Introduction to Computer Programming

Week 9.2: Curve Fitting

It can be useful to define a relationship between two variables, x and y.

We often want to 'fit' a function to a set of data points (e.g. experimental data).

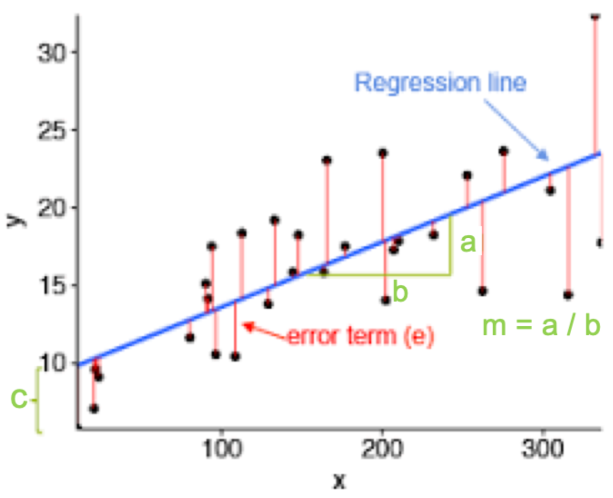
Python has several tools (e.g. Numpy and Scipy packages) for finding relationships in a set of data.

In [31]:
```
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline
```

Fitting a linear function

> ***Linear function:***
> *Has form*
> $$f(x) = mx + c$$
> *where m and c are constants.*

Linear regression calculates a **linear function** that minimizes the combined error between the fitted line and the data points.



Fitting a polynomial function

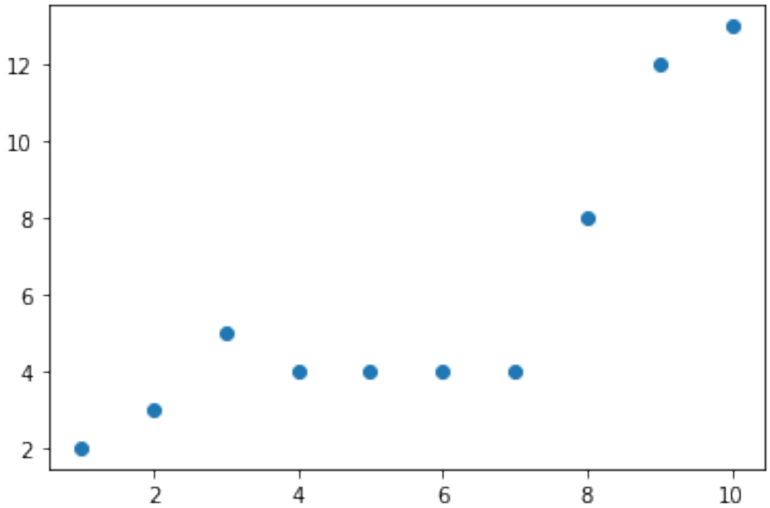
> ***Polynomial function:*** *a function involving only non-negative integer powers of x.*

1st degree polynomial $y = \mathrm{a}x^1 + \mathrm{b}x^0$
(linear function)

2nd degree polynomial $y = \mathrm{c}x^2 + \mathrm{d}x^1 + \mathrm{e}x^0$

3rd degree polynomial $y = \mathrm{f}x^3 + \mathrm{g}x^2 + \mathrm{h}x^1 + \mathrm{i}x^0$

In [32]:
```
x = np.array([1, 6, 3, 4, 10, 2, 7, 8, 9, 5])
y = np.array([2, 4, 5, 4, 13, 3, 4, 8, 12, 4])

plt.plot(x,y,'o')
plt.show()
```



Fitted function

A polynomial function can be fitted using the `numpy.polyfit` function.

Inputs:

- independent variable
- dependent variable
- degree of the polynomial

Returns:

- coefficients of each term of the polynomial.

Example 1:

Fit a first degree polynomial (linear function) to the `x,y` data.

Print the coefficients of the fitted function.

In [34]:
```
x = np.array([1, 6, 3, 4, 10, 2, 7, 8, 9, 5])
y = np.array([2, 4, 5, 4, 13, 3, 4, 8, 12, 4])

c1 = np.polyfit(x, y, 1)

print(c1)

print(c1[0], c1[1])
```

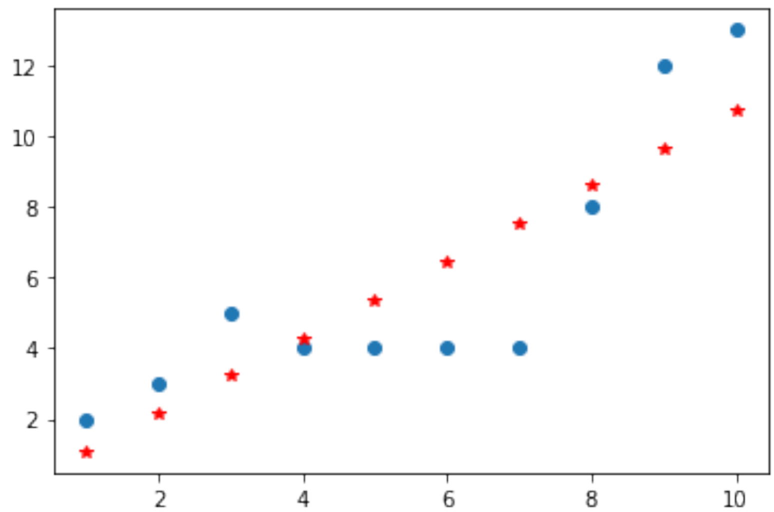
```
[ 1.07272727e+00 -5.61733355e-15]
1.0727272727272728 -5.61733354972272e-15
```

We can now plot the fitted linear function

$$y = ax^1 + bx^0$$

In [35]:
```
a, b = c1[0], c1[1]     # coefficients a and b

y_new = a*x + b         # fitted line
```

In [37]:
```
plt.plot(x,y,'o')
plt.plot(x,y_new,'r*')
plt.show()
```



Try it yourself

Example 2:

Fit a second degree polynomial to the `x,y` data.
(Remember to import numpy to use `polyfit`).

Print the coefficients of the fitted function.

In [39]:
```
x = np.array([1, 6, 3, 4, 10, 2, 7, 8, 9, 5])
y = np.array([2, 4, 5, 4, 13, 3, 4, 8, 12, 4])

c2 = np.polyfit(x, y, 2)

print(c2[0], c2[1], c2[2])
```

```
0.19318181818181812 -1.0522727272727261 4.249999999999994
```

Fitted data

As the degree increases, the code to generate the fitted line gets longer.

In [15]:
```
yfit1 = c1[0]*x + c1[1]

yfit2 = c2[0]*x**2 + c2[1]*x + c2[2]
```

Fitted data

`numpy.polyval` : generates fitted y values.

Inputs:

- coefficients of the fitted polynomial function
- x data (monotonically sorted if plotting a line graph)

Returns:

- fitted y data

Example 3:

Use `numpy.polyval` to generate x,y data of the fitted linear function.

In [40]:
```
x_new = np.array(sorted(x))

yfit1 = np.polyval(c1, x_new)
```

Try it yourself

Example 4:

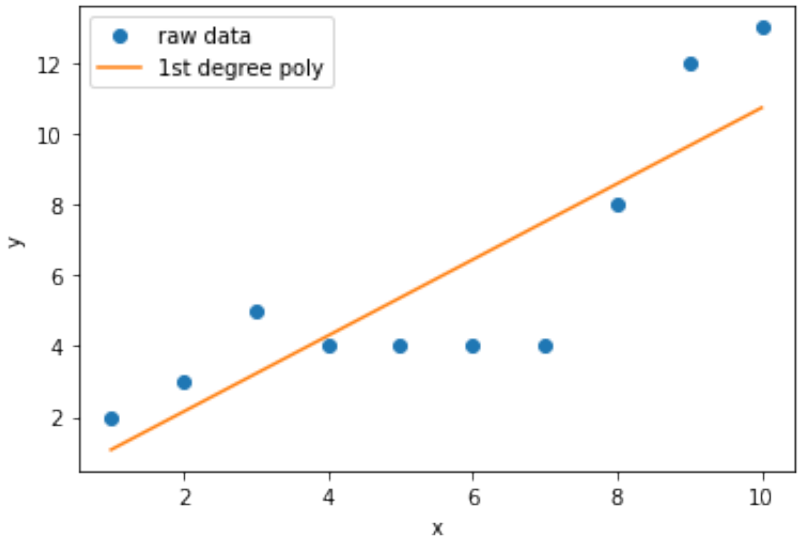
Use `numpy.polval` to generate x,y data of the fitted second degree polynomial function.

In [41]:
```
x_new = np.array(sorted(x))

yfit2 = np.polyval(c2, x_new)


```

Plotting fitted data

Example 5: Plot the raw data as a scatter plot and fitted linear function as a line graph ont eh same figure.

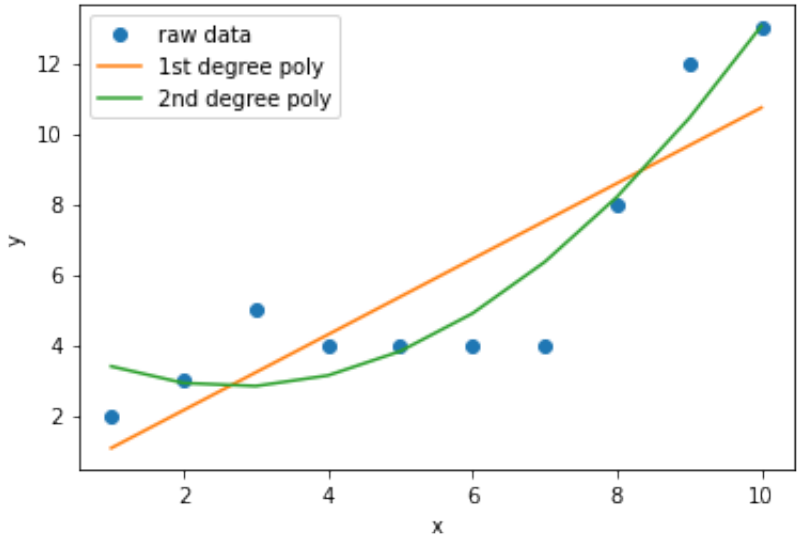
In [42]:
```
# plot data
plt.plot(x, y, 'o', label='raw data')

plt.plot(x_new, yfit1, label='1st degree poly')

plt.legend()

plt.xlabel('x')
plt.ylabel('y')

plt.show()
```



Try it yourself

Example 6: Plot the raw data as a scatter plot and second degree polynomial function as a line graph on the same figure.

In [44]:
```
# plot data
plt.plot(x, y, 'o', label='raw data')

plt.plot(x_new, yfit1, label='1st degree poly')

plt.plot(x_new, yfit2, label='2nd degree poly')

plt.legend()

plt.xlabel('x')
plt.ylabel('y')

plt.show()
```



Fitting an Arbitrary Function

Curve fitting is not limited to polynomial functions.

We can fit any function with unknown constants to the data using the function `curve_fit` from the `scipy` package.

Fitted function

Choose a function to fit e.g.

$$y = ae^{bx}$$

Define the function in the following format:

In [45]:
```
def exponential(x, a, b): # input arguments are independent var
    y = a * np.exp(b*x)
    return y
```

Fitted function

Use `scipy.optimize.curve_fit` to find the constants that best fit the function to the data.
Inputs:

- the function to fit
- the independent variable
- the dependent variable

Returns:

- constants of fitted function
- the covariance of the parameters (measure of the tendancy of one parameter to vary linearly with the other)

In [48]:
```
from scipy.optimize import curve_fit

# constants, covariance of fitted function
c, cov = curve_fit(exponential, x, y)
```

Fitted data

Generate fitted data by runnig the function we defined (`exponential`), on:

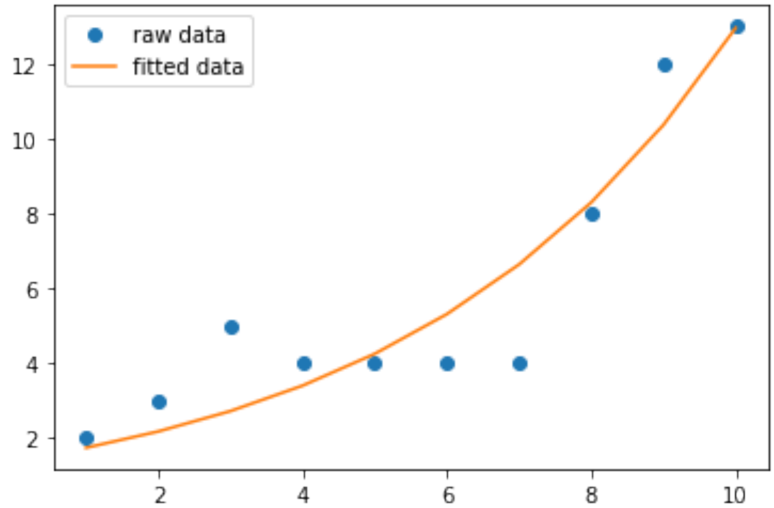
- x data (sorted monotonically if plotting)
- fitted constants (`*` allows `c` to be a *data structure* of any length)
- remember `c` is the variable we created to store the output of `curve_fit`

In [49]:
```
# input  to function to get fitted data
# use monotonically sorted x data
x_new = np.array(sorted(x))

yfit = exponential(x_new, *c)

```

Plotting fitted data

In [50]:
```
# plot data
plt.plot(x, y, 'o',    label='raw data')       # raw data
plt.plot(x_new, yfit, label='fitted data');  # fitted function
plt.legend()

# equation of the fitted line
print(f'y={round(c[0],2)}exp({round(c[1],2)}x)')
```

```
y=1.4exp(0.22x)
```



How does `polyfit` / `curve_fit` determine which coefficients/constants give the best fit?

How can we measure 'goodness' of fit e.g. when choosing degree of polynomial for best fit line?

Root Mean Square Error (RMSE)

(*least squares* approach)

A widely used measure of the error between fitted values and raw data.

Error/residual, ε:
The difference between the raw value $y(x)$ and the fitted value $a(x)$.

$$\varepsilon = a(x) - y(x)$$

Sum of the squared errors for N data points:
(error squared so that negative and positive errors do not cancel)

$$S = \sum_{i=1}^{N} \varepsilon_i^2$$

RMSE:

$$RMSE = \sqrt{\frac{1}{N} S} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \varepsilon_i^2}$$

Smaller RMSE indictes smaller error (i.e. a better fit between raw and fitted data).

We can optimise the fitted function by minimising the RMSE (used by `curve_fit`).

RMSE tells us statistically which line gives the best fit.

In [51]:

```
def RMSE(x, y, yfit):
    "Returns the RMSE of a y data fitted to x-y raw data"
    # error
    e = (yfit - y)

    # RMSE
    return np.sqrt(np.sum(e**2)/ len(x))

```

Let's compare the RMSE of each polynomial we fitted to the x,y data earlier

In [52]:

```
for degree in range(1, 3):

    c = np.polyfit(x, y, degree)        # coefficients of fitte

    yfit = np.polyval(c,x)              # no need to sort x mon

    rmse = RMSE(x, y, yfit)             # goodness of fit

    print(f'polynomial order {degree}, RMSE = {rmse}')
```

```
polynomial order 1, RMSE = 1.8964080880347554
polynomial order 2, RMSE = 1.2751140333327013
```

The second order polynomial gives a better fit.

Example 7

Fit the function $y = ae^{bx}$ which we defined earlier as `exponential` and find the RMSE:

In [53]:
```
c, cov = curve_fit(exponential, x, y)

yfit = exponential(x, *c)

rmse = RMSE(x, y, yfit)

print(f'RMSE = {rmse}')

```

```
RMSE = 1.3338248760975626
```

Of the three functions tested, the second order polynomial gives a better fit, statitically.

Summary

1. Find constants of fitted function

    - **Polynomial functions:** Find coefficients of polynomial by running `polyfit` on data and specifying degree of polynomial.
    - **Arbitrary functions:** Find constants of arbitrary function by defining function to fit and running `curve_fit` on raw data and function to fit.

2. Generate fitted data (arrange x data monotonically if plotting as graph):

    - **Polynomial functions:** Use `polyval` to generate the fitted data using fitted coefficients for given input range.
    - **Arbitrary functions:** Call function defined in step 1 using a range of x data and fitted coefficents as inputs.

3. Test goodness of fit: RMSE or other optimisation method.