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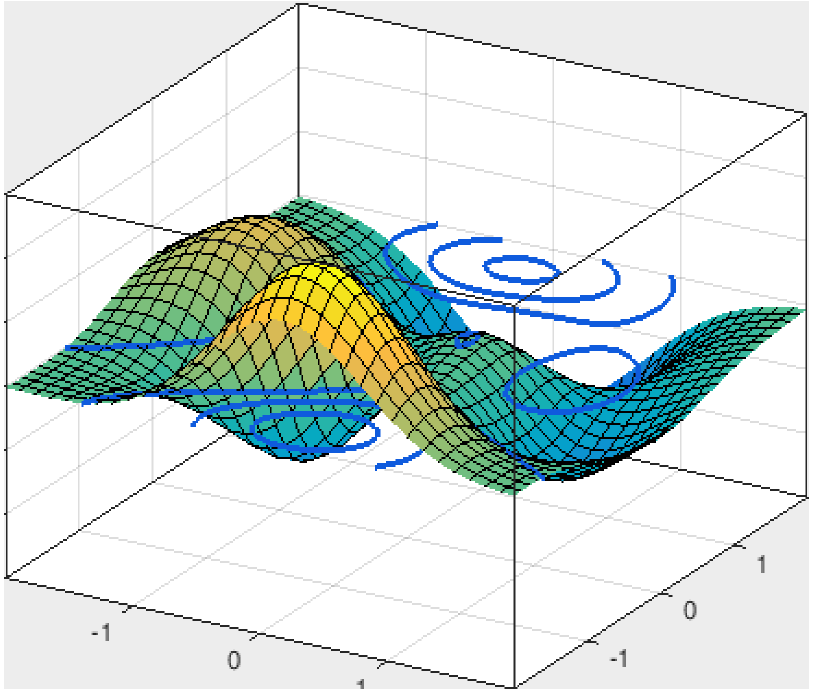
CITS2401 Computer Analysis and Visualization

School of Computer Science and Software Engineering

Lecture 9

Interpolation and curve fitting



Summary

- Interpolation
- Curve fitting
- Linear regression (for single variables)
- Polynomial regression
- Multiple variable regression
- Non-linear terms in regression

Interpolation

- Suppose you have some *known* data points, and you wish to predict what other data points might be – how can you do this?
- For example:
  - If at t = 1 second, distance traveled = 2m, and
  - at t = 5 seconds, distance traveled = 10m ...
  - What would be the distance traveled at, say, t = 3 seconds?

Linear interpolation

- The simplest interpolation technique is *linear interpolation*:

  it assumes that data follows a straight line between adjacent measurements.

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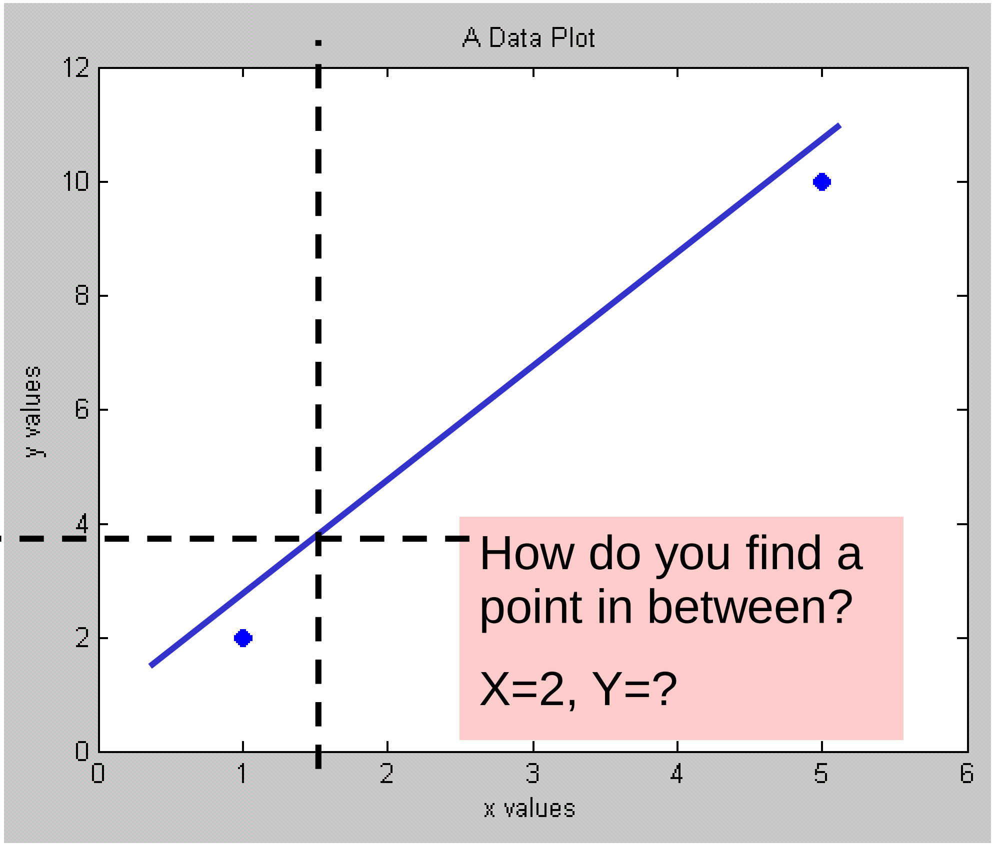
Linear interpolation (2)

- Assume the function between two points is a straight line
- Find equation of the line that passes through the two points
- Put a value of x in the equation to find y
- Put a value of y in the equation to find x



Linear interpolation in python

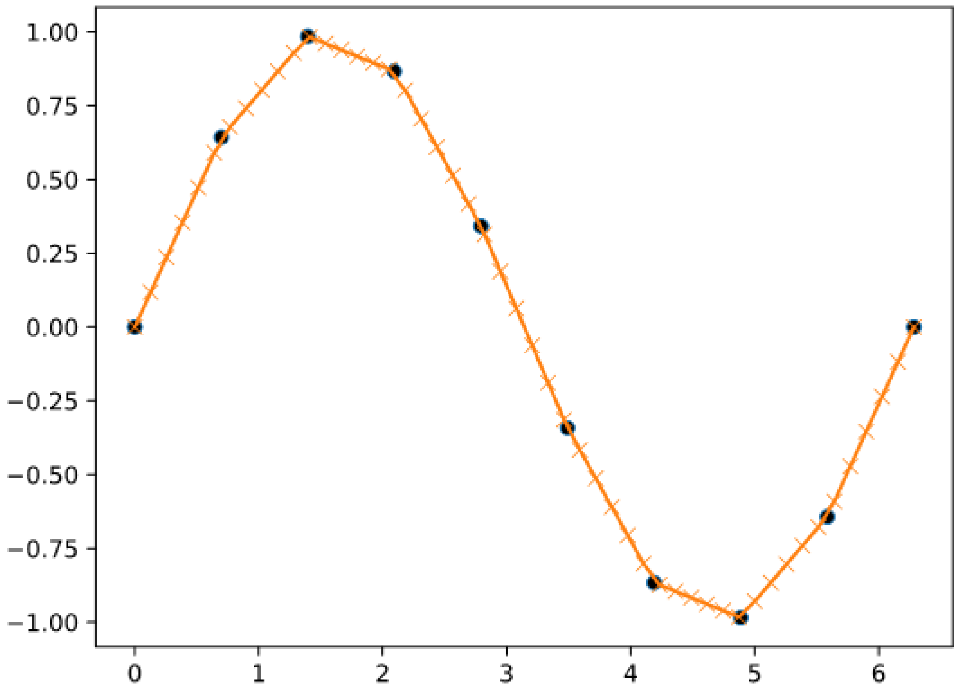
- `numpy.interp(x, xp, yp)`:
  - `xp` and `yp` give the x and y coordinates of the data points we have
  - `x` contains the x coordinates that we want interpolated y-values for.

Linear interpolation in python – example

Linear interpolation of the sin() function:

```
>>> import numpy as np
>>> import matplotlib.pyplot as plt
>>> x_pts = np.linspace(0, 2*np.pi, 10)
    # 10 equidistant x coords from 0 to 10
>>> y_pts = np.sin(x_pts)
>>> x_vals = np.linspace(0, 2*np.pi, 50)
    # 50 desired points
>>> y_vals = np.interp(x_vals, x_pts, y_pts)
>>> plt.plot(x_pts, y_pts, 'o') # plot known data points
>>> plt.plot(x_vals, y_vals, '-x') # plot interpolated points
>>> plt.show()
```

Linear interpolation in python – example (2)



Cubic spline interpolation

- Just as a *linear* interpolation is made up of linear segments – a cubic spline interpolation is made of segments of cubic polynomials, whose gradients match up at the measured data points.
- These cubic polynomials are continuous up to their 2nd derivative.

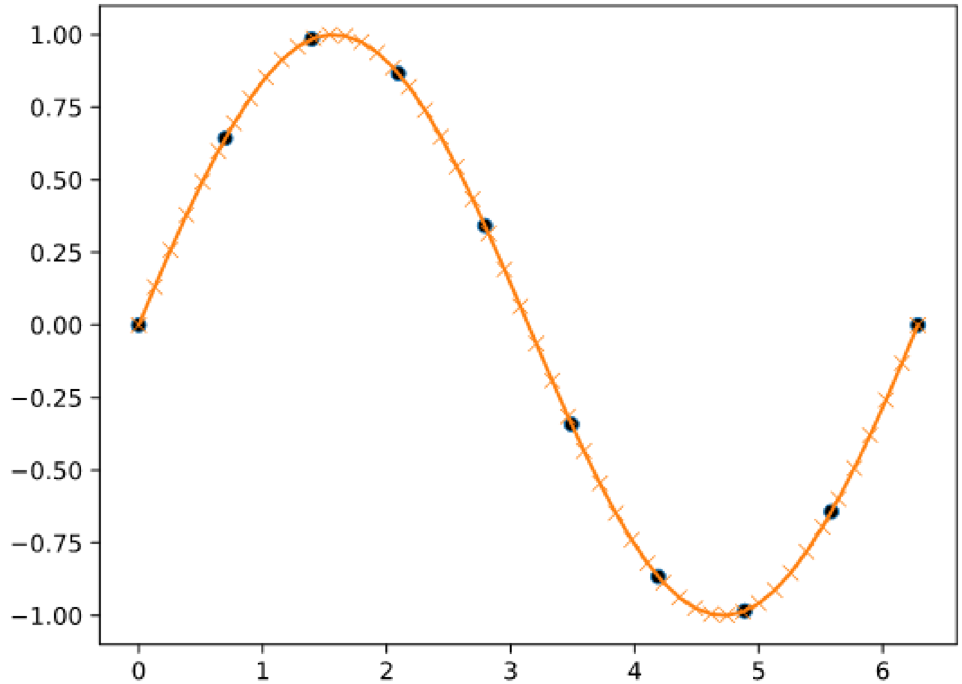
Cubic spline interpolation (2)

- Using numpy and scipy, interpolation is done in 2 steps:
  - `scipy.interpolate.splrep(x_pts, y_pts)` – returns a tuple representing the spline formulas needed
  - `scipy.interpolate.splev(x_vals, splines)` ("spline evaluate") – evaluate the spline data returned by `splrep`, and use it to estimate y values.

Cubic spline interpolation example

```
>>> import numpy as np
>>> from scipy import interpolate
>>> import matplotlib.pyplot as plt
>>> x_pts = np.linspace(0, 2*np.pi, 10)
    # 10 equidistant x coords from 0 to 10
>>> y_pts = np.sin(x_pts)
>>> splines = interpolate.splrep(x_pts, y_pts)
>>> x_vals = np.linspace(0, 2*np.pi, 50)
    # 50 desired points
>>> y_vals = interpolate.splev(x_vals, splines)
>>> plt.plot(x_pts, y_pts, 'o') # plot known data points
>>> plt.plot(x_vals, y_vals, '-x') # plot interpolated points
>>> plt.show()
```

Cubic spline interpolation example (2)



2D interpolation

- Just as we can do linear interpolation to estimate y values given x values – i.e. estimating a one-variable function f(x) – we can also do linear interpolation of a two-variable function f(x,y).

2D interpolation – original data (1)

- We will generate some data, and demonstrate what the original data points look like, and the interpolated version.

```
from mpl_toolkits.mplot3d import axes3d, Axes3D
import matplotlib.pyplot as plt
from matplotlib import cm
import numpy as np
from matplotlib.mlab import bivariate_normal
...
```

2D interpolation – original data (2)

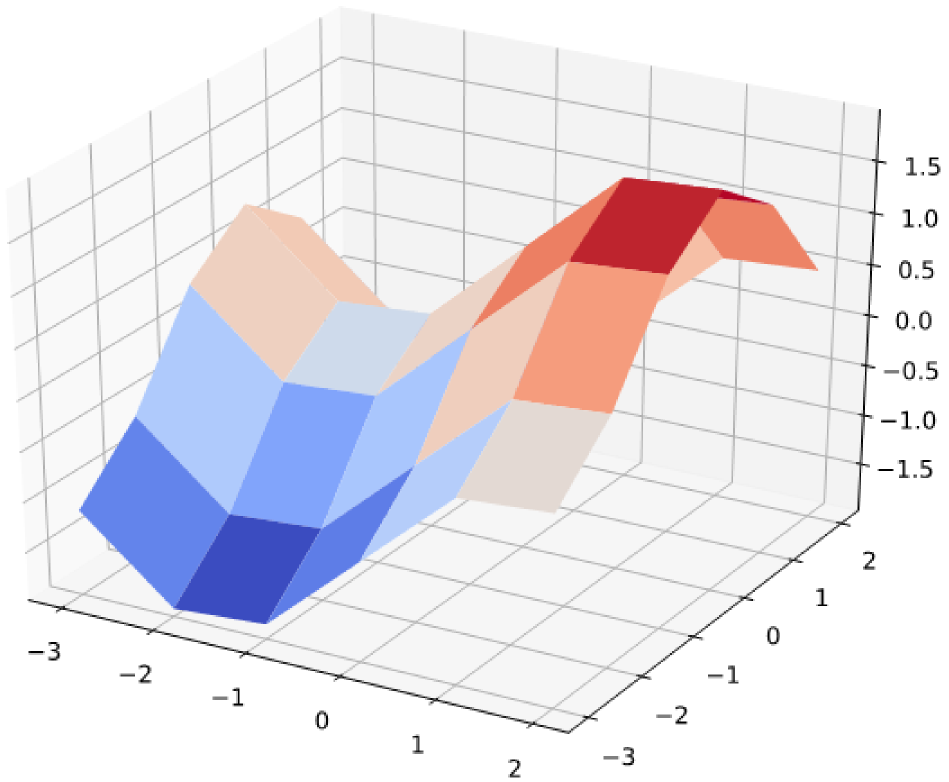
```
...

# a function to plot the surface.
# x, y and z should be arrays of data
def plot_data(x, y, z):
    fig = plt.figure()
    #ax = fig.gca(projection='3d')
    ax = Axes3D(fig)
    surf = ax.plot_surface(x, y, z, cmap=cm.coolwarm,
                           linewidth=0, antialiased=False)
    plt.show()
```

2D interpolation – original data (3)

```
>>> x_pts = np.arange(-3, 3, 1)
>>> y_pts = np.arange(-3, 3, 1)
>>> xx, yy = np.meshgrid(x_pts, y_pts)
    # the plotting functions require the x and
    # y values in a grid format
>>> zz = np.sin(xx) + np.cos(yy)
>>> plot_data(xx,yy,zz)
```

2D interpolation – original data (4)

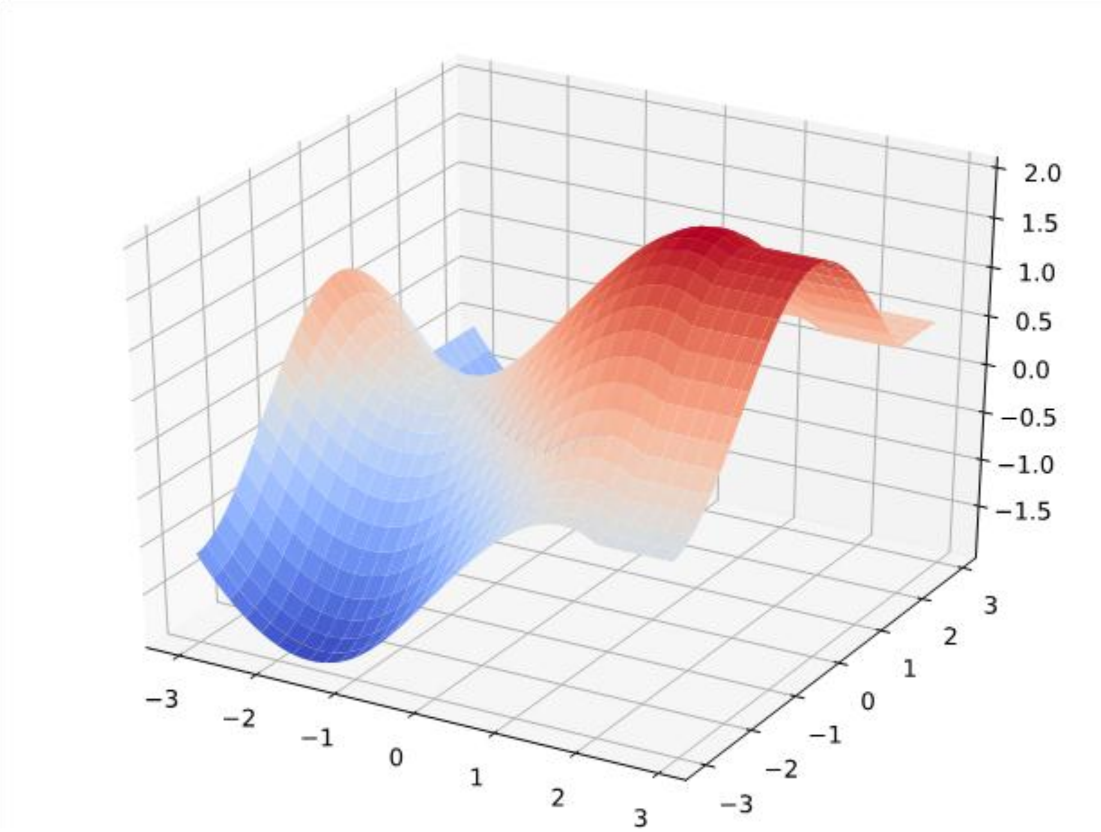


2D interpolation – linearly interpolated data

- Now we'll perform linear interpolation.
- `interpolate.interp2d(x, y, z, kind='linear')` returns a function which, when called, returns the actual interpolated values.

```
>>> from scipy import interpolate
>>> f = interpolate.interp2d(x_pts, y_pts, zz, kind='linear')
    # "kind" specifies whether we're doing linear, cubic, etc.
>>> x_vals = np.arange(-3, 3, 0.1)
>>> y_vals = np.arange(-3, 3, 0.1)
>>> xx_v, yy_v = np.meshgrid(x_vals, y_vals)
>>> zz_v = f(x_vals, y_vals)
>>> plot_data(xx_v,yy_v,zz_v)
```

2D interpolation – linearly interpolated data (2)

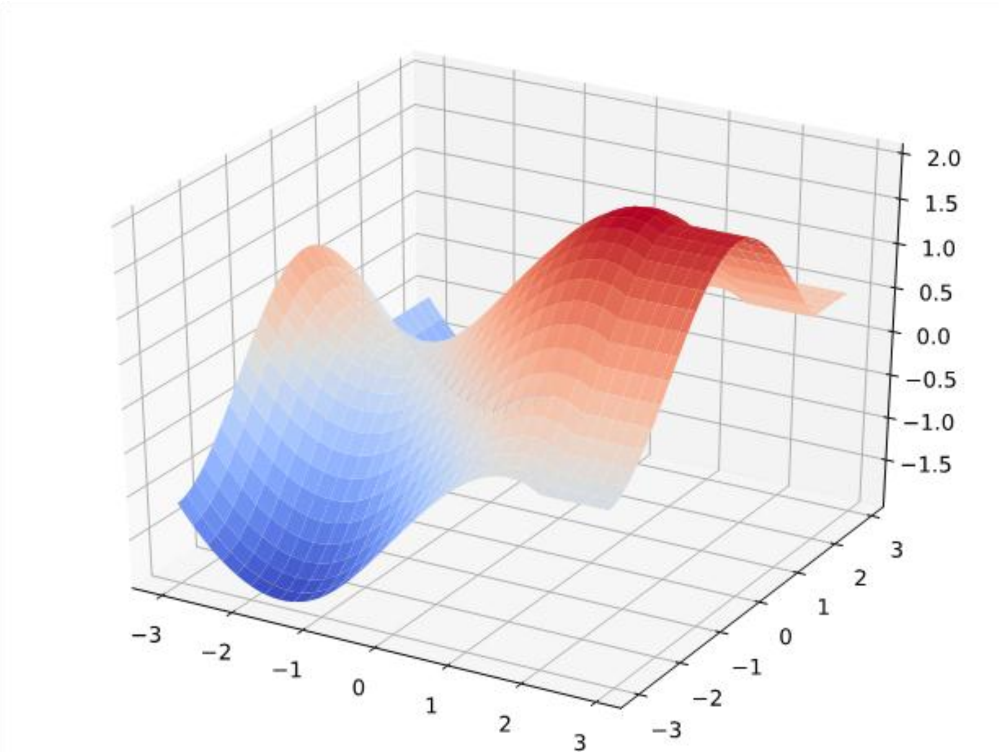


2D interpolation – cubic interpolated data

- Now we'll perform cubic interpolation.
- `interpolate.interp2d(x, y, z, kind='linear')` returns a function which, when called, returns the actual interpolated values.

```
>>> from scipy import interpolate
>>> f = interpolate.interp2d(x_pts, y_pts, zz, kind='cubic')
>>> x_vals = np.arange(-3, 3, 0.1)
>>> y_vals = np.arange(-3, 3, 0.1)
>>> xx_v, yy_v = np.meshgrid(x_vals, y_vals)
>>> zz_v = f(x_vals, y_vals)
>>> plot_data(xx_v,yy_v,zz_v)
```

2D interpolation – cubic interpolated data (2)

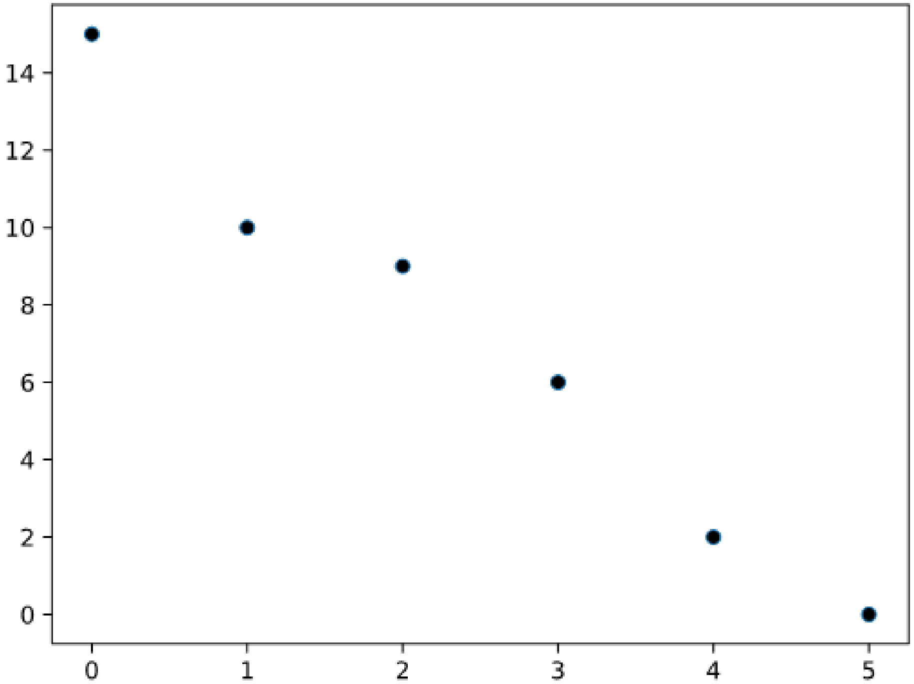


Curve fitting

- Collected data always contains some degree of error or imprecision
- Whereas interpolation is used when we assume that all data points are accurate and we want to infer new intermediate data points – *curve fitting* is used when we want to match an analytical (or symbolic) model to a set of measurements which may contain some error.

Curve fitting (2)

- For instance, we may have data points which seem to represent noisy data obtained from an underlying linear relationship – how can we estimate or model that underlying relationship?



Linear regression

- One method of curve fitting is linear regression – it minimizes the "square of the errors" (where the "error" is the distance each point is from the line).

  (In Excel, there is a function called "`SLOPE`" which performs linear regression on a set of data points, similar to the Python functions we will see here.)

Polynomial regression

- Linear regression is a special case of *polynomial regression* –

  since a line (i.e., an equation of the form $ax + b$) is a simple polynomial.
- But your data may not reflect a linear relationship – a polynomial of a higher order may be a better fit.

Linear regression (2)

- Both linear and non-linear polynomial regression can be done with Numpy's `polyfit` function:

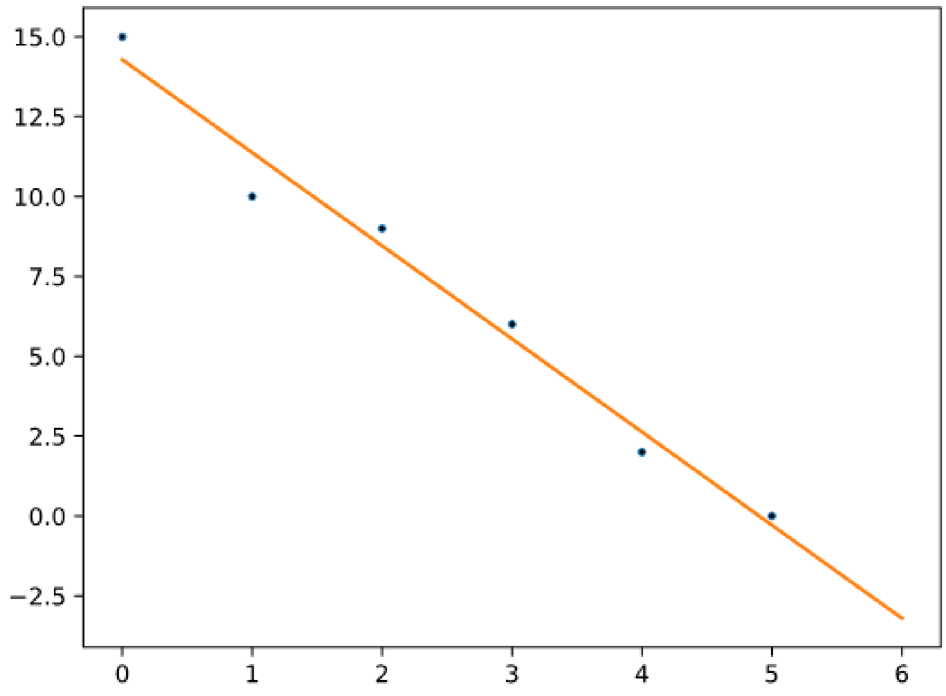
```
numpy.polyfit(x, y, degree)
```

- It returns the coeffficients for the polynomial;

  the easiest way to then use these in code is to use the `numpy.poly1d` class.

```
>>> import numpy as np
>>> from scipy.stats import linregress
>>> x_pts = np.arange(0,6,1)
>>> y_pts = np.array([15, 10, 9, 6, 2, 0])
>>> f = np.poly1d( np.polyfit(x_pts, y_pts, 1))
    # linear regression
>>> x_vals = np.linspace(0, 6, 100)
>>> plt.plot(x_pts, y_pts, '.')
>>> plt.plot(x_vals, f(x_vals), '-')
```

Linear regression (3)



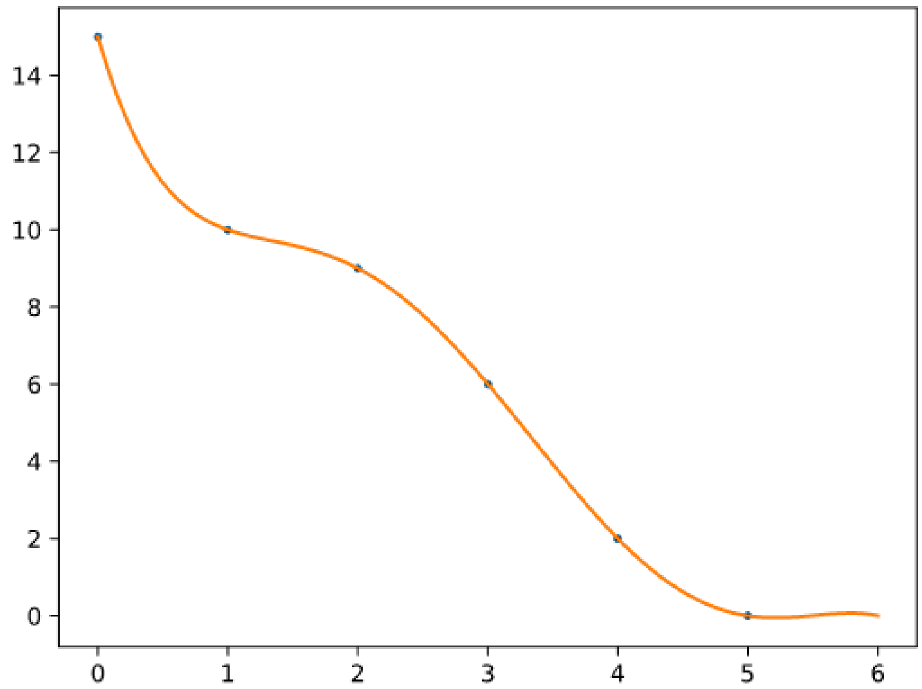
Polynomial regression

- If we have 6 data points, then a fifth-order polynomial will be able to give a perfect fit for them

  (i.e., there is some fifth-order polynomial on which all the data points fall exactly).

```
>>> import numpy as np
>>> from scipy.stats import linregress
>>> x_pts = np.arange(0,6,1)
>>> y_pts = np.array([15, 10, 9, 6, 2, 0])
>>> f = np.poly1d( np.polyfit(x_pts, y_pts, 5))
    # 5th-order polynomial
>>> x_vals = np.linspace(0, 6, 100)
>>> plt.plot(x_pts, y_pts, '.')
>>> plt.plot(x_vals, f(x_vals), '-')
```

Polynomial regression (2)



Interpolation and curve fitting – part 2

Overview

- Multiple variable regression
- Non-linear terms in regression

Multiple variable data

- In our regression examples, we have used models where a single output variable changes with respect to a single input variable.But real data may have multiple input variables.
- For example, the top speed of a vehicle will depend on many variables such as engine size, weight, air resistance etc.

Predictor and response variables

- The input variables are called the
  - independent variables, OR
  - predictor variables, OR
  - experimental variables
- The output variable is referred to as the
  - dependent variable, OR
  - response variable, OR
  - outcome variable

Predictor and response variables (2)

- We can use regression to find the relationship between input and output variables.
- We will use the following for our data points:

```
import numpy as np
x_pts = np.arange(-5,5,0.5)
y_pts = np.arange(-5,5,0.5)
xx, yy = np.meshgrid(x_pts, y_pts)
# our dependent variable is a linear function of
# x and y, plus random noise.
zz = 3*xx - 0.5*yy - 5 + 8 * np.random.normal(size=xx.shape)
```

Predictor and response variables (3)

- We build a model – i.e., we estimate the coefficients for *x*, *y* and intercept – by expressing our data as a matrix equation, and getting Python to give us a "least squares" solution for it.
- The `lstsq` function from Numpy will return a range of information about the solution as a tuple – the coefficients we want are the first member of that tuple:

```
numpy.linalg.lstsq(independent_vars, dependent_var)
```

- e.g.:

```
model_coefficients = numpy.linalg.lstsq(independent_vars,
dependent_var)[0]
```

Predictor and response variables (4)

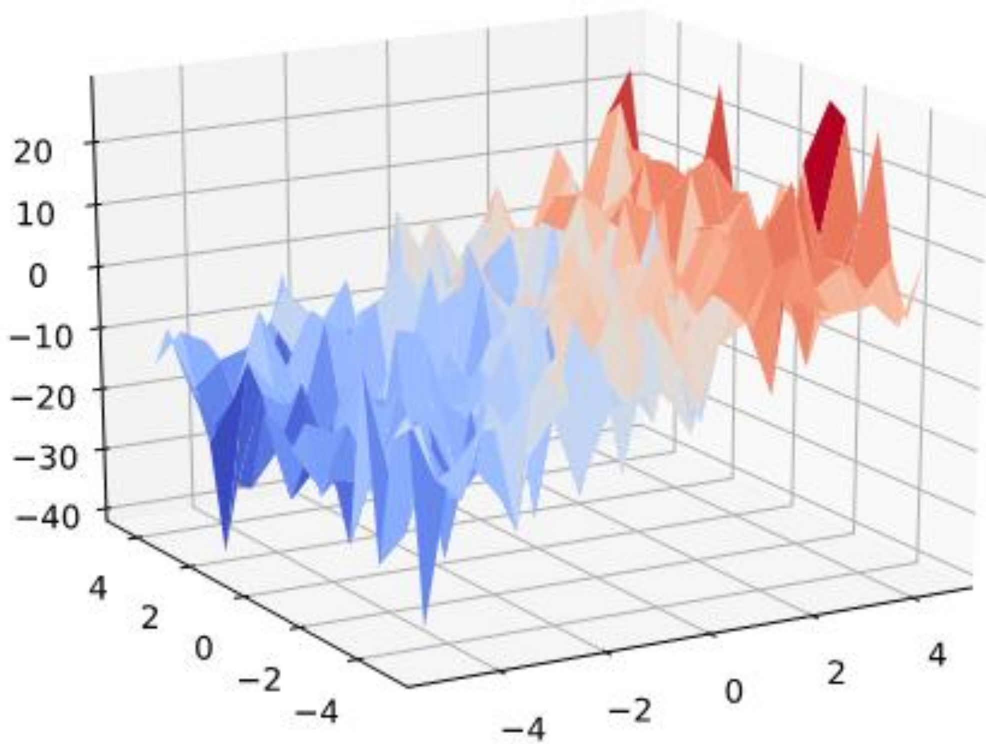
- Let's see what our input data looks like:

```
from mpl_toolkits.mplot3d import axes3d, Axes3D
import matplotlib.pyplot as plt
from numpy.linalg import lstsq

def plot_points(x, y, z):
  fig = plt.figure()
  ax = fig.gca(projection='3d')
  surf = ax.plot_surface(x, y, z, cmap=plt.cm.coolwarm)
  ax.view_init(20, -120)
  plt.show()

plot_points(xx,yy,zz)
```

Predictor and response variables (5)



Predictor and response variables (6)

- To estimate the coefficients in our underlying relationship, we will ask Python to solve a matrix equation of the form

  $$\mathbf{Dc} = \mathbf{z}$$

  where **D** is a matrix of representing our observations of independent variables, **c** are the unknown coefficients we want to estimate, and **z** represents our observations of the z values.

- So that Python will estimate values of the intercept – the "-5" in our underlying relationship – we will need a column of ones in the **D** matrix.

- So the equation will look like:

$$\begin{bmatrix} x_1 & y_1 & 1 \\ x_2 & y_2 & 1 \\ x_3 & y_3 & 1 \\ \dots & & \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ \dots \end{bmatrix} = \begin{bmatrix} z_1 \\ z_2 \\ z_3 \\ \dots \end{bmatrix}$$

Predictor and response variables (7)

```
# matrix for observations of independent variables
>>> ones = [ [1] * len( xx.flatten() )]
>>> indep = np.column_stack( [xx.flatten(), yy.flatten()] + ones )
>>> model = lstsq(indep, zz.flatten())[0]
>>> model
array([ 3.27248794, -0.6004752 , -5.26689769])
```

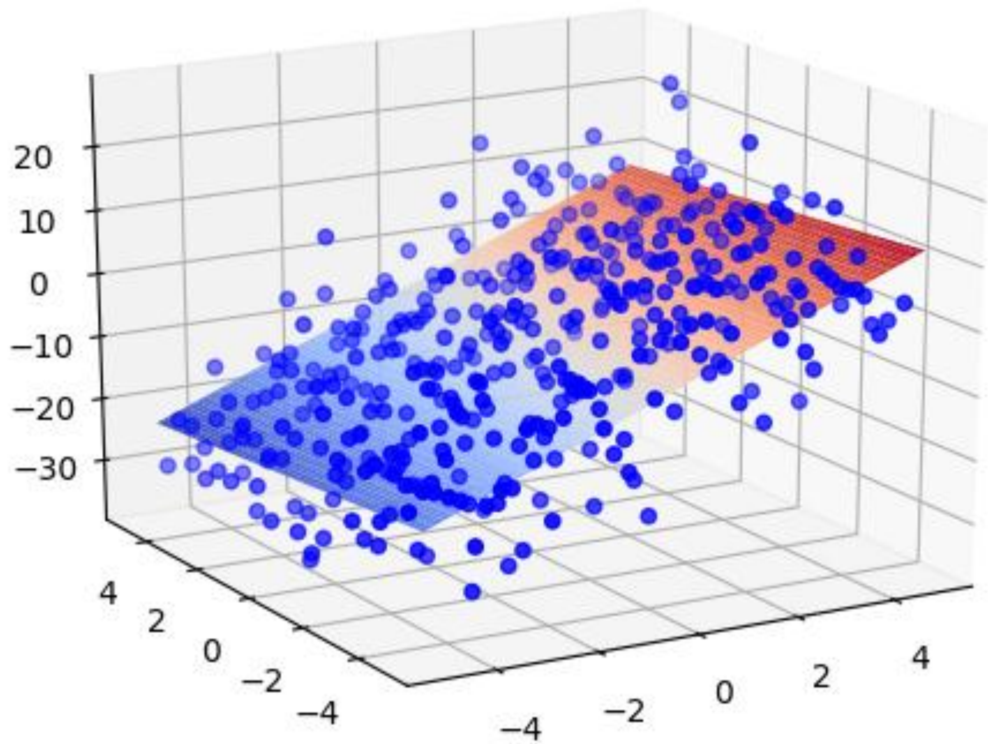
- Compare the estimated coefficients with the actual ones (3, -0.5 and -5).

Predictor and response variables (8)

- We can plot the least squares solution:

```
>>> x_vals = np.arange(-5,5,0.1)
>>> y_vals = np.arange(-5,5,0.1)
>>> xx_vals, yy_vals = np.meshgrid(x_vals, y_vals)
>>> zz_vals = model[0] * xx_vals + model[1] * yy_vals + model[2]
>>> fig = plt.figure()
>>> ax = fig.gca(projection='3d')
>>> ax.plot_surface(xx_vals, yy_vals, zz_vals, cmap=plt.cm.coolwarm)
    # the surface is our least-squares estimate
>>> ax.scatter( xx, yy, zz)
    # the scatter plot shows our original data points
>>> ax.view_init(20, -120)
>>> plt.show()
```

Predictor and response variables (9)



Curve-fitting using non-linear terms in linear regression

- What if we have a non-linear relationship between our variables?
- We can actually still use linear regression, as we did in the previous example: but in our matrix of independent variables, we'll include terms which are a non-linear function of our observations.

```
>>> xx_flat = xx.flatten()
>>> yy_flat = yy.flatten()
>>> zz_flat = zz.flatten()
>>> ones = [ [1] * len( xx_flat )]
>>> indep = np.column_stack( [xx_flat, yy_flat,
                             3 * np.sin(2 * xx_flat) ] + ones )
    # the 3rd column is *3sin(2x)*
>>> model = lstsq(indep, zz.flatten())[0]
>>> model
array([ 2.88268949, -0.30450846, -0.02530611, -4.46351387])
```

Curve-fitting using non-linear terms in linear regression (2)

- As with the linear case, we can use this model to estimate z-values.

```
>>> x_vals = np.arange(-5,5,0.1)
>>> y_vals = np.arange(-5,5,0.1)
>>> xx_vals, yy_vals = np.meshgrid(x_vals, y_vals)
>>> zz_vals = model[0] * xx_vals +
              model[1] * yy_vals +
              model[2] * 3 * np.sin(2 * xx_vals) +
              model[3]
>>> fig = plt.figure()
>>> ax = fig.gca(projection='3d')
>>> ax.plot_surface(xx_vals, yy_vals, zz_vals, cmap=plt.cm.coolwarm)
    # the surface is our least-squares estimate
>>> ax.scatter( xx, yy, zz)
    # the scatter plot shows our original data points
>>> ax.view_init(20, -120)
>>> plt.show()
```

Curve-fitting using non-linear terms in linear regression (3)