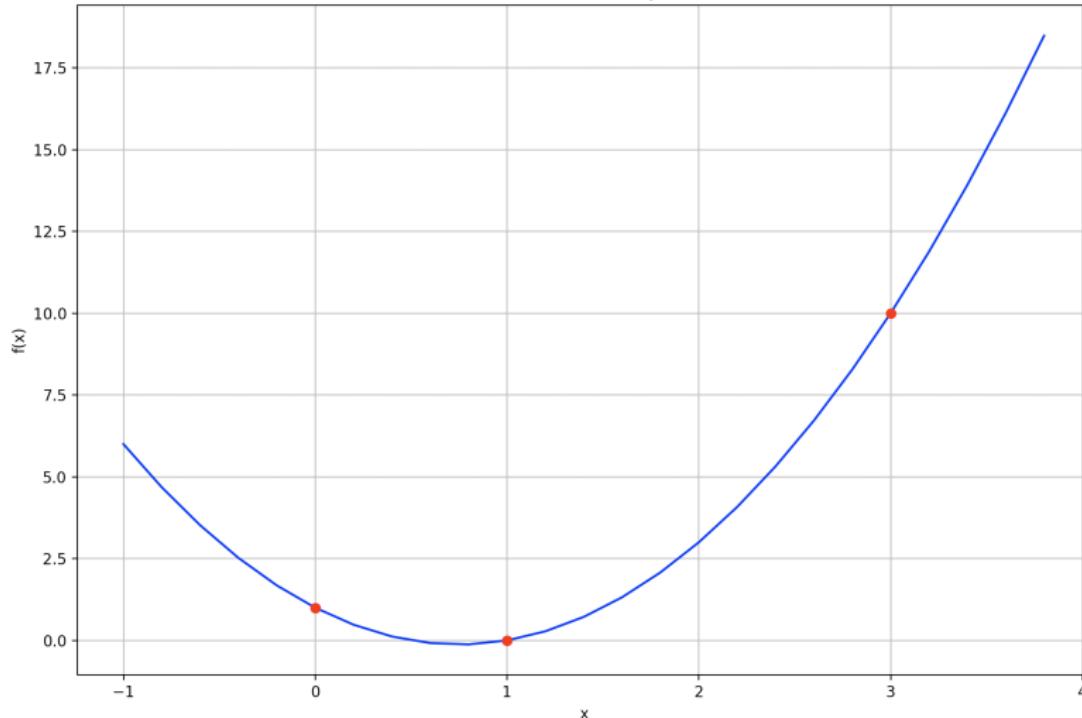
## Abbreviated Output:

Matrix: divided difference table

1.0000	-1.0000	2.0000
0.0000	5.0000	0.0000
10.0000	0.0000	0.0000

# Method of Divided Differences

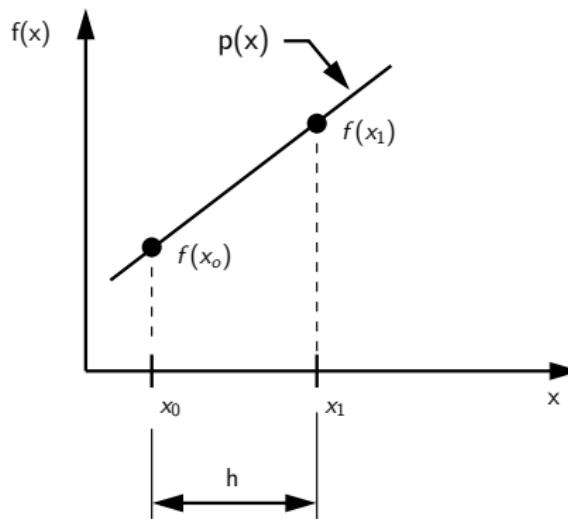
Divided Difference Polynomial



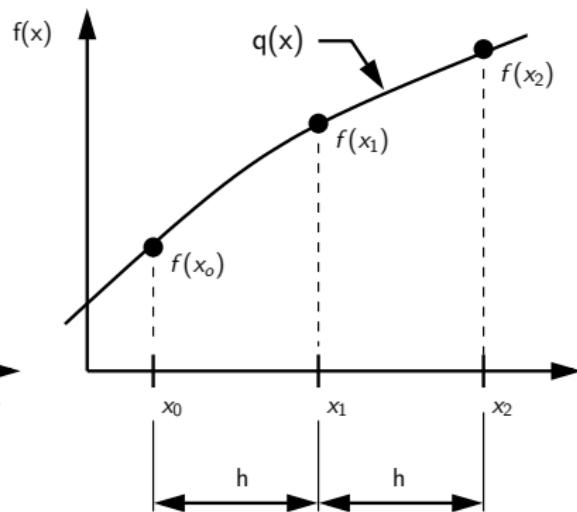
# Method of Divided Differences

**Example 2.** Derive formulae for linear and quadratic interpolation when data points are equally spaced.

Linear Interpolation  $p(x)$



Quadratic Interpolation  $q(x)$



# Method of Divided Differences

**Linear Interpolation  $p(x)$ .** Divided difference table is:

$x_i$	$f[x_i] = f(x_i)$	$f[,]$
$x_0$	$f(x_0)$	$f[x_0, x_1]$
$x_1$	$f(x_1)$	

where

$$f[x_0, x_1] = \left[ \frac{f(x_1) - f(x_0)}{x_1 - x_0} \right] = \left[ \frac{f(x_1) - f(x_0)}{h} \right]. \quad (7)$$

**Interpolated Polynomial:**

$$p(x) = f[x_0] + f[x_0, x_1](x - x_0) = f(x_0) + \left[ \frac{f(x_1) - f(x_0)}{h} \right] (x - x_0). \quad (8)$$

# Method of Divided Differences

**Quadratic Interpolation  $q(x)$ .** Divided difference table is:

$x_i$	$f[x_i] = f(x_i)$	$f[,]$	$f[,,]$
$x_0$	$f(x_0)$	$f[x_0, x_1]$	$f[x_0, x_1, x_2]$
$x_1$	$f(x_1)$	$f[x_1, x_2]$	
$x_2$	$f(x_2)$		

where

$$f[x_0, x_1] = \left[ \frac{f(x_1) - f(x_0)}{x_1 - x_0} \right] = \left[ \frac{f(x_1) - f(x_0)}{h} \right]. \quad (9)$$

$$f[x_1, x_2] = \left[ \frac{f(x_2) - f(x_1)}{x_2 - x_1} \right] = \left[ \frac{f(x_2) - f(x_1)}{h} \right]. \quad (10)$$

# Method of Divided Differences

$$f[x_0, x_1, x_2] = \left[ \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0} \right] = \left[ \frac{f(x_2) - 2f(x_1) + f(x_o)}{2h^2} \right]. \quad (11)$$

## Interpolated Polynomial:

$$q(x) = f[x_0] + f[x_o, x_1](x - x_o) + f[x_o, x_1, x_2](x - x_o)(x - x_1). \quad (12)$$

**Validate:**  $q(x_o) = f(x_o)$ ,  $q(x_1) = f(x_1)$ ,  $q(x_2) = f(x_2)$ .

# Method of Divided Differences

## Integration of $p(x)$ :

$$\begin{aligned}\int_{x_0}^{x_1} p(x) dx &= \int_{x_0}^{x_1} f(x_o) dx + \left[ \frac{f(x_1) - f(x_0)}{h} \right] \int_{x_0}^{x_1} (x - x_o) dx \\ &= \frac{h}{2} [f(x_o) + f(x_1)].\end{aligned}$$

## Integration of $q(x)$ :

$$\int_{x_0}^{x_1} q(x) dx = \frac{h}{3} [f(x_o) + 4f(x_1) + f(x_2)].$$

## Method of Divided Differences

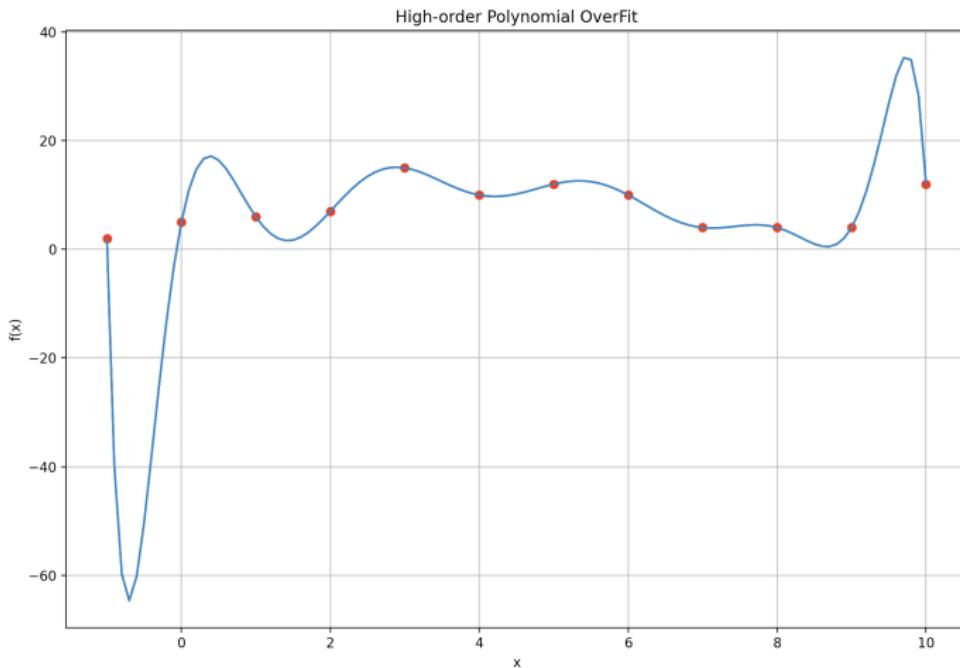
**Example 3.** High-order polynomial overfit for the dataset:

## **Abbreviated Output:**

Matrix: divided difference table

2	3	-1.0	0.33	0.21	-0.27	0.14	-0.05	0.01	-0.002	0.000	-0.0001
5	1	0.0	1.17	-1.13	0.56	-0.19	0.05	-0.01	0.002	-0.000	0.0000
6	1	3.5	-3.33	1.67	-0.59	0.16	-0.03	0.00	-0.000	0.000	0.0000
7	8	-6.5	3.33	-1.29	0.35	-0.06	0.00	0.00	0.000	0.000	0.0000
15	-5	3.5	-1.83	0.46	-0.01	-0.04	0.02	0.00	0.000	0.000	0.0000
10	2	-2.0	0.00	0.42	-0.22	0.08	0.00	0.00	0.000	0.000	0.0000
12	-2	-2.0	1.67	-0.67	0.25	0.00	0.00	0.00	0.000	0.000	0.0000
10	-6	3.0	-1.00	0.58	0.00	0.00	0.00	0.00	0.000	0.000	0.0000
4	0	0.0	1.33	0.00	0.00	0.00	0.00	0.00	0.000	0.000	0.0000
4	0	4.0	0.00	0.00	0.00	0.00	0.00	0.00	0.000	0.000	0.0000
4	8	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.000	0.000	0.0000
12	0	0.0	0.00	0.00	0.00	0.00	0.00	0.00	0.000	0.000	0.0000

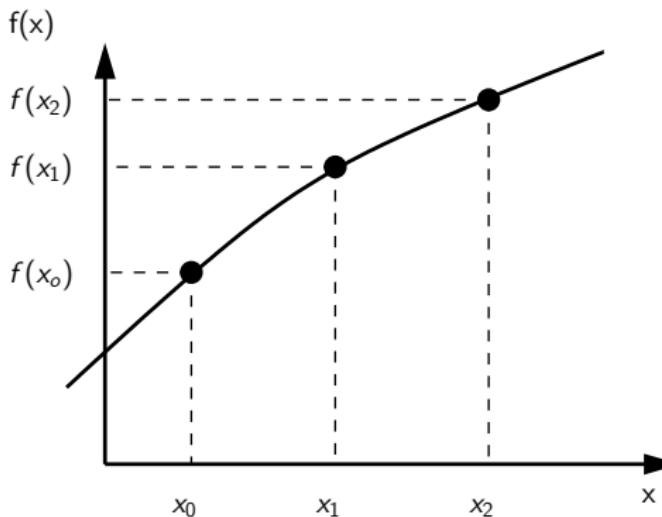
# Method of Divided Differences



# Lagrange Interpolation

# Lagrange Interpolation

**Basic Idea.** Assume that a curve passes through set of point:  
 $(x_0, f(x_0)), (x_1, f(x_1)), (x_2, f(x_2)), \dots, (x_n, f(x_n))$ .



We propose that:

# Lagrange Interpolation

$$f_o = f_o p_o(x_o) + f_1 p_1(x_o) + \cdots + f_n p_n(x_o).$$

$$f_1 = f_o p_o(x_1) + f_1 p_1(x_1) + \cdots + f_n p_n(x_1).$$

$\cdots = \cdots$

$$f_n = f_o p_o(x_n) + f_1 p_1(x_1) + \cdots + f_n p_n(x_n).$$

where  $p_i(x_j) = 1, i = j$ , and  $p_i(x_j) = 0, i \neq j$ .

**Lagrange Formula:**  $f(x) = p_0(x)f_o + p_1(x)f_1 + p_2(x)f_2 + \dots$ ,  
where

$$p_i(x) = \frac{\prod_{i=0, i \neq j}^{n-1} (x - x_i)}{\prod_{i=0, i \neq j}^{n-1} (x_j - x_i)} \quad (13)$$

# Lagrange Interpolation

**Example 1.** Find a polynomial that interpolates the data set:

x		0	1	3
-----* -----</td <td data-kind="ghost"></td> <td data-kind="ghost"></td> <td data-kind="ghost"></td> <td data-kind="ghost"></td>				
f(x)		1	0	10

**Solution.** For the given dataset,

$$f(x) = f(x_0)p_0(x) + f(x_1)p_1(x) + f(x_2)p_2(x) \quad (14)$$

where

$$p_0(x) = \frac{(x - 1)(x - 3)}{(0 - 1)(0 - 3)} = \left[ \frac{x^2 - 4x + 3}{3} \right]. \quad (15)$$

$$p_1(x) = \frac{(x - 0)(x - 3)}{(1 - 0)(1 - 3)} = \left[ \frac{x^2 - 3x}{-2} \right]. \quad (16)$$

# Lagrange Interpolation

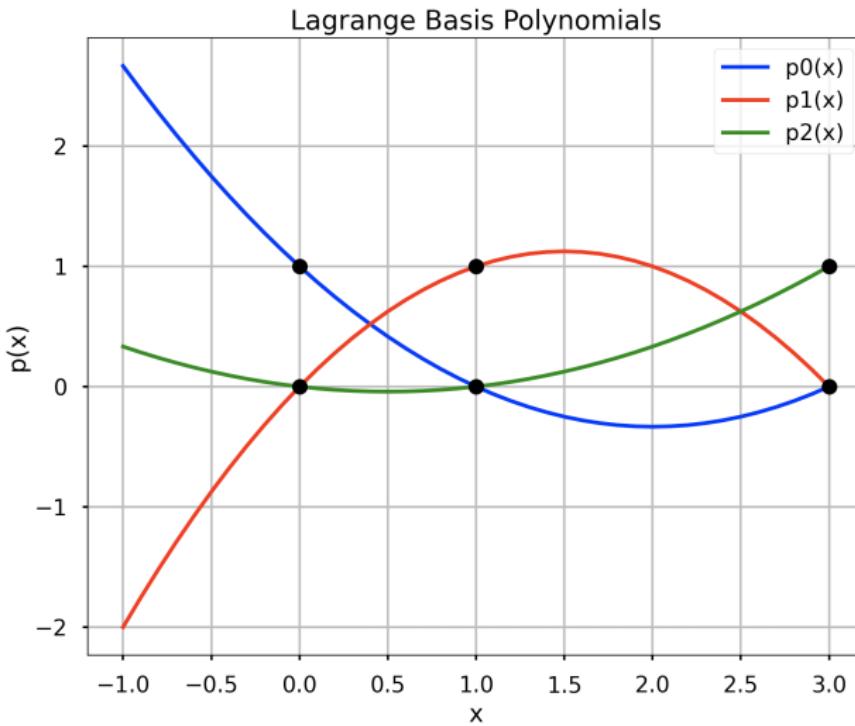
$$p_2(x) = \frac{(x - 0)(x - 1)}{(3 - 0)(3 - 1)} = \left[ \frac{x^2 - x}{6} \right]. \quad (17)$$

Plugging equations (15) - (17) into (14):

$$\begin{aligned} f(x) &= f(x_0)p_0(x) + f(x_1)p_1(x) + f(x_2)p_2(x) \\ &= 1 \cdot \left[ \frac{x^2 - 4x + 3}{3} \right] + 0 \cdot \left[ \frac{x^2 - 4x + 3}{2} \right] + 10 \cdot \left[ \frac{x^2 - x}{6} \right], \\ &= 1 - 3x + 2x^2. \end{aligned}$$

**Validate:**  $f(0) = 1$ ;  $f(1) = 0$ ;  $f(3) = 1 - 9 + 18 = 10$ .

# Lagrange Interpolation



# Lagrange Interpolation

**Example 2.** For the set of data,

x	-1	2	4	5	6
-----* -----</td <td data-kind="ghost"></td> <td data-kind="ghost"></td> <td data-kind="ghost"></td> <td data-kind="ghost"></td> <td data-kind="ghost"></td>					
f(x)	2	7	10	3	0

use the Lagrange interpolation formula to approximate the functional value at  $x = 3.5$

**Solution.** For the given dataset,

$$f(x) = 2p_0(x) + 7p_1(x) + 10p_2(x) + 3p_3(x), \quad (18)$$

where

$$\begin{aligned} p_0(x) &= \frac{(x - 2)(x - 4)(x - 5)(x - 6)}{(-1 - 2)(-1 - 4)(-1 - 5)(-1 - 6)} \\ &= (x - 2)(x - 4)(x - 5)(x - 6)/(630). \end{aligned}$$

# Lagrange Interpolation

Similarly,

$$p_1(x) = (x + 1)(x - 4)(x - 5)(x - 6)/(-72). \quad (19)$$

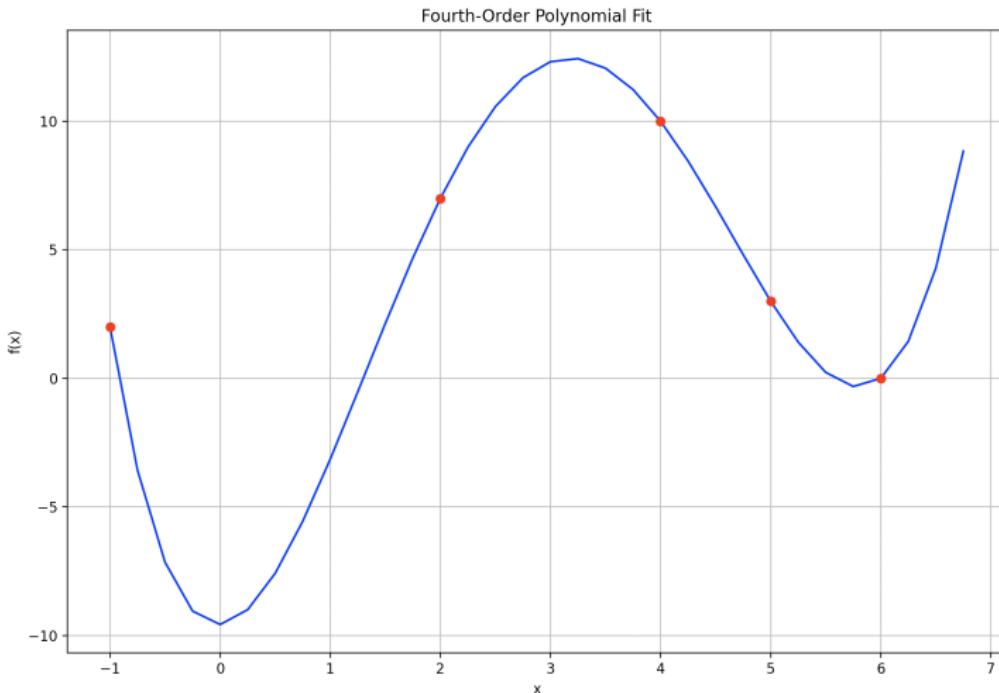
$$p_2(x) = (x + 1)(x - 2)(x - 5)(x - 6)/(20). \quad (20)$$

$$p_3(x) = (x + 1)(x - 2)(x - 4)(x - 6)/(-18). \quad (21)$$

**Let  $x = 3.5$ .**  $p_0(3.5) = (3.5 - 2)(3.5 - 4)(3.5 - 5)(3.5 - 6)/630 = -2.81/630$ . Similarly,  $p_1(3.5) = -8.43/-72$ ,  $p_2(3.5) = 25.31/20$  and  $p_3(3.5) = 8.43/-18$ . Hence,

$$f(3.5) = 2p_0(3.5) + 7p_1(3.5) + 10p_2(3.5) + 3p_3(3.5) = 12.06. \quad (22)$$

# Lagrange Interpolation



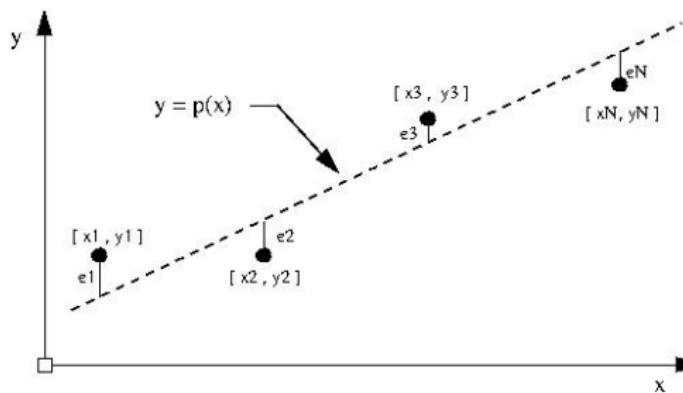
# Least Squares Analysis

# Least Squares Analysis

## Least Squares Analysis

Given a set of data points, least squares analysis is a numerical procedures for finding a best fit curve.

**Mathematical Approach.** Minimize the sum of the squares of the residuals between the data and data provided by the fitted model.



# Least Squares Analysis

**Least Squares Data:**  $(x_0, y_0), (x_1, y_1), (x_2, y_2), \dots, (x_n, y_n)$ .

## Mathematical Procedure:

- Let  $e_i = y_i - p(x_i)$ .
- We aim to determine the curve fit parameters that minimize:

$$S = \sum_{i=0}^n e_i^2 = \sum_{i=0}^n [y_i - p(x_i)]^2. \quad (23)$$

- Mean square error (MSE) =  $\left[\frac{S}{n}\right]$ .

## Practical Considerations:

- What sort of function,  $p(x)$ , do we want to fit? Linear?  
Quadratic? Exponential? Sinusoidal? Which function provides  
the best fit?

# Least Squares Analysis

**Model 1.** Linear Approximation to the Data:

Let:  $p(x) = a_0 + a_1x$ . The sum of the squares:

$$S(a_0, a_1) = \sum_{i=0}^n e_i^2 = \sum_{i=0}^n [y_i - a_0 - a_1 x_i]^2. \quad (24)$$

has a minimum value when:

$$\frac{\partial S}{\partial a_0} = 0. \rightarrow \left( \sum_{i=0}^n x_i \right) a_0 + \left( \sum_{i=0}^n 1 \right) a_1 = \left( \sum_{i=0}^n y_i \right). \quad (25)$$

$$\frac{\partial S}{\partial a_1} = 0 \rightarrow \left( \sum_{i=0}^n x_i \right) a_0 + \left( \sum_{i=0}^n x_i^2 \right) a_1 = \left( \sum_{i=0}^n x_i y_i \right). \quad (26)$$

# Least Squares Analysis

Writing equations 25 and 26 in matrix form:

$$\begin{bmatrix} n & \sum_{i=0}^n x_i \\ \sum_{i=0}^n x_i & \sum_{i=0}^n x_i^2 \end{bmatrix} \cdot \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} = \begin{bmatrix} \sum_{i=0}^n y_i \\ \sum_{i=0}^n x_i y_i \end{bmatrix} \quad (27)$$

# Least Squares Analysis

**Model 2.** Quadratic Approximation to the Data:

Let:  $p(x) = a_0 + a_1x + a_2x^2$ . The sum of the squares:

$$S(a_0, a_1, a_2) = \sum_{i=0}^n e_i^2 = \sum_{i=0}^n [y_i - a_0 - a_1x - a_2x^2]^2. \quad (28)$$

has a minimum value when:

$$\frac{\partial S}{\partial a_0} = \frac{\partial S}{\partial a_1} = \frac{\partial S}{\partial a_2} = 0. \quad (29)$$

The individual equations are:

$$\left( \sum_{i=0}^n \right) a_0 + \left( \sum_{i=0}^n x_i \right) a_1 + \left( \sum_{i=0}^n x_i^2 \right) a_2 = \left( \sum_{i=0}^n y_i \right). \quad (30)$$

# Least Squares Analysis

$$\left( \sum_{i=0}^n x_i \right) a_0 + \left( \sum_{i=0}^n x_i^2 \right) a_1 + \left( \sum_{i=0}^n x_i^3 \right) a_2 = \left( \sum_{i=0}^n x_i y_i \right). \quad (31)$$

$$\left( \sum_{i=0}^n x_i^2 \right) a_0 + \left( \sum_{i=0}^n x_i^3 \right) a_1 + \left( \sum_{i=0}^n x_i^4 \right) a_2 = \left( \sum_{i=0}^n x_i^2 y_i \right). \quad (32)$$

Writing equations 30 and 32 in matrix form:

$$\begin{bmatrix} n & \sum_{i=0}^n x_i & \sum_{i=0}^n x_i^2 \\ \sum_{i=0}^n x_i & \sum_{i=0}^n x_i^2 & \sum_{i=0}^n x_i^3 \\ \sum_{i=0}^n x_i^2 & \sum_{i=0}^n x_i^3 & \sum_{i=0}^n x_i^4 \end{bmatrix} \cdot \begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \sum_{i=0}^n y_i \\ \sum_{i=0}^n x_i y_i \\ \sum_{i=0}^n x_i^2 y_i \end{bmatrix} \quad (33)$$

# Least Squares Analysis

**Example 1.** Find linear and quadratic least squares approximations to the set of data:

x		0	3	6
-----*-----				
f(x)		1	2	0

find linear and quadratic least squares approximations.

**Note:** Because there are only three data points, we expect that the quadratic model will interpolate the data exactly.

## Abbreviated Output:

Matrix: data array

0.0000000e+00	1.0000000e+00
3.0000000e+00	2.0000000e+00
6.0000000e+00	1.0000000e+00

# Least Squares Analysis

## Abbreviated Output: Continued ...

--- Part 1: Linear least squares fit ...

---

Matrix: A1

3.0000000e+00	9.0000000e+00
9.0000000e+00	4.5000000e+01

Matrix: B1

4.0000000e+00
1.2000000e+01

--- Least squares coefficients and polynomial ...

Matrix: Coeff ----->  $p(x) = 1.333333333333333 + 0.0 \cdot x^1$

1.3333333e+00
0.0000000e+00

--- Mean square error = 0.222 ...

--- Part 2: Quadratic least squares fit ...

---

Matrix: A2

3.0000000e+00	9.0000000e+00	4.5000000e+01
---------------	---------------	---------------

# Least Squares Analysis

**Abbreviated Output:** Continued ...

9.0000000e+00	4.5000000e+01	2.4300000e+02
4.5000000e+01	2.4300000e+02	1.3770000e+03

Matrix: B2

4.0000000e+00
1.2000000e+01
5.4000000e+01

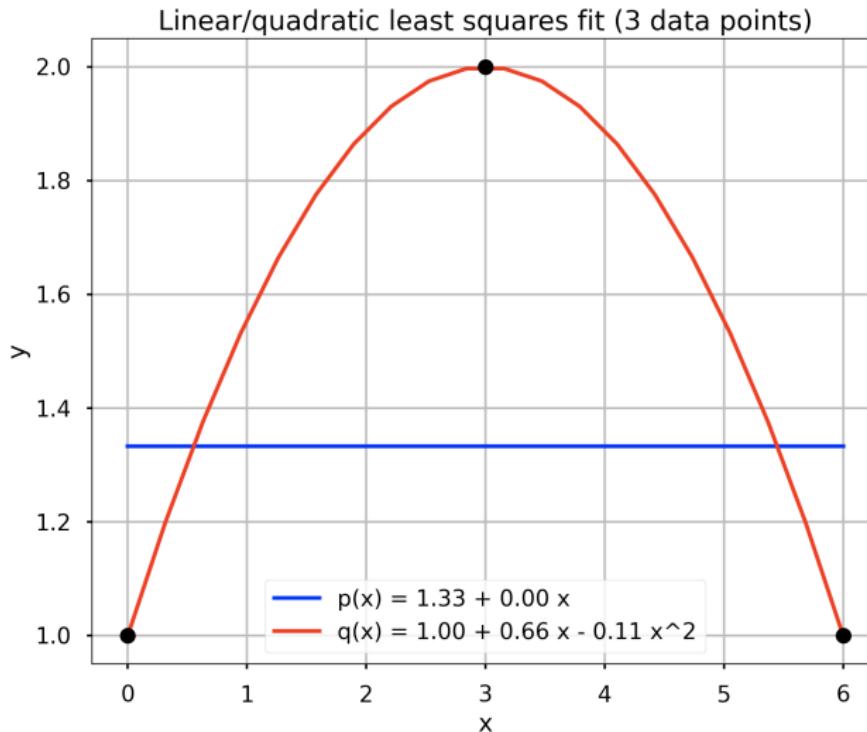
--- Least squares coefficients and polynomial ...

Matrix: Coeff

1.0000000e+00	---> $q(x) = 1.000 + 0.667 \cdot x^1 - 0.111 \cdot x^2$
6.6666667e-01	
-1.1111111e-01	

--- Mean square error = 0.000 ...

# Least Squares Analysis



# Least Squares Analysis

**Example 2.** Find linear and quadratic least squares approximations to the set of data:

x		0	1	2	3	4	5	6	7	8	9	10
<hr/>												
f(x)		0	1	2	3	4	5	6	6	6	6	6

## Abbreviated Output:

Matrix: data array

0.0000000e+00	0.0000000e+00
1.0000000e+00	1.0000000e+00
2.0000000e+00	2.0000000e+00
....	....
8.0000000e+00	6.0000000e+00
9.0000000e+00	6.0000000e+00
1.0000000e+01	6.0000000e+00

# Least Squares Analysis

## Abbreviated Output: Continued ...

--- Part 1: Linear least squares fit ...

---

Matrix: A1

1.1000000e+01	5.5000000e+01
5.5000000e+01	3.8500000e+02

Matrix: B1

4.5000000e+01
2.9500000e+02

--- Least squares coefficients and polynomial ...

Matrix: Coeff      --->  $p(x) = 0.909 + 0.636 \cdot x^1$

9.0909091e-01
6.3636364e-01

--- Mean square error = 0.579 ...

--- Part 2: Quadratic least squares fit ...

---

Matrix: A2

1.1000000e+01	5.5000000e+01	3.8500000e+02
---------------	---------------	---------------

# Least Squares Analysis

**Abbreviated Output:** Continued ...

```
5.5000000e+01    3.8500000e+02    3.0250000e+03  
3.8500000e+02    3.0250000e+03    2.5333000e+04
```

Matrix: B2

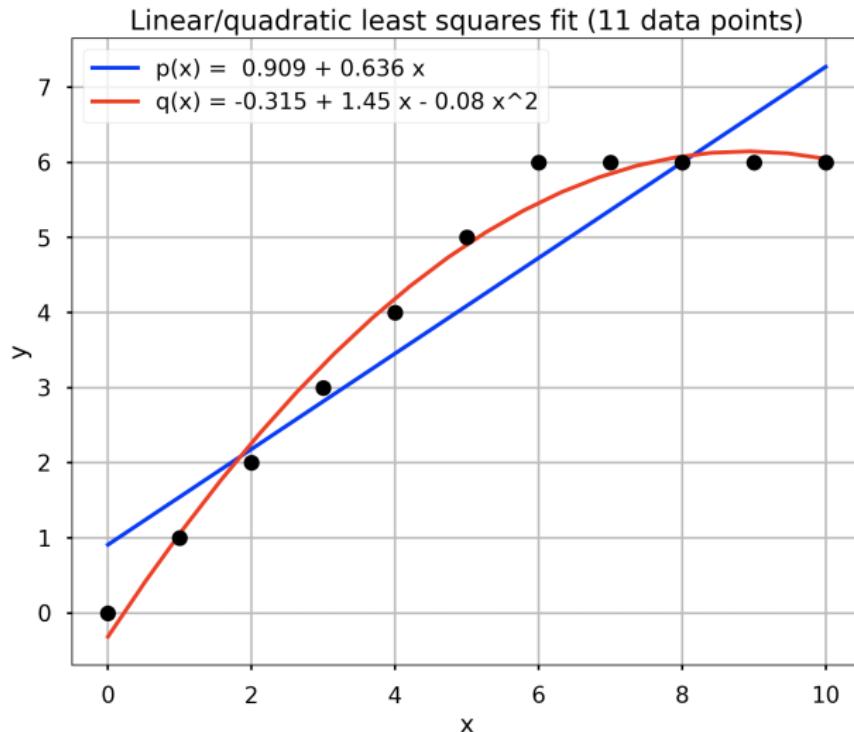
```
4.5000000e+01  
2.9500000e+02  
2.2050000e+03
```

--- Least squares coefficients and polynomial ...

Matrix: Coeff ---> q(x) = -0.314 + 1.452·x<sup>1</sup> - 0.081·x<sup>2</sup>  
-3.1468531e-01  
1.4522145e+00  
-8.1585082e-02

--- Mean square error = 0.059 ... <-- Much better !!!

# Least Squares Analysis



# Python Code Listings

# Code 1: Method of Divided Differences

```
1 # =====
2 # Interpolation.py: Functions to compute interpolation polynomial fits ...
3 # =====
4
5 import math
6 import numpy as np
7
8 # =====
9 # LinearMatrixEquations.printmatrix(): Print two-dimensional matrices.
10 #
11 # Args: name: string description of matrix.
12 #       A (nxn) matrix.
13 #
14 # Returns: void.
15 # =====
16
17 def printmatrix(name, a):
18     print("");
19     print("Matrix: {:s} ".format(name));
20     for row in a:
21         for col in row:
22             print("{:8.4f}".format(col), end=" ")
23     print("")
24
25 # =====
26 # Interpolation.divideddifference(): Compute Newton's divided difference table ..
27 #
28 # Args: x (float): array of x coordinates.
```

# Code 1: Method of Divided Differences

```
29     #           y (float): array of y values.
30 #
31 # Returns:
32 #         dtable (float): divided difference matrix/table.
33 # =====
34
35 def divideddifference(x, y):
36
37     # Create divided difference table ...
38
39     n = len(y)
40     dtable = np.zeros([n, n])
41
42     # First column of table is y ...
43
44     dtable[:,0] = y
45     for j in range(1,n):
46         for i in range(n-j):
47             dtable[i][j] = (dtable[i+1][j-1] - dtable[i][j-1]) / (x[i+j]-x[i])
48
49     # Print divided difference table ...
50
51     printmatrix("divided difference table", dtable);
52
53     return dtable
54
55 # =====
56 # Interpolation.newtonpolynomial(): Evaluate Newton's polynomial at x.
57 #
58 # Args: dtable (float): divided difference matrix / table.
```

# Code 1: Method of Divided Differences

```
59  #           y (float): array of y values.
60  #           x_data (float): array of x_data points.
61  #
62  # Returns:
63  #           p (float): value of newtons polynomial evaluated at x.
64  # =====
65
66 def newtonpolynomial( dtable, x_data, x):
67     n = len(x_data) - 1
68     p = dtable[n]
69     for k in range(1,n+1):
70         p = dtable[n-k] + (x -x_data[n-k])*p
71     return p
```

## Code 2: Lagrange Interpolation

```
1 # =====
2 # Interpolation.py: Functions to compute interpolation polynomial fits ...
3 # =====
4
5 import math
6 import numpy as np
7
8 # =====
9 # Interpolation.lagrange(): Compute Lagrange polynomial through the
10 # points (x, y) and return its value at t.
11 #
12 # Args: x (float): array of x values ...
13 #       y (float): array of y values ...
14 #       t (float): evaluate polynomial at point t.
15 #
16 # Returns:
17 #       t (float): polynomial value evaluated at point t.
18 # =====
19
20 def lagrange(x, y, t):
21
22     # Check that the input arrays have the same length
23
24     if len(x) != len(y):
25         raise ValueError("The arrays x and y must have the same length.")
26
27     # Initialize the polynomial
```

## Code 2: Lagrange Interpolation

```
29     p = 0
30
31     # Loop over the points
32
33     for i in range(len(x)):
34
35         # Get the current point
36         xi, yi = x[i], y[i]
37
38         # Initialize the term
39         term = yi
40
41         # Loop over the other points
42         for j in range(len(x)):
43             # Skip the current point
44             if i == j:
45                 continue
46
47             # Multiply the term by the appropriate factor
48             term *= (t - x[j]) / (xi - x[j])
49
50         # Add the term to the polynomial
51         p += term
52
53     return p
```

# Code 3: Lagrange Basis Polynomials

```
1 # =====
2 # TestInterpolationLagrange02.py: Work with Lagrange basis polynomials ...
3 #
4 # Written By: Mark Austin
5 # =====
6
7 import math;
8
9 import numpy as np
10 import numpy.polynomial.polynomial as poly
11 import matplotlib.pyplot as plt
12
13 plt.style.use('seaborn-poster')
14
15 def main():
16     print("--- Case Study 1. Interpolation.lagrange() ... ");
17
18     x = [0, 1, 3]
19     y = [1, 0, 10]
20
21     print("--- Create arrays of basis function coefficients ... ");
22
23     P0_coeff = [ 1, -4.0/3.0, 1.0/3.0 ]
24     P1_coeff = [ 0, 1.5, -0.5 ]
25     P2_coeff = [ 0, -1.0/6.0, 1.0/6.0 ]
26
27     # Get the polynomial function
```

## Code 3: Lagrange Basis Polynomials

```
29     print(" --- Create and print polynomials ... ");
30
31     P0 = poly.Polynomial( P0_coeff )
32     P1 = poly.Polynomial( P1_coeff )
33     P2 = poly.Polynomial( P2_coeff )
34
35     np.polynomial.set_default_printstyle('ascii')
36
37     print(" --- Create array of x values for plotting ... ");
38
39     x_new = np.arange(-1.0, 3.1, 0.1)
40
41     print(" --- Plot Lagrange polynomials ... ");
42
43     fig = plt.figure(figsize = (10,8))
44     plt.plot( x_new, P0(x_new), 'b', label = 'p0(x)')
45     plt.plot( x_new, P1(x_new), 'r', label = 'p1(x)')
46     plt.plot( x_new, P2(x_new), 'g', label = 'p2(x)')
47
48     plt.plot(x, np.ones(len(x)), 'ko', x, np.zeros(len(x)), 'ko')
49     plt.title('Lagrange Basis Polynomials')
50     plt.xlabel('x')
51     plt.ylabel('p(x)')
52     plt.grid()
53     plt.legend()
54     plt.show()
55
56 # call the main method ...
57
58 main()
```

# Code 4: Least Squares Analysis

```
1 # =====
2 # TestLeastSquares01.py: Compute least squares analysis for linear and quadratic
3 # fits to test data.
4 # =====
5
6 import math
7 import numpy as np
8 import numpy.polynomial.polynomial as poly
9 import matplotlib.pyplot as plt
10
11 import LinearMatrixEquations as lme
12
13 plt.style.use('seaborn-poster')
14
15 def main():
16     print(" --- Enter TestLeastSquares01.main()           ... ");
17     print(" --- ===== ... ");
18
19     print(" --- Step 1: Create (x,y) data array ... ");
20
21     data = np.array([ [ 0, 1], [ 3, 2], [ 6, 1] ]);
22
23     lme.printmatrix("data array", data );
24
25     print(" --- Step 2: Extract x and y arrays from data array ... ");
26
27     x = data [:,0];
28     y = data [:,1];
```

# Code 4: Least Squares Analysis

```
29
30     lme.printvector("x", x);
31     lme.printvector("y", y);
32
33     print(" --- Part 1: Linear least squares fit ... ");
34     print(" --- ----- ... ");
35
36     n      = len(x);      # <-- number of data points ....
37
38     a11 = n;           a12 = sum(x);
39     a21 = sum(x);       a22 = np.dot(x,x)
40     b11 = sum(y)
41     b21 = np.dot(x,y)
42
43     A1 = np.array([ [ a11, a12 ], [ a21, a22 ] ]);
44     B1 = np.array([ [ b11 ], [ b21 ] ]);
45
46     lme.printmatrix("A1", A1);
47     lme.printmatrix("B1", B1);
48
49     print(" --- Step 4: Compute least squares coefficients ... ");
50
51     coeff = lme.solvesystem( A1, B1);
52     lme.printmatrix("Coeff", coeff );
53
54     print(" --- Step 5: Create and print polynomials ...");
55
56     p_coeff = [ coeff[0][0], coeff[1][0] ]
57     p = poly.Polynomial( p_coeff )
58     print (p)
```

# Code 4: Least Squares Analysis

```
59
60     print(" --- Step 6: Compute mean square error ...");
61
62     yfit = p(x)
63     print( y - yfit )
64     mse = np.dot(y - yfit, y- yfit)/len(y)
65
66     print(" --- Mean square error = {:.3f} ...".format(mse))
67
68     print(" --- Part 2: Quadratic least squares fit ... ");
69     print(" --- ----- ... ");
70
71     n      = len(x);           # <-- number of data points ...
72     a11 = n;                  a12 = sum(x);
73     a21 = sum(x);            a22 = np.dot(x,x)
74     a31 = np.dot(x,x)
75
76     b11 = sum(y)
77     b21 = np.dot(x,y)
78
79     # manually assemble array coefficients ...
80
81     a23 = 0; a32 = 0; a33 = 0
82     b31 = 0;
83     i = 0
84     while i < n:
85         xi = x[i]
86         yi = y[i]
87         a32 = a32 + xi**3
```

# Code 4: Least Squares Analysis

```
88         a33 = a33 + xi**4
89         b31 = b31 + xi*xi*yi
90         i = i + 1
91
92     a13 = np.dot(x,x)
93     a23 = a32
94
95     A2 = np.array([ [ a11, a12, a13 ],
96                     [ a21, a22, a23 ],
97                     [ a31, a32, a33 ] ]);
98
99     B2 = np.array([ [ b11 ], [ b21 ], [ b31 ] ]);
100
101    lme.printmatrix("A2", A2);
102    lme.printmatrix("B2", B2);
103
104    print(" --- Step 8: Compute least squares coefficients ... ");
105
106    coeff = lme.solvesystem( A2, B2);
107    lme.printmatrix("Coeff", coeff );
108
109    print(" --- Step 9: Create and print polynomials ...");
110
111    q_coeff = [ coeff[0][0], coeff[1][0], coeff[2][0] ]
112    q = poly.Polynomial( q_coeff )
113    print (q)
114
115    print(" --- Step 10: Compute mean square error ...");
```

# Code 4: Least Squares Analysis

```
116
117     yfit = q(x)
118     print( y - yfit )
119     mse  = np.dot(y - yfit, y- yfit)/len(y)
120
121    print("--- Mean square error = {:.3f} ...".format(mse))
122
123    print("--- Step 11: Graph data and least squares fit equations ... ");
124    print("--- ----- ... ");
125
126    x_new = np.linspace(0.0, 6.0, num=20)
127
128    fig = plt.figure(figsize = (10,8))
129    plt.plot(x_new, p(x_new), 'b', label = 'p(x) = 1.33 + 0.00 x')
130    plt.plot(x_new, q(x_new), 'r', label = 'q(x) = 1.00 + 0.66 x - 0.11 x^2')
131    plt.plot(x, y, 'ko')
132    plt.title('Linear/quadratic least squares fit (3 data points)')
133    plt.xlabel('x')
134    plt.ylabel('y')
135    plt.grid()
136    plt.legend()
137    plt.show()
138
139    print("--- ===== ... ");
140    print("--- Leave TestLeastSquares01.main() ... ");
141
142 # call the main method ...
143
144 main()
```