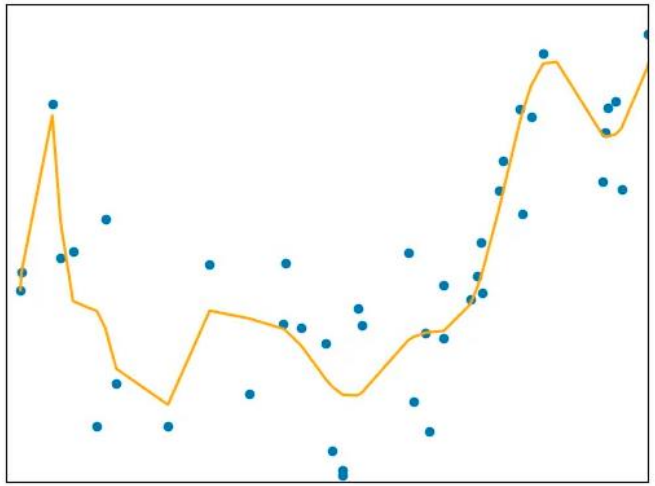
Polynomial regression

Polynomial regression

- Linear regression requires the relation between the dependent variable and the independent variable to be linear.
- What if the distribution of the data was more complex as shown in the below figure?
- Can linear models be used to fit non-linear data?
- How can we generate a curve that best captures the data as shown below?

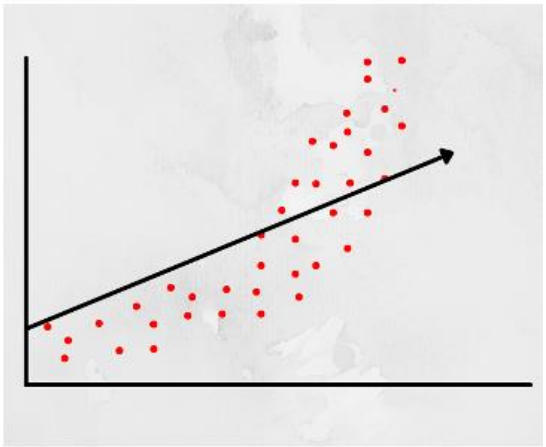


A polynomial regression model takes the following form:

$Y = \beta 0 + \beta 1X + \beta 2X^2 + \ldots + \beta hX^n + \varepsilon$

In this equation, n is the degree of the polynomial.

- A simple linear regression algorithm only works when the relationship between the data is linear.
- But suppose we have non-linear data, then linear regression will not be able to draw a best-fit line.
- Simple regression analysis fails in such conditions.
- Consider the below diagram, which has a non-linear relationship
- See the linear regression does not perform well
- Hence, we introduce polynomial regression to overcome this problem, which helps identify the curvilinear relationship between independent and dependent variables.



Polynomial regression

What is Polynomial Regression?

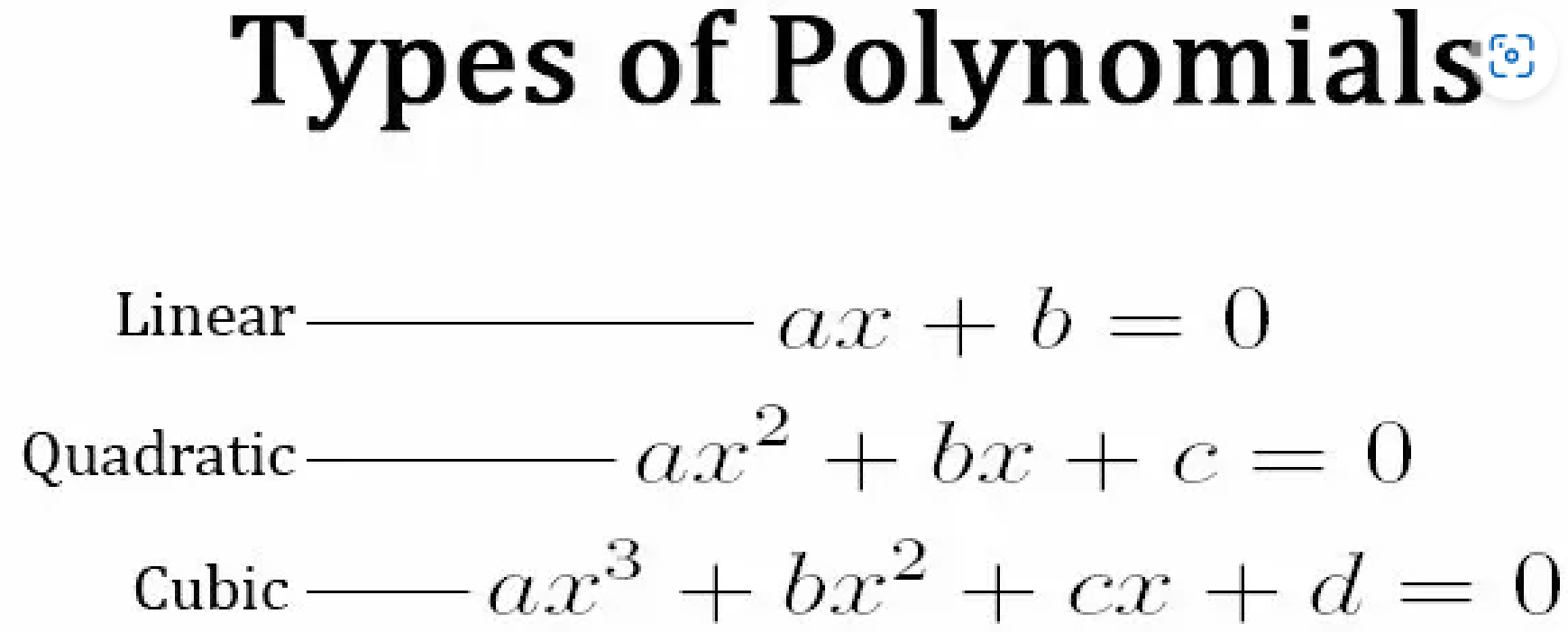
- Polynomial Regression is a form of *regression analysis in which the relationship between the independent variables and dependent variables are modeled in the nth degree polynomial.*

- Polynomial Regression models are usually fit with the method of **least squares**. The least square method **minimizes the variance of the coefficients**, under the Gauss Markov Theorem.

- Polynomial Regression is a special case of Linear Regression where we *fit the polynomial equation on the data with a curvilinear relationship between the dependent and independent variables*.

- A Quadratic Equation is a Polynomial Equation of 2nd Degree. However, this degree can increase to nth values.

Polynomial regression



- In polynomial regression, the relationship between the dependent variable and the independent variable is modeled as an nth-degree polynomial function.
- When the polynomial is of degree 2, it is called a quadratic model;
- when the degree of a polynomial is 3, it is called a cubic model

Polynomial regression

Assumptions of Polynomial Regression:

•The behavior of a dependent variable can be explained by a linear, or curvilinear, additive relationship between the dependent variable and a set of *k* independent variables *(xi, i=1 to k).*

•The relationship between the dependent variable and any independent variable is linear or curvilinear (specifically polynomial).

•The independent variables are independent of each other.

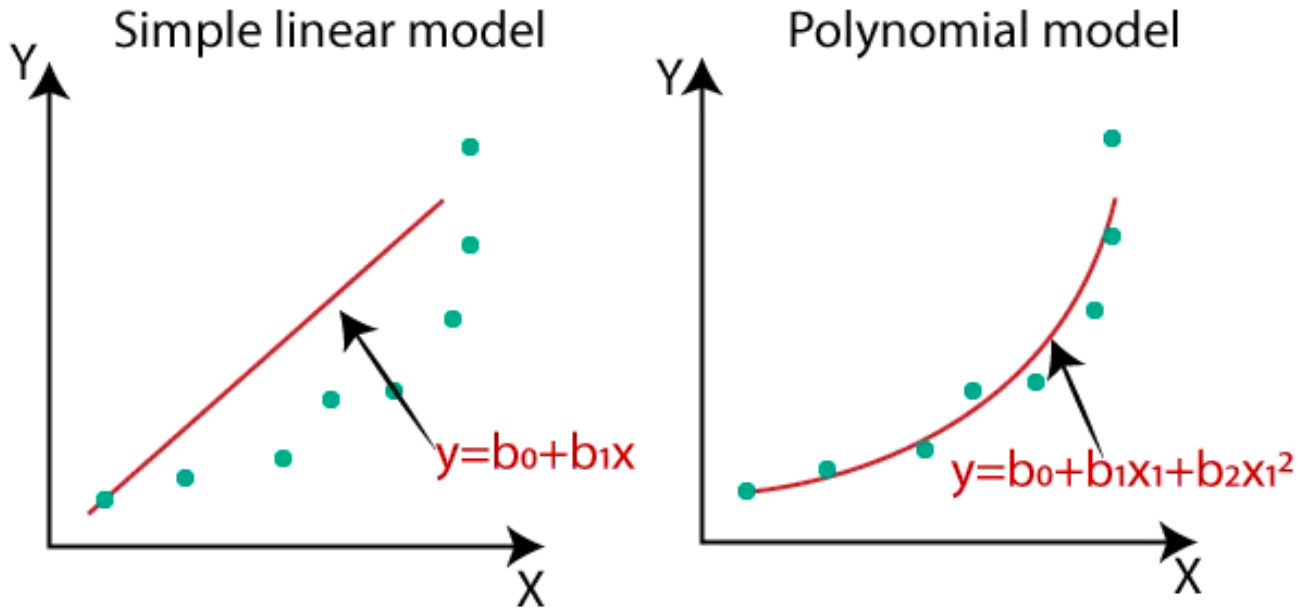
•The errors are independent, normally distributed with mean zero and a constant variance (*OLS*).

Polynomial regression

Why do we need Polynomial Regression?

Let's consider a case of ***Simple Linear Regression***.

- We make our model and find out that it performs very badly,
- We observe between the actual value and the best fit line, which we predicted and it seems that the actual value has some kind of curve in the graph and our line is no where near to cutting the mean of the points.
- This where polynomial Regression comes to the play, it predicts the best fit line that follows the pattern(curve) of the data, as shown in the pic below:



When to Use Polynomial Regression

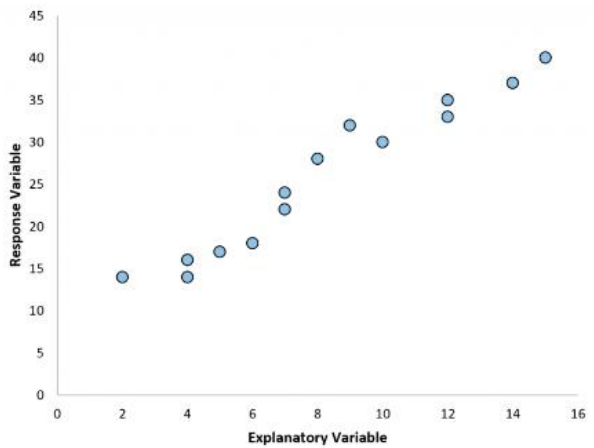
Use polynomial regression when the relationship between a predictor and response variable is nonlinear.

Way to detect a nonlinear relationship:

1. Create a Scatterplot.

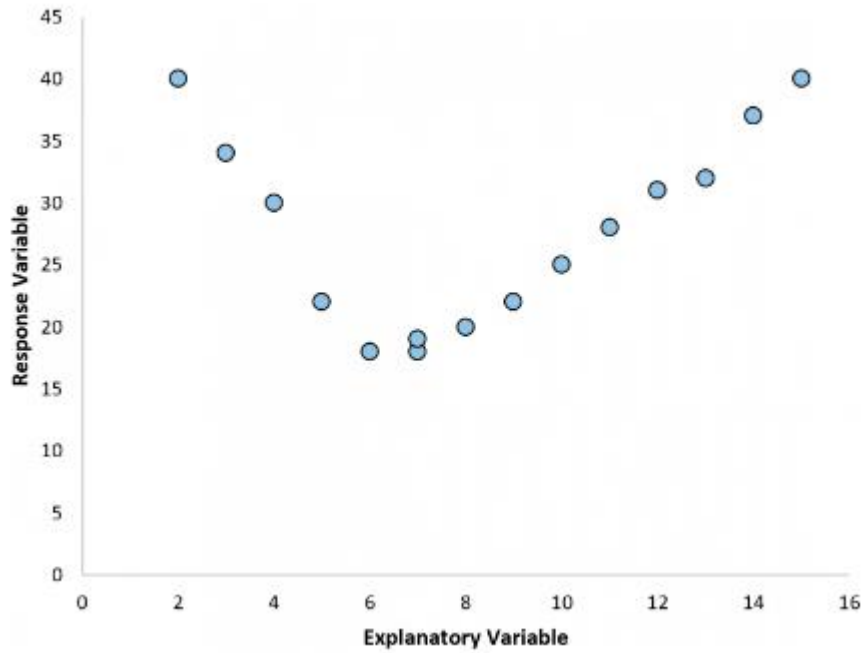
The easiest way to detect a nonlinear relationship is to create a scatterplot of the response vs. predictor variable.

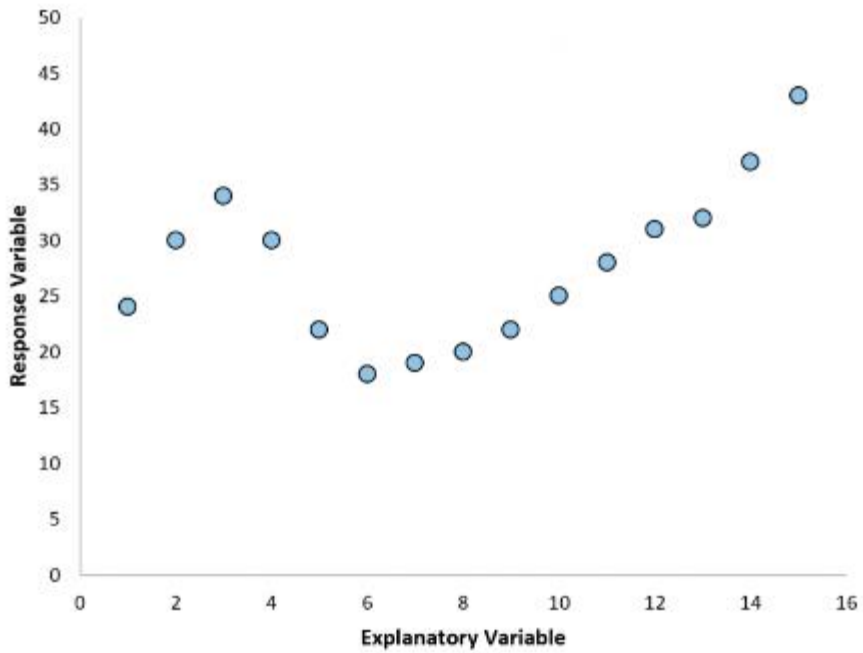
Ex1: In the following scatterplot we can see that the relationship between the two variables is roughly linear, thus simple linear regression would likely perform fine on this data.



When to Use Polynomial Regression

Ex2: In the following scatterplot we can see that the relationship between the two variables is nonlinear and thus polynomial regression would be a good idea

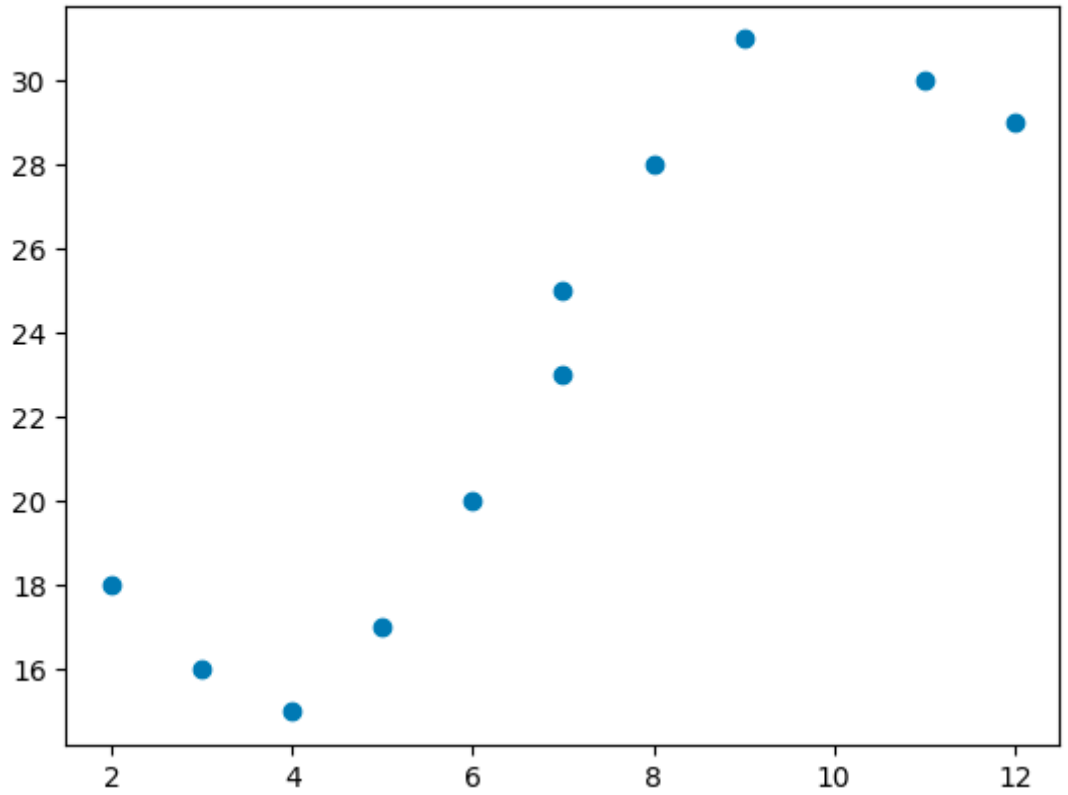




When to Use Polynomial Regression - Example

```
import matplotlib.pyplot as plt
x = [2, 3, 4, 5, 6, 7, 7, 8, 9, 11, 12]
y = [18, 16, 15, 17, 20, 23, 25, 28, 31, 30, 29]
plt.scatter(x, y) # #create scatterplot
```

```
[9]: <matplotlib.collections.PathCollection at 0x26f54dbd690>
```



Polynomial regression

- Polynomial Regression *does not require the relationship between the independent and dependent variables to be linear in the data set*, This is also one of the main difference between the Linear and Polynomial Regression.

- **Polynomial Regression is generally used when the points in the data are not captured by the Linear Regression Model and the Linear Regression fails in describing the best result clearly**.

As we increase the degree in the model, it tends to increase the performance of the model. However, increasing the degrees of the model also increases the risk of over-fitting and under-fitting the data.

- using a high degree of polynomial tries to overfit the data
- and for smaller values of degree, the model tries to underfit
- so we need to find the optimum value of a degree

Polynomial regression

How to find the right degree of the equation?

In order to find the right degree for the model to prevent over-fitting or under-fitting, we can use:

1.Forward Selection:

This method increases the degree until it is significant enough to define the best possible model.

2.Backward Selection:

This method decreases the degree until it is significant enough to define the best possible model.

Polynomial regression

Let there be only one independent variable x and the relationship between x, and dependent variable y, be modeled as,

$y=a0+a1*x+a2*x^2+\ldots\ldots\ldots+an*x^n$

for some positive integer n >1, then we have a polynomial regression.

Problem Definition:

Find a quadratic regression model for the following data:

X	Y
3	2.5
4	3.2
5	3.8
6	6.5
7	11.5

First, draw a scatter plot and check whether the relationship between x and y is non-linear.

Polynomial regression

Solution:

Let the quadratic polynomial regression model be

$y=a0+a1*x+a2*x^2$

The values of a0, a1, and a2 are calculated using the following system of equations:

n- is number of data points, here it is 5.

$$\sum y_i = na_0 + a_1\left(\sum x_i\right) + a_2\left(\sum x_i^2\right)$$

$$\sum y_i x_i = a_0\left(\sum x_i\right) + a_1\left(\sum x_i^2\right) + a_2\left(\sum x_i^3\right)$$

$$\sum y_i x_i^2 = a_0\left(\sum x_i^2\right) + a_1\left(\sum x_i^3\right) + a_2\left(\sum x_i^4\right)$$

Polynomial regression

First, we calculate the required variables and note them in the following table.

	x	y	x^2	x^3	x^4	y*x	$y*x^2$
	3	2.5	9	27	81	7.5	22.5
	4	3.2	16	64	256	12.8	51.2
	5	3.8	25	125	625	19	95
	6	6.5	36	216	1296	39	234
	7	12	49	343	2401	80.5	563.5
Σ	25	27.5	135	775	4659	158.8	966.2

Using the given data,

$$27.5 = 5a_0 + 25a_1 + 135a_2$$

$$158.8 = 25a_0 + 135a_1 + 775a_2$$

$$966.2 = 135a_0 + 775a_1 + 4659a_2$$

Solving Systems of Linear Equations Using Matrices

The three equations could be represented in matrix form AX = B

Matrix A is 3x3 below:

5	25	135	= 27.5
25	135	775	=158.8
135	775	4659	=966.2

Matrix X is 3 x 1 below:

ao
a1
a2

Matrix B is 3 x 1 below:

27.5
158.8
966.2

Find $X = A^{-1}B$

Solving Systems of Linear Equations Using Matrices

Find $X = A^{-1}B$

Inverse of 3*3 matrix = A1

40.485714285714286524	-16.928571428571428891	1.64285714285714289
-16.928571428571428891	7.2428571428571430002	-0.7142857142857143
1.64285714285714289	-0.7142857142857143	0.07142857142857143

Matrix Multiplication of A1 with B

12.428571428571428882
-5.51285714285714296744
0.7642857142857143001

a0=12.4285714
a1=-5.5128571
a2=0.7642857

Polynomial regression

Solving this system of equations we get

a_0=12.4285714

a_1=-5.5128571

a_2=0.7642857

The required quadratic polynomial model is

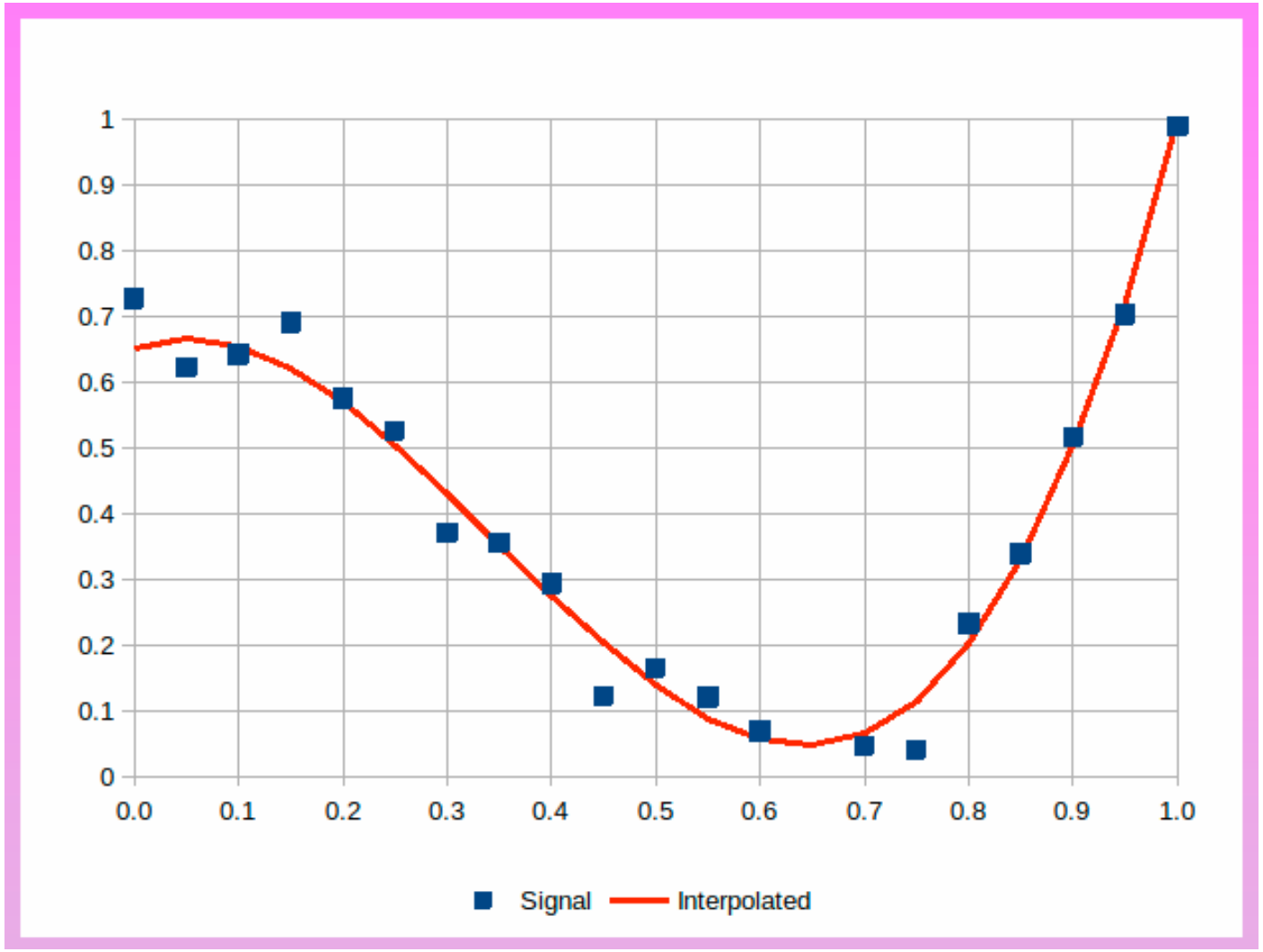
$$\mathbf{y=12.4285714 -5.5128571 * x +0.7642857 * x^2}$$

Now, given the value of x (independent variable), we can calculate the value of y (dependent or output variable).

Cost function - MSE

Polynomial regression

Simply put polynomial regression is an attempt to create a polynomial function that approximates a set of data points. This is easier to demonstrate with a visual example.

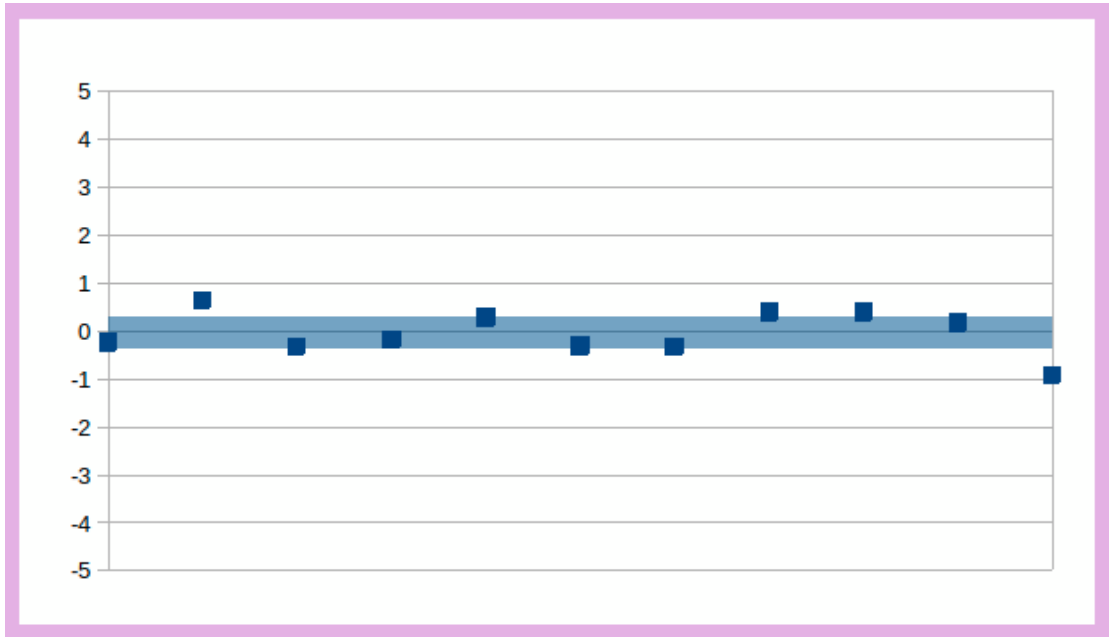


Polynomial regression

- Polynomial regression is one of several methods of **curve fitting**.
- With polynomial regression, the data is approximated using a polynomial function.
- A polynomial is a function that takes the form $f(x) = c_0 + c_1 x + c_2 x^2 \cdots c_n x^n$
  where *n* is the degree of the polynomial and *c* is a set of coefficients.

A polynomial of degree 0 is just a constant because $f(x) = c_0 x^0 = c_0$.

Likewise preforming polynomial regression with a degree of 0 on a set of data returns a single constant value. It is the same as the mean average of that data. This makes sense because the average is an approximation of all the data points.

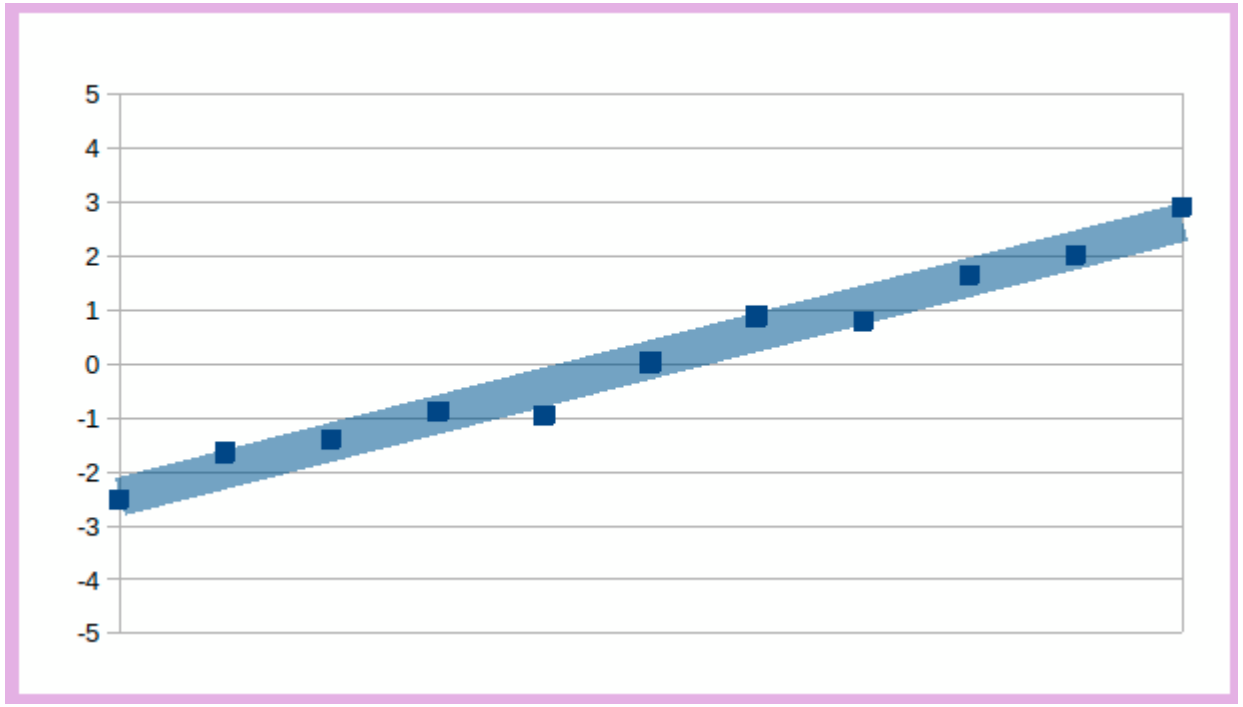


Polynomial regression

Linear regression is polynomial regression of degree 1, and generally takes the form

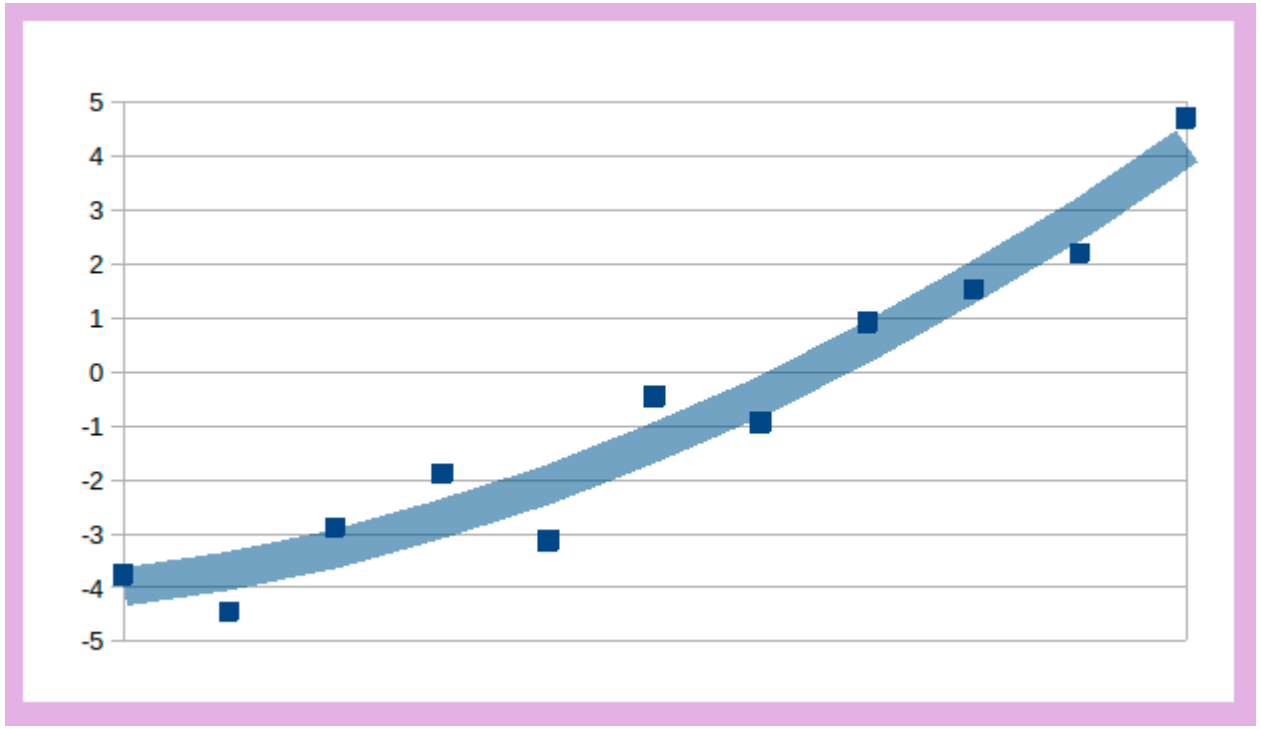
$y = m\,x + b$ where m is the slope, and b is the y-intercept.

It could just as easily by written $f(x) = c_0 + c_1\,x$ with c_1 being the slope and c_0 the y-intercept.



Polynomial regression

Quadratic regression is a 2nd degree polynomial and not nearly as common. Now the regression becomes non-linear and the data is not restricted to straight lines.



Polynomial regression

We need a way of calculating coefficients that takes all our data points into consideration. This is where least squares come in.

To preform a least square approach we need to define a **residual** function.

For any point (x_i, y_i) on the line, the residual would be:

$$r_i(x_i) = y_i - (mx_i + b)$$

Where i is the index into the set of known data points.

We can generalize it for any function:

$$r_i(x_i) = y_i - f(x_i)$$

Polynomial regression

What does the residual tell us?

Well, for each data point the *residual denotes the amount of error between our estimation and the true data*.

How about the overall error?

To get this, we could just *sum up the error for all data points*.

However error can be *positive or negative*.

So we could end up with a lot of error uniformly distributed between negative and positive values.

$$r(x) = \sum_{i=0}^{n} \left[y_i - f(x_i) \right]^2$$

So now that we have a function that measures residual, what do we do with it?

Well, if we are trying to produce a function that models a set of data, we want the residual to be as small as possible—we want to **minimize** it.

Polynomial regression

Let's try using a 2nd degree polynomial to get the results for quadratic regression.

First, the quadratic function:

$$y = c_0 + c_1 x + c_2 x^2$$

Now the sum of squares for n known data points:

$$r(x) = \sum_{i=0}^{n} (c_0 + c_1 x_i + c_2 x^2 - y_i)^2$$