10-numpy-part2

December 5, 2019

Contents

1 NumPy - Part 2

NumPy has long list of functions, difficult to go over all of them. Please refer to its manual. You can use tab to see the available functions as well.

In this notebook we'll cover more features of NumPy.

> Most of the code in this notebook has been taken or adapted from Bootcamp for Biology notebook prepared by Mickey Atwal, Cold Spring Harbor Laboratory. (Lab website) A gentle introduction to some elements of scientific programming in Python.

1.0.1 1. Loading data

We will be working with the text file containing the nucleotide counts of the E. Coli DNA binding sites of the transcription factor CRP (cAMP receptor protein) also known as CAP (catabolite gene activator protein). You can find a copy at http://atwallab.cshl.edu/links/crp_counts_matrix.txt.

[ ]:
```
# web URL address of the file
# http://atwallab.cshl.edu/links/crp_counts_matrix.txt

# name of the file to be saved into
filename="data/crp_counts_matrix.txt"
```

This is a small tab-delimited text file where the counts data at each of the 42 nucleotide positions is stored as a series of strings. Let's take a look using the Unix command "head"

[2]:
```
!head data/crp_counts_matrix.txt
```

```
109     61      57      115
95      74      62      111
111     70      70      91
```

```
89      68      83      102
99      79      72      92
93      66      72      111
83      79      77      103
91      85      70      96
121     63      71      87
143     38      57      104
```

We need to convert this to a numerical array of numbers where we can perform computations. The genfromtxt function in NumPy automatically generates a NumPy array from a text file

[3]:
```
# loads data from text file and store in an integer NumPy array called 'counts'
import numpy as np
counts=np.genfromtxt(filename,dtype=int)
```

There's an alternative function to read txt files: `np.loadtxt()`

1.0.2 2. Working with numerical arrays

[4]:
```
counts.ndim # what is the dimensionality of the array?
```

[4]:
```
2
```

[5]:
```
counts.shape # what is the size of the array? (rows, columns)
```

[5]:
```
(42, 4)
```

[6]:
```
counts.dtype # what is the data type of the array?
```

[6]:
```
dtype('int64')
```

Array indexing Let's practise some array indexing to remember how they work in Python

[7]:
```
# let's have a look at the first five rows
counts[:5]
```

[7]:
```
array([[109,  61,  57, 115],
       [ 95,  74,  62, 111],
       [111,  70,  70,  91],
       [ 89,  68,  83, 102],
       [ 99,  79,  72,  92]])
```

[8]:
```
# the first row
counts[0]
```

[8]:
```
array([109,  61,  57, 115])
```

```
[9]: # rows 2 to 3, i.e. the second to third rows
     counts[1:3]
```

```
[9]: array([[ 95,  74,  62, 111],
            [111,  70,  70,  91]])
```

```
[10]: # the second column
      counts[:,1]
```

```
[10]: array([ 61,  74,  70,  68,  79,  66,  79,  85,  63,  38,  25,  28,  43,
              40,  16,  36,  18,  41,  54, 106,  81,  45,  74,  60,  31, 247,
              29, 232,  35,  62,  39,  43,  51,  62,  72,  62,  90,  71,  76,
              74,  72,  49])
```

```
[11]: # the last two rows
      counts[-2:]
```

```
[11]: array([[121,  72,  44, 105],
             [130,  49,  52, 111]])
```

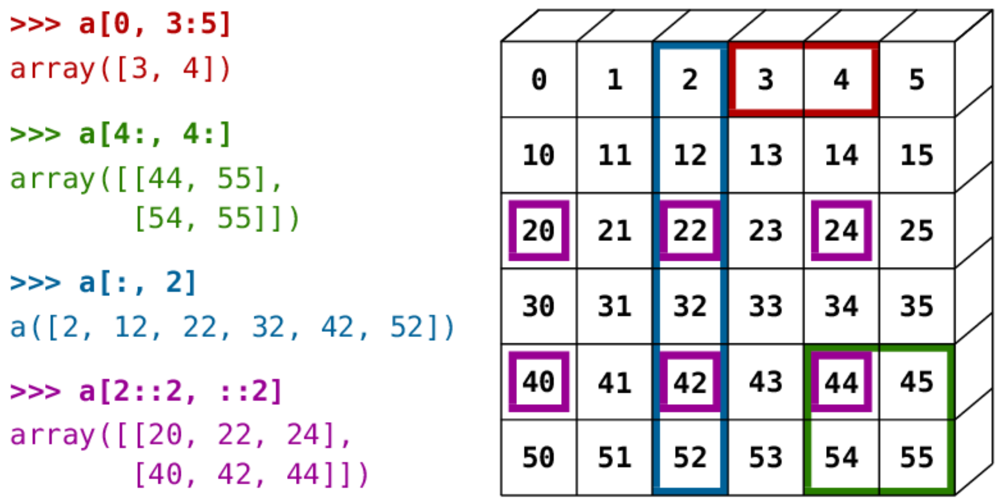
```
[12]: # every third row beginning with the first
      counts[::3]
```

```
[12]: array([[109,  61,  57, 115],
             [ 89,  68,  83, 102],
             [ 83,  79,  77, 103],
             [143,  38,  57, 104],
             [127,  43,  46, 126],
             [ 30,  36,  27, 249],
             [ 74,  54,  53, 161],
             [131,  45,  88,  78],
             [ 32,  31,  30, 249],
             [ 60, 232,  16,  34],
             [116,  39,  20, 167],
             [100,  62,  58, 122],
             [108,  90,  65,  79],
             [102,  74,  66, 100]])
```

```
[13]: # rows 3 to 4, and columns 2 to 4
      counts[2:4,1:4]
```

```
[13]: array([[ 70,  70,  91],
             [ 68,  83, 102]])
```

Here's a summary of indexing and slicing.



```
>>> a[0, 3:5]
array([3, 4])

>>> a[4:, 4:]
array([[44, 55],
       [54, 55]])

>>> a[:, 2]
a([2, 12, 22, 32, 42, 52])

>>> a[2::2, ::2]
array([[20, 22, 24],
       [40, 42, 44]])
```

Reshaping

[14]:
```
counts.reshape(21,8)
```

[14]:
```
array([[109,  61,  57, 115,  95,  74,  62, 111],
       [111,  70,  70,  91,  89,  68,  83, 102],
       [ 99,  79,  72,  92,  93,  66,  72, 111],
       [ 83,  79,  77, 103,  91,  85,  70,  96],
       [121,  63,  71,  87, 143,  38,  57, 104],
       [162,  25,  38, 117, 155,  28,  43, 116],
       [127,  43,  46, 126,  40,  40,  29, 233],
       [ 32,  16, 240,  54,  30,  36,  27, 249],
       [ 29,  18, 254,  41, 227,  41,  46,  28],
       [ 74,  54,  53, 161,  68, 106,  77,  91],
       [ 70,  81,  55, 136, 131,  45,  88,  78],
       [ 77,  74, 100,  91, 134,  60,  59,  89],
       [ 32,  31,  30, 249,  46, 247,  14,  35],
       [238,  29,  41,  34,  60, 232,  16,  34],
       [217,  35,  45,  45,  94,  62,  49, 137],
       [116,  39,  20, 167, 113,  43,  24, 162],
       [ 89,  51,  38, 164, 100,  62,  58, 122],
       [110,  72,  67,  93, 105,  62,  76,  99],
       [108,  90,  65,  79, 110,  71,  72,  89],
       [ 93,  76,  65, 108, 102,  74,  66, 100],
       [121,  72,  44, 105, 130,  49,  52, 111]])
```

[15]:
```
counts.reshape(4,2,21)
```

[15]:
```
array([[[109,  61,  57, 115,  95,  74,  62, 111, 111,  70,  70,  91,
          89,  68,  83, 102,  99,  79,  72,  92,  93],
        [ 66,  72, 111,  83,  79,  77, 103,  91,  85,  70,  96, 121,
          63,  71,  87, 143,  38,  57, 104, 162,  25]],
        [[ 38, 117, 155,  28,  43, 116, 127,  43,  46, 126,  40,  40,
           29, 233,  32,  16, 240,  54,  30,  36,  27],
         [249,  29,  18, 254,  41, 227,  41,  46,  28,  74,  54,  53,
          161,  68, 106,  77,  91,  70,  81,  55, 136]],

        [[131,  45,  88,  78,  77,  74, 100,  91, 134,  60,  59,  89,
           32,  31,  30, 249,  46, 247,  14,  35, 238],
         [ 29,  41,  34,  60, 232,  16,  34, 217,  35,  45,  45,  94,
           62,  49, 137, 116,  39,  20, 167, 113,  43]],

        [[ 24, 162,  89,  51,  38, 164, 100,  62,  58, 122, 110,  72,
           67,  93, 105,  62,  76,  99, 108,  90,  65],
         [ 79, 110,  71,  72,  89,  93,  76,  65, 108, 102,  74,  66,
          100, 121,  72,  44, 105, 130,  49,  52, 111]]])
```

Computations on arrays

[16]:
```python
# the minimum and maximum element of the array
np.min(counts), np.max(counts)
```

[16]:
```
(14, 254)
```

[17]:
```python
# select the elements greater than 200
counts[counts>200]
```

[17]:
```
array([233, 240, 249, 254, 227, 249, 247, 238, 232, 217])
```

[18]:
```python
counts >200
```

[18]:
```
array([[False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False,  True],
       [False, False,  True, False],
       [False, False, False,  True],
       [False, False,  True, False],
       [ True, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False,  True],
       [False,  True, False, False],
       [ True, False, False, False],
       [False,  True, False, False],
       [ True, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False],
       [False, False, False, False]])
```

[19]:
```
# what are the indices of the elements greater than 200?
# The Numpy function "where" returns the indices in separate arrays of rows and␣
 ↪columns.
np.where(counts>200)
```

[19]:
```
(array([13, 14, 15, 16, 17, 24, 25, 26, 27, 28]),
 array([3, 2, 3, 2, 0, 3, 1, 0, 1, 0]))
```

[20]:
```
# select elements that are greater than 200 and also divisible by 3, i.e. counts␣
 ↪mod 3 = 0
counts[(counts>200) & (counts%3==0)]
```

[20]:
```
array([240, 249, 249])
```

Dot Product. Frequently when performing operations on arrays we have to take the dot product of two list of numbers, or two vectors, e.g. $\vec{x} = \{x_1, x_2, x_3\}$ and $\vec{y} = \{y_1, y_2, y_3\}$. The dot product $\vec{x} \cdot \vec{y}$ is defined as

$$x \cdot y = \sum_{i=1}^{3} x_i y_i$$

NumPy provides an efficient way of doing this without explicitly writing a 'for loop'

[21]:
```
# dot product between rows 3 and 4s
counts[:5]
```

[21]:
```
array([[109,  61,  57, 115],
       [ 95,  74,  62, 111],
       [111,  70,  70,  91],
       [ 89,  68,  83, 102],
       [ 99,  79,  72,  92]])
```

[22]:
```
np.dot(counts[2],counts[3])
```

[22]:
```
29731
```

[23]:
```
111*89+70*68+70*83+91*102
```

[23]:
```
29731
```

[24]:
```
# sum each column of the array, i.e. sum along the rows, the dimension indexed␣
 ↪as 0
np.sum(counts,0)
```

[24]:
```
array([4374, 2747, 2688, 4555])
```

[25]:
```
# sum each row of the array, i.e. sum along the columns, the dimension indexed␣
 ↪as 1
np.sum(counts,1)
```

[25]:
```
array([342, 342, 342, 342, 342, 342, 342, 342, 342, 342, 342, 342, 342,
       342, 342, 342, 342, 342, 342, 342, 342, 342, 342, 342, 342, 342,
       342, 342, 342, 342, 342, 342, 342, 342, 342, 342, 342, 342, 342,
       342, 342, 342])
```

[26]:
```
# mean, median and standard deviation of each column
np.mean(counts,0), np.median(counts,0), np.std(counts,0)
```

[26]:
```
(array([104.14285714,  65.4047619 ,  64.        , 108.45238095]),
 array([101. ,  62. ,  57.5, 102.5]),
 array([47.21106177, 43.99245581, 45.42759807, 50.88933015]))
```

We can add pseudocounts to each element. This is usually a good idea if your count data is undersampled.

[27]:
```
# add 1 to EVERY element of the counts matrix to form a new matrix 'new_counts'
new_counts=counts+1
```

Let's calculate the probabilities of each nucleotide at each position, e.g. the probability of seeing an A at position i is

$$p_i(A) = \frac{counts_i(A)}{counts_i(A) + counts_i(T) + counts_i(G) + counts_i(C)} \tag{1}$$

The total counts is the same for all positions, so we might just as well use only the first position to evaluate it.

[28]:
```
total_counts=sum(new_counts[0])
prob=new_counts/total_counts
print(prob)
```

```
[[0.31791908 0.17919075 0.16763006 0.33526012]
 [0.27745665 0.21676301 0.18208092 0.32369942]
 [0.32369942 0.20520231 0.20520231 0.26589595]
 [0.26011561 0.19942197 0.24277457 0.29768786]
 [0.28901734 0.23121387 0.21098266 0.26878613]
 [0.2716763  0.19364162 0.21098266 0.32369942]
 [0.24277457 0.23121387 0.22543353 0.30057803]
 [0.26589595 0.24855491 0.20520231 0.28034682]
 [0.35260116 0.1849711  0.20809249 0.25433526]
 [0.41618497 0.11271676 0.16763006 0.30346821]
 [0.47109827 0.07514451 0.11271676 0.34104046]
 [0.45086705 0.08381503 0.12716763 0.33815029]
 [0.3699422  0.12716763 0.13583815 0.36705202]
 [0.11849711 0.11849711 0.0867052  0.67630058]
 [0.09537572 0.04913295 0.69653179 0.15895954]
 [0.08959538 0.10693642 0.08092486 0.72254335]
 [0.0867052  0.05491329 0.73699422 0.12138728]
 [0.65895954 0.12138728 0.13583815 0.08381503]
 [0.21676301 0.15895954 0.15606936 0.46820809]
 [0.19942197 0.30924855 0.22543353 0.26589595]
 [0.20520231 0.23699422 0.16184971 0.39595376]
 [0.38150289 0.13294798 0.25722543 0.2283237 ]
 [0.22543353 0.21676301 0.29190751 0.26589595]
 [0.39017341 0.17630058 0.1734104  0.26011561]
 [0.09537572 0.09248555 0.08959538 0.72254335]
 [0.13583815 0.71676301 0.0433526  0.10404624]
 [0.69075145 0.0867052  0.12138728 0.10115607]
 [0.17630058 0.6734104  0.04913295 0.10115607]
 [0.6300578  0.10404624 0.13294798 0.13294798]
 [0.27456647 0.18208092 0.14450867 0.39884393]
 [0.33815029 0.11560694 0.06069364 0.48554913]
 [0.32947977 0.12716763 0.07225434 0.47109827]
 [0.26011561 0.15028902 0.11271676 0.47687861]
 [0.29190751 0.18208092 0.17052023 0.35549133]
 [0.32080925 0.21098266 0.19653179 0.2716763 ]
 [0.30635838 0.18208092 0.22254335 0.28901734]
 [0.3150289  0.26300578 0.19075145 0.23121387]
 [0.32080925 0.20809249 0.21098266 0.26011561]
 [0.2716763  0.22254335 0.19075145 0.3150289 ]
 [0.29768786 0.21676301 0.19364162 0.29190751]
 [0.35260116 0.21098266 0.1300578  0.30635838]
 [0.37861272 0.14450867 0.15317919 0.32369942]]
```

[29]:
```
new_counts[0]
```

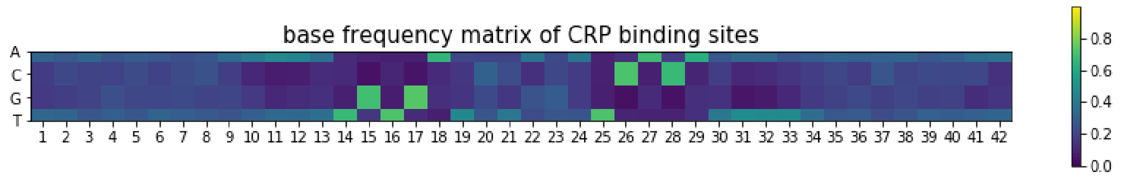
[29]:
```
array([110,  62,  58, 116])
```

[30]:
```
total_counts
```

[30]:
```
346
```

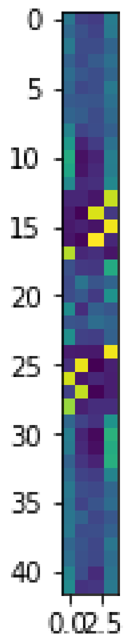
It's often a good idea to represent the data graphically to glean what's going on

[31]:
```
%matplotlib inline

import matplotlib.pyplot as plt

# set the size of the figure
plt.figure(figsize=[15,2])

# show the array flipped (transposed) and with no colour interpolation smoothing
plt.imshow(prob.T,interpolation='nearest')

# set the ticks
plt.xticks(range(0,42),range(1,43))
plt.yticks(range(4),['A','C','G','T'])

# set the colorbar
plt.clim([0,1])
plt.colorbar(ticks=np.arange(0,1,0.2))

# title
plt.title('base frequency matrix of CRP binding sites',fontsize=15)

# show the figure
plt.show()
```



```
[32]: import matplotlib.pyplot as plt
      plt.imshow(prob,interpolation='nearest')
```

```
[32]: <matplotlib.image.AxesImage at 0x7f9f68b6e5c0>
```



1.0.3 3. Random sampling, correlations and statistical tests

Gaussian distribution A frequent task in scientific programming is to analyze random samples from a known distribution. A commonly used distribution is the gaussian (normal distribution)

$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \tag{2}$$

where σ is the standard deviation and μ is the mean

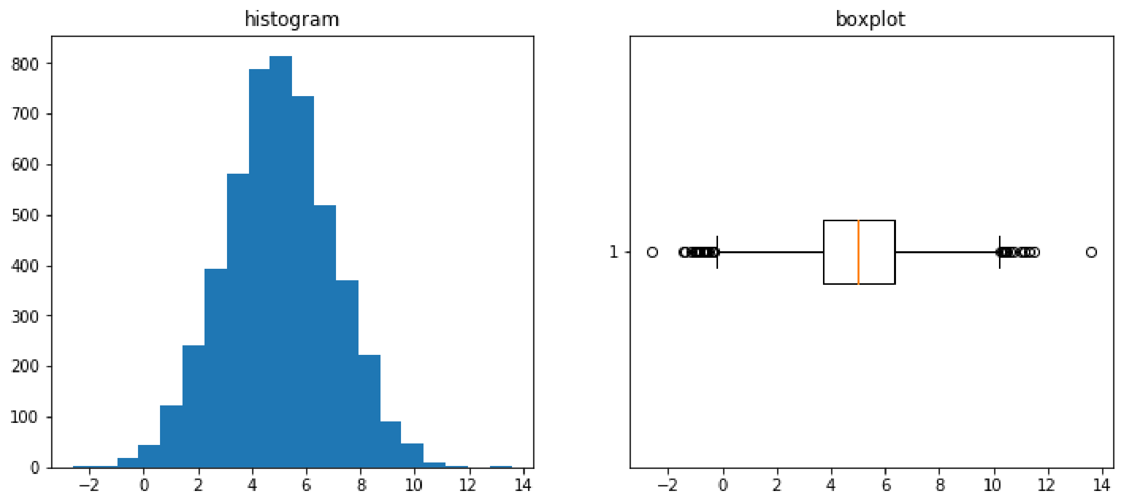
```
[33]: # number of samples
      N_gauss = 5000

      # standard deviations
      s = 2

      # mean
      u = 5

      # draw random samples from gaussian distribution
      samples=np.random.normal(u,s,N_gauss)
```

```
[34]: samples
```

```
[34]: array([4.61811608, 7.79977054, 3.83690571, ..., 1.584546  , 3.76935005,
             7.48291947])
```

We can plot the data in two different ways:

```
[35]: plt.figure(figsize=(12,5))

      # plot histogram
      plt.subplot(1,2,1)
      plt.hist(samples,bins=20)
      plt.title('histogram')

      # plot boxplot
      plt.subplot(1,2,2)
      # the default is to produce a vertical boxplot. Setting vert=False gives a␣
       ↪horizontal plot
      plt.boxplot(samples,vert=False)
      plt.title('boxplot')

      plt.show()
```



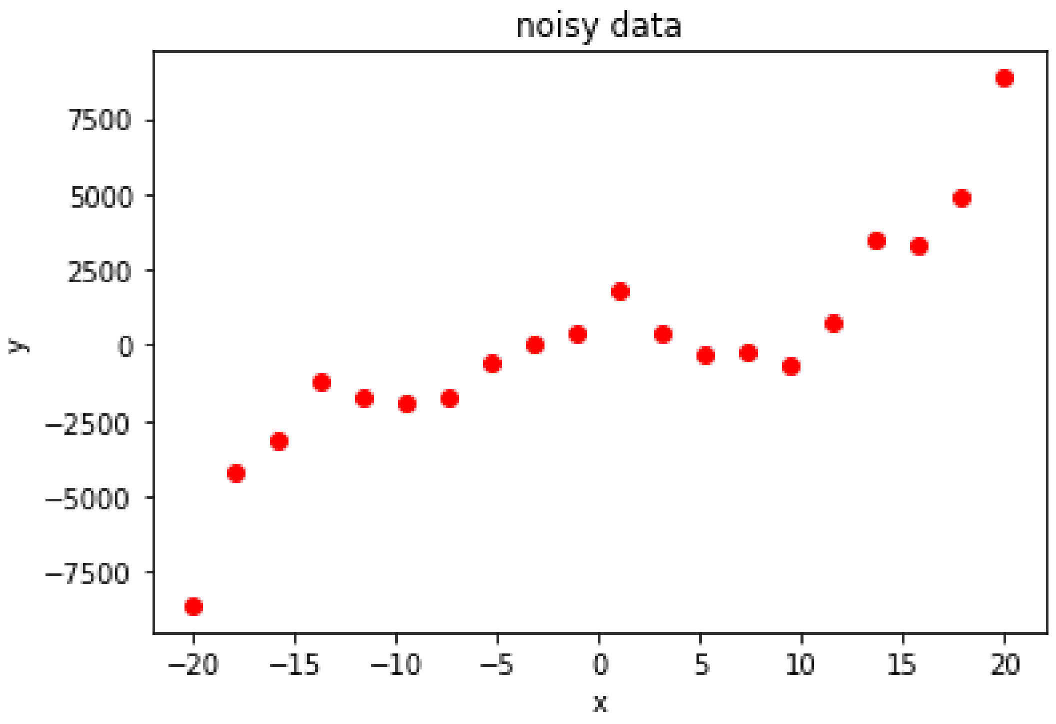
1.0.4 Curve Fitting

A frequent task in science is to fit a curve to data, and guess the underyling generative model. Let's make up some fake noisy data of the form $y = x^3 + \eta$, where η is noise drawn from a gaussian (normal) distribution.

[36]:
```
# number of data points
N=20

# N equalled spaced x values, from -20 to 20
x=np.linspace(-20,20,N)

# noise term: N samples from a gaussian distribution with mean 0 and standard␣
 ↪deviation 1000
noise=np.random.normal(0,1000,N)

# y values
y=x**3+noise
```

Let's plot our fake noisy data.

[37]:
```
plt.plot(x,y,'ro') # 'r' indicates red, 'o' indicates a small circle
plt.title('noisy data')
plt.xlabel('x')
plt.ylabel('y')
plt.show()
```

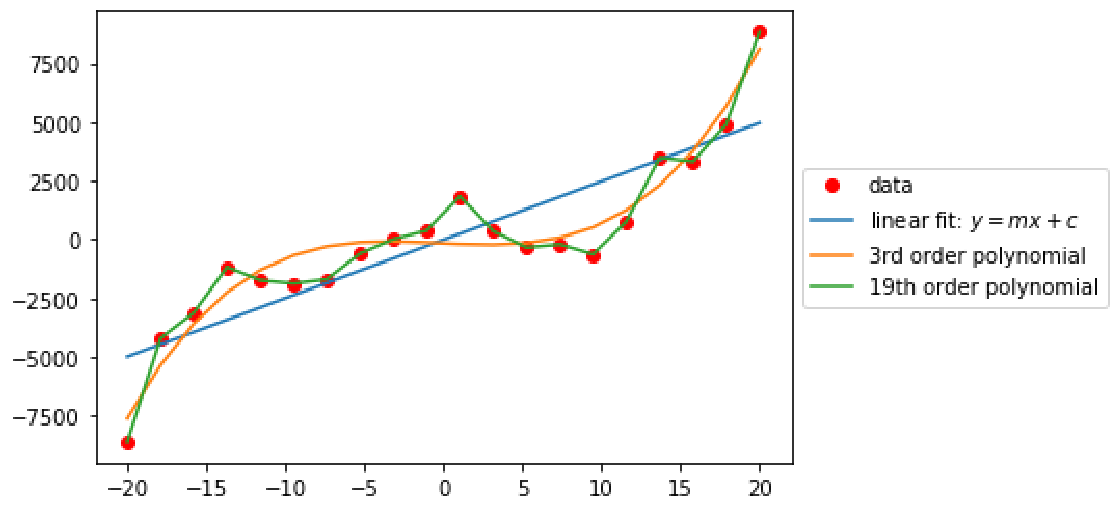


Now we will try to fit polynomials of various orders using the Numpy "polyfit" function.

[38]:
```
# straight line fit. The "fit1" array consists of the coefficients of the best␣
 ↪linear fit
fit1=np.polyfit(x,y,1)

# 3rd order polynomial fit
fit3=np.polyfit(x,y,3)

# 19th order polynomial fit
fit19=np.polyfit(x,y,19)

# create functions from the fits
y_1=np.poly1d(fit1)
y_3=np.poly1d(fit3)
y_19=np.poly1d(fit19)

print('linear fit: y_1=(%.2f)x+(%.2f)' % (fit1[0],fit1[1]))
print('3rd order fit: y_3=(%.2f)x^3 + (%.2f)x^2 + (%.2f)x + (%.2f)' %␣
 ↪(fit3[0],fit3[1],fit3[2],fit3[3]))
```

```
linear fit: y_1=(248.81)x+(-14.61)
3rd order fit: y_3=(1.07)x^3 + (1.05)x^2 + (-32.88)x + (-168.77)
```

[39]:
```
plt.plot(x,y,'ro')
plt.plot(x,y_1(x))
plt.plot(x,y_3(x))
plt.plot(x,y_19(x))

# add a legend to the right of the plot
legend_text=('data','linear fit: $y=mx+c$ ','3rd order polynomial','19th order␣
 ↪polynomial')
plt.legend(legend_text, loc='center left', bbox_to_anchor=(1,0.5))

plt.show()
```



The high order (19th) fit clearly tracks the data better. However, the 19th order polynomial in fact overfits the data since it will perform poorly on new data sampled from the original noisy curve.