Multi-dimensional data

- NumPy
- matrix multiplication, @
- numpy.linalg.solve, numpy.polyfit

Array programming with NumPy
Harris et al.
Nature, volume 585, pages 357–362, 2020
DOI 10.1038/s41586-020-2649-2

NumPy

- NumPy is a Python package for dealing with multi-dimensional data

www.numpy.org

docs.scipy.org/doc/numpy/user/quickstart.html

pylab ?

- Guttag [2nd edition] uses pylab in the examples, but...

> *"pylab is a convenience module that bulk imports matplotlib.pyplot (for plotting) and numpy (for mathematics and working with arrays) in a single name space. Although many examples use pylab, it is no longer recommended."*

matplotlib.org/faq/usage_faq.html

NumPy arrays (example)

Python shell

```
> range(0, 1, .3)
| TypeError: 'float' object cannot be
  interpreted as an integer
> [1 + i / 4 for i in range(5)]
| [1.0, 1.25, 1.5, 1.75, 2.0]
```

python only supports ranges of int

generate 5 uniform values in range [1,2]

Python shell

```
> import numpy as np
> np.arange(0, 1, 0.3)
| array([0. , 0.3, 0.6, 0.9])
> type(np.arange(0, 1, 0.3))
| <class 'numpy.ndarray'>
> help(numpy.ndarray)
| +2000 lines of text
> np.linspace(1, 2, 5)
| array([1.  , 1.25, 1.5 , 1.75, 2.  ])
```

numpy can generate ranges with float

returns a ”NumPy array” (not a list)

”arange” ≡ ”array range” and generates the array explicitly

generate n uniformly spaced values

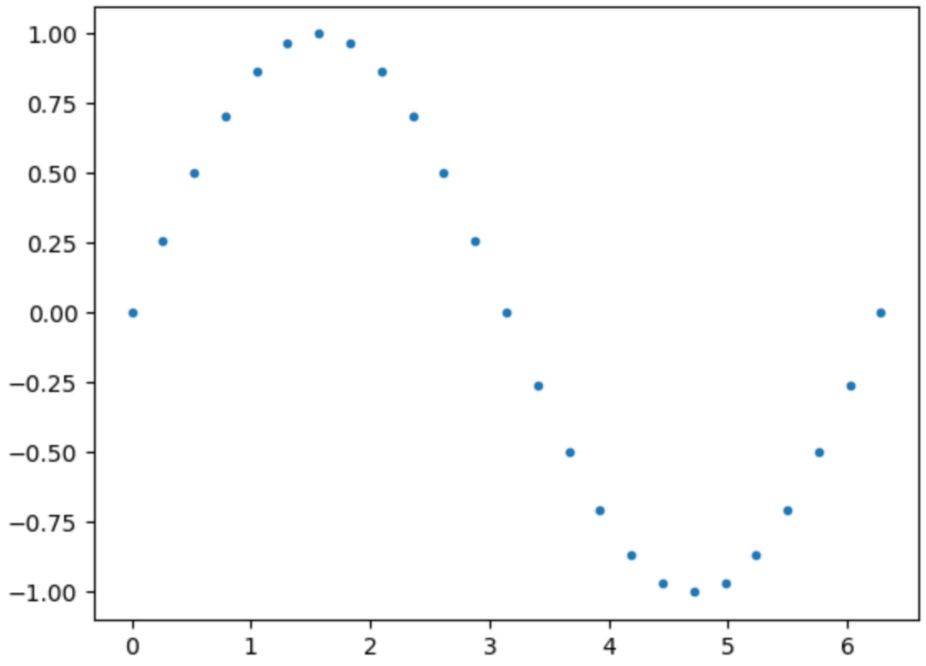
Plotting a function (example)

sin.py

```
import matplotlib.pyplot as plt
import math
n = 25
x = [2 * math.pi * i / (n - 1) for i in range(n)]
y = [math.sin(v) for v in x]
plt.plot(x, y, '.')
plt.show()
```

sin_numpy.py

```
import matplotlib.pyplot as plt
import numpy as np
x = np.linspace(0, 2 * np.pi, 25)
y = np.sin(x)
plt.plot(x, y, '.')
plt.show()
```

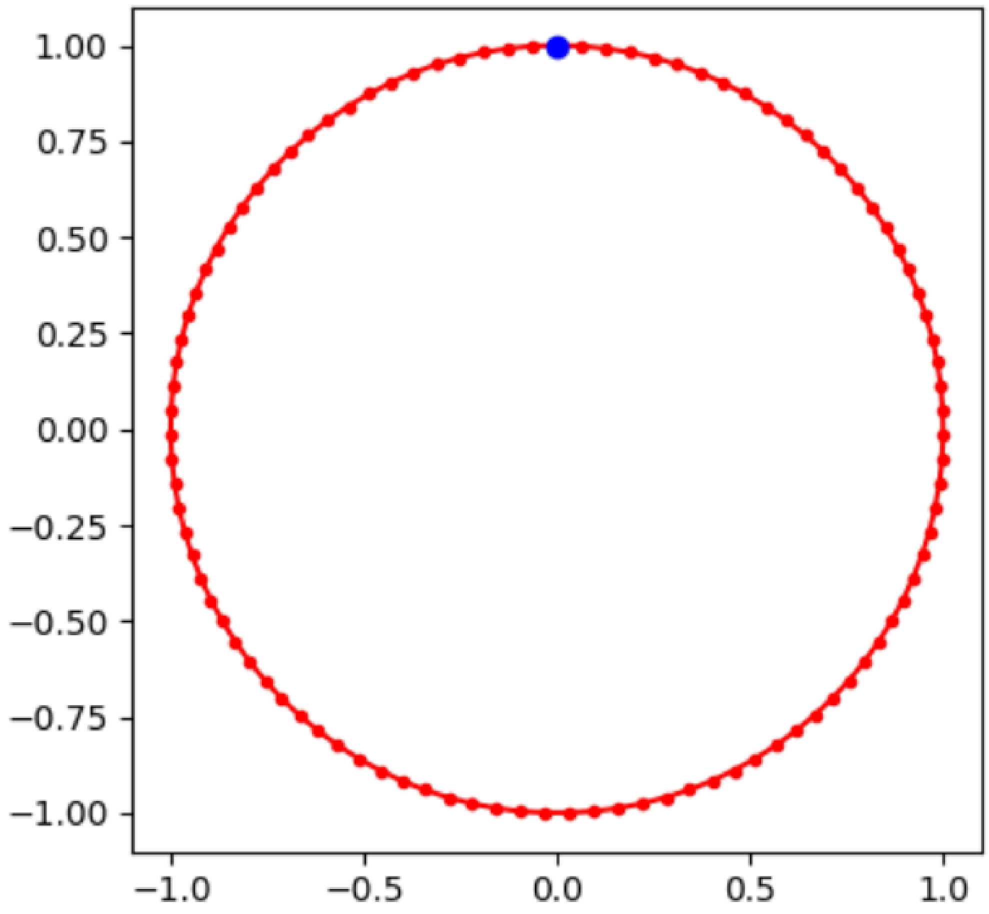


- `np.sin` applies the `sin` function *to each* element of `x`
- `pyplot` accepts NumPy arrays
- `math.pi == np.pi` $\approx \frac{22}{7}$

A circle

circle.py

```
import matplotlib.pyplot as plt
import numpy as np

a = np.linspace(0, 2 * np.pi, 100)
x = np.sin(a)
y = np.cos(a)

plt.plot(x, y, 'r.-')
plt.plot(x[0], y[0], 'bo')
plt.show()
```

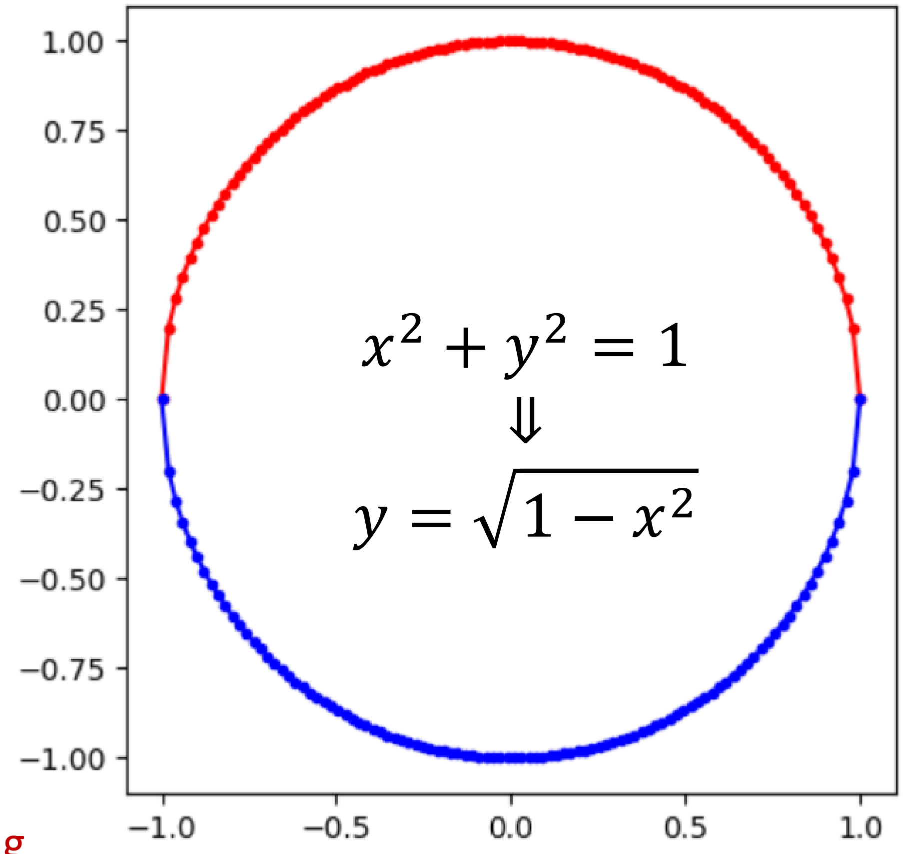


Two half circles

half_circles.py

```
import matplotlib.pyplot as plt
import numpy as np

x = np.linspace(-1, 1, 100)
plt.plot(x, np.sqrt(1 - x ** 2), 'r.-')
plt.plot(x, -np.sqrt(1 - x ** 2), 'b.-')
plt.show()
```

compact expression computing something quite comlicated



- `x` is a NumPy array
- `**` NumPy method `__pow__` squaring each element in `x`
- binary – NumPy method `__rsub__` that for each element e in `x` computes 1 - e
- `np.sqrt` NumPy method computing the square root of each element in `x`
- unary – NumPy method `__neg__` that negates each element in `x`

Creating one-dimensional NumPy arrays

Python shell

```
> np.array([1, 2, 3])
| array([1, 2, 3])
> np.array((1, 2, 3))
| array([1, 2, 3])
> np.array(range(1, 4))
| array([1, 2, 3])
> np.arange(1., 4., 1.)
| array([1., 2., 3.])
> np.linspace(1, 3, 3)
| array([1., 2., 3.])
> np.zeros(3)
| array([0., 0., 0.])
> np.ones(3)
| array([1., 1., 1.])
> np.full(3, 7)
| array([7, 7, 7])
> np.random.random(3)
| array([0.73761651,
  0.60607355, 0.3614118 ])
```

```
> np.array([1, 2, 3]).dtype    # type of all values
| dtype('int32')
> np.arange(3, dtype='float')
| array([0., 1., 2.])
> np.arange(3, dtype='int16') # 16 bit integers
| array([0, 1, 2], dtype=int16)
> np.arange(3, dtype='int32') # 32 bit integers
| array([0, 1, 2])
> 1000 ** np.arange(5)
| array([1, 1000, 1000000, 1000000000,
  -727379968], dtype=int32)    # OOPS.. overflow
> 1000 ** np.arange(5, dtype='O')
| array([1, 1000, 1000000, 1000000000,
  1000000000000], dtype=object) # Python integer
> np.arange(3, dtype='complex')
| array([0.+0.j, 1.+0.j, 2.+0.j])
```

Elements of a NumPy array are not arbitrary precision integers by default – you can select between +25 number representations

docs.scipy.org/doc/numpy-1.13.0/user/basics.types.html

Mantissa size in various numpy floats

Python shell

```
> for data_type in ['half', 'float', 'single', 'double', 'longdouble', 'float32', 'float64']:
    x = np.array([1], dtype=data_type)
    for i in range(100):
      if x == x + (x / 2) ** i:
        break
    print(data_type, i - 1, 'bits mantissa')
| half 10 bits mantissa
| float 52 bits mantissa
| single 23 bits mantissa
| double 52 bits mantissa
| longdouble 52 bits mantissa
| float32 23 bits mantissa            # platform independent
| float64 52 bits mantissa            # platform independent
```

$$1.\overbrace{\underbrace{00001}_{i}00000}^{\text{mantissa}}{}_2$$

docs.scipy.org/doc/numpy-1.13.0/user/basics.types.html

Creating multi-dimensional NumPy arrays

Python shell

```
> np.array([[1, 2, 3], [4, 5, 6]])
| array([[1, 2, 3],
|        [4, 5, 6]])
> np.arange(1, 7).reshape(2, 3)
| array([[1, 2, 3],
|        [4, 5, 6]])
> x = np.arange(12).reshape(2, 2, 3)
> x
| array([[[ 0,  1,  2],
|         [ 3,  4,  5]],
|
|        [[ 6,  7,  8],
|         [ 9, 10, 11]]])
> numpy.zeros((2, 5), dtype='int32')
| array([[0, 0, 0, 0, 0],
|        [0, 0, 0, 0, 0]])
```

```
> x.size
| 12
> x.ndim
| 3
> x.shape
| (2, 2, 3)
> x.dtype
| dtype('int32')
> x.flatten()
| array([0,1,2,3,4,5,6,7,8,9,10,11])
> list(x.flat)  # flat is an iterator
| [0,1,2,3,4,5,6,7,8,9,10,11]
> np.eye(3)     # diagonal 2D array
| array([[1., 0., 0.],
|        [0., 1., 0.],
|        [0., 0., 1.]])
```

View vs Copy

- Numpy is optimized to handle big multi-dimensional arrays
- To *avoid copying* data, **views** allows one to look at the underlying data in different ways (data can be shared by multiple views)
- `reshape`, `ravel` and slicing are examples creating views
- `flatten` and `ravel` both turn multiple dimensional arrays into one dimensional arrays but `flatten` creates an explicit copy whereas `ravel` creates a space efficient view

Python shell

```
> x = np.arange(6)
> y = x.reshape(2, 3)   # view
> y[0][0] = 42          # updates x
> x
| array([42, 1, 2, 3, 4, 5])
> y
| array([[42, 1, 2],
|        [ 3, 4, 5]])
> z = y.flatten()       # copy
> z[5] = 0
> z
| array([42, 1, 2, 3, 4, 0])
> x
| array([42, 1, 2, 3, 4, 5])
> w = y.ravel()        # view
> w[5] = -1
> w
| array([42, 1, 2, 3, 4, -1])
> x
| array([42, 1, 2, 3, 4, -1])
```

NumPy operations

Python shell

```
> x = numpy.arange(3)
> x
| array([0, 1, 2])
> x + x  # elementwise addition
| array([0, 2, 4])
> 1 + x  # add integer to each element
| array([1, 2, 3])
> x * x  # elementwise multiplication
| array([0, 1, 4])
> np.dot(x, x)  # dot product
| 5
> np.cross([1, 2, 3], [3, 2, 1]) # cross product
| array([-4,  8, -4])
```

```
> a = np.arange(6).reshape(2,3)
> a
| array([[0, 1, 2],
|        [3, 4, 5]])
> a.T  # matrix transposition, view
| array([[0, 3],
|        [1, 4],
|        [2, 5]])
> a @ a.T  # matrix multiplication
| array([[ 5, 14],
|        [14, 50]])
> a += 1
> a
| array([[1, 2, 3],
|        [4, 5, 6]])
```

PEP 465 - A dedicated infix operator for matrix multiplication

Universal functions (apply to each entry)

Python shell

```
> x = np.array([[1, 2], [3, 4]])
> np.sin(x)  # also: cos, exp, sqrt, log, ceil, floor, abs
| array([[ 0.84147098,  0.90929743],
|        [ 0.14112001, -0.7568025 ]])
> np.sign(np.sin(x))
| array([[ 1.,  1.],
|        [ 1., -1.]])
> np.mod(np.arange(10), 3)  # same as: np.arange(10) % 3
| array([0, 1, 2, 0, 1, 2, 0, 1, 2, 0], dtype=int32)
```

Axis

Python shell

```
> x = np.arange(1, 7).reshape(2, 3)
> x
| array([[1, 2, 3],
|        [4, 5, 6]])
> x.sum()   # = x.sum(axis=(0, 1))
| 21
> x.sum(axis=0)
| array([5, 7, 9])
> x.sum(axis=1)
| array([6, 15])
> x.min()   # = x.min(axis=(0, 1))
| 1
```

Python shell

```
> x.min(axis=0)
| array([1, 2, 3])
> x.min(axis=1)
| array([1, 4])
> x.cumsum()
| array([ 1,  3,  6, 10, 15, 21], dtype=int32)
> x.cumsum(axis=0)
| array([[1, 2, 3],
|        [5, 7, 9]], dtype=int32)
> x.cumsum(axis=1)
| array([[ 1,  3,  6],
|        [ 4,  9, 15]], dtype=int32)
```

Slicing

Python shell

```
> x = numpy.arange(20).reshape(4,5)
> x
| array([[ 0,  1,  2,  3,  4],
|        [ 5,  6,  7,  8,  9],
|        [10, 11, 12, 13, 14],
|        [15, 16, 17, 18, 19]])
> x[2, 3]  # = x[(2, 3)]
| 13
> x[1:4:2, 2:4:1]  # rows 1 and 3, and columns 2 and 3, view
| array([[ 7,  8],
|        [17, 18]])
> x[:, 3]
| array([ 3,  8, 13, 18])
> x[..., 3]  # ... is placeholder for ':' for all missing dimensions
| array([ 3,  8, 13, 18])
> type(...)
| <class 'ellipsis'>
```

Broadcasting (stretching arrays to get same size)

- Numpy tries to apply *broadcasting*, if array shapes do not match, i.e. adds missing leading dimensions and repeats a dimension with only one element:

```
  [[1],[2]] + [10,20]          column + row vector
≡ [[1],[2]] + [[10,20]]        both ndim = 2
≡ [[1,1],[2,2]] + [[10,20]]
≡ [[1,1],[2,2]] + [[10,20],[10,20]]
≡ [[11,21],[12,22]]
```

- To prevent unexpected broadcasting, add an assertion to your program:

```
assert x.shape == y.shape
```

docs.scipy.org/doc/numpy/user/basics.broadcasting.html

Python shell

```
> x = np.array([[1, 2, 3], [4, 5, 6]])
> y = np.array([1, 2, 3])   # one row
> z = np.array([[1], [2]]) # one column
> x + 3   # add 3 to each entry
| array([[4, 5, 6],
|        [7, 8, 9]])
> x + y   # add y to each row
| array([[2, 4, 6],
|        [5, 7, 9]])
> x + z   # add z to each column
| array([[2, 3, 4],
|        [6, 7, 8]])
> y + z   # 2 rows with y + 3 columns with z
| array([[2, 3, 4],
|        [3, 4, 5]])
> z == z.T   # [[1,1],[2,2]] == [[1,2],[1,2]]
| array([[ True, False],
|        [False,  True]])
```

Masking

Python shell

```
> x = np.arange(1, 11).reshape(2, 5)
> x
| array([[ 1,  2,  3,  4,  5],
|        [ 6,  7,  8,  9, 10]])
> x % 3
| array([[1, 2, 0, 1, 2],
|        [0, 1, 2, 0, 1]], dtype=int32)
> x % 3 == 0
| array([[False, False,  True, False, False],
|        [ True, False, False,  True, False]])
> x[x % 3 == 0]  # use Boolean matrix to select entries
| array([3, 6, 9])
> x[:, x.sum(axis=0) % 3 == 0]  # columns with sum divisible by 3
| array([[ 2,  5],
|        [ 7, 10]])
```

Numpy is fast... but be aware of dtype ⚠

Python shell

```
> sum([x**2 for x in range(1000000)])
| 333332833333500000
> (np.arange(1000000)**2).sum()
| 584144992   # wrong since overflow when default dtype='int32'
> (np.arange(1000000, dtype="int64")**2).sum()
| 333332833333500000  # 64 bit integers do not overflow
> import timeit from timeit
> timeit('sum([x**2 for x in range(1000000)])', number=1)
| 0.5614346340007614
> timeit('(np.arange(1000000)**2).sum()', setup='import numpy as np', number=1)
| 0.01436296700012462  # ridiculous fast but also wrong result...
> timeit('(np.arange(1000000, dtype="int64")**2).sum()',
  setup='import numpy as np', number=1)
| 0.04801707799924770  # fast and correct
> np.iinfo(np.int32).min
| -2147483648
> np.iinfo(np.int32).max
| 2147483647
```

numpy.int32 – 32 bit signed two's-complement integers

32 bits $b_{31}b_{30}b_{29}b_{28}\cdots b_2b_1b_0$ represent the value

$$-b_{31}\cdot 2^{31}+\sum_{i=0}^{30} b_i\cdot 2^i$$

10000000000000000000000000000000	-2147483648
10000000000000000000000000000001	-2147483647
⋮	
11111111111111111111111111111110	-2
11111111111111111111111111111111	-1
00000000000000000000000000000000	0
00000000000000000000000000000001	1
⋮	
01111111111111111111111111111110	2147483646
01111111111111111111111111111111	2147483647

Note: There is one more negative number than positive

Python shell

```
> np.int32(- 2 ** 31)
| -2147483648
> np.int32(- 2 ** 31) + 1
| -2147483647
> np.int32(- 2 ** 31) - 1
| 2147483647
> np.int32(2 ** 31)
| OverflowError: Python int too
  large to convert to C long
> np.int32(2 ** 31 - 1)
| 2147483647
> np.int32(2 ** 31 - 1) + 1
| -2147483648
> abs(np.int32(-2147483647))
| 2147483647
> abs(np.int32(-2147483648))
| -2147483648
```

numpy.org/doc/stable/user/basics.types.html

en.wikipedia.org/wiki/Two's_complement

Linear algebra

numpy.matrix

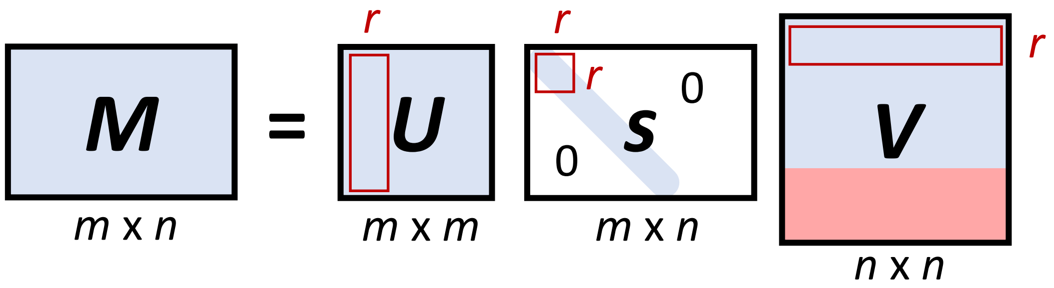
"It is no longer recommended to use this class, even for linear algebra. Instead use regular arrays. The class may be removed in the future."

Python shell

```
> x = np.arange(1, 5, dtype=float).reshape(2, 2)
> x
| array([[1., 2.],
|        [3., 4.]])
> x.T  # matrix transpose
| array([[1., 3.],
|        [2., 4.]])
> np.linalg.det(x)  # matrix determinant
| -2.0000000000000004
> np.linalg.inv(x)  # matrix inverse
| array([[-2. ,  1. ],
|        [ 1.5, -0.5]])
> np.linalg.eig(x)  # eigenvalues and eigenvectors
| (array([-0.37228132,  5.37228132]),
   array([[-0.82456484, -0.41597356], [0.56576746, -0.90937671]]))
> y = np.array([[5.], [7.]])
> np.linalg.solve(x, y)  # solve linear matrix equations
| array([[-3.],   # z1
|        [ 4.]])  # z2
```

$$\begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix} = \begin{pmatrix} 5 \\ 7 \end{pmatrix}$$

Singular value decomposition, `np.linalg.svd`

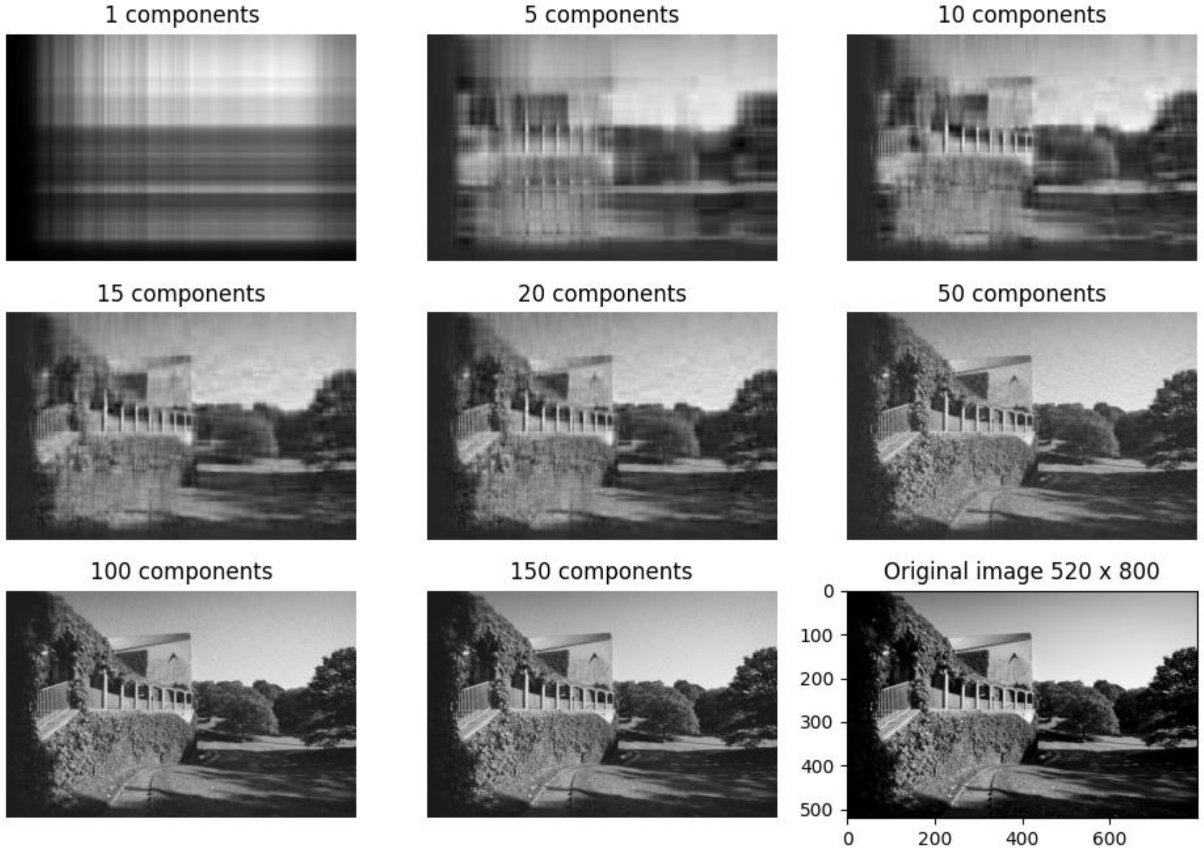


- U and V unitary matrix ($UU^{\mathsf{T}} = I$)
- S diagonal matrix, decreasing singular values

np.ndarray shape=(520, 800) dtype=uint8 min=0 max=252

image-reconstruction.py

```python
import numpy as np
import cv2  # Computer Vision, opencv.org
import matplotlib.pyplot as plt

color = cv2.imread('university.jpg')              # color image
gray = cv2.cvtColor(color, cv2.COLOR_BGR2GRAY)   # convert to gray

u, s, v = np.linalg.svd(gray)  # Calculating the SVD

for i, r in enumerate([1, 5, 10, 15, 20, 50, 100, 150], start=1):
    rank_r = u[:, :r] @ np.diag(s[:r]) @ v[:r, :]
    plt.subplot(3, 3, i)
    plt.imshow(rank_r, cmap='gray', vmin=0, vmax=255)
    plt.title(f'{r} components')
    plt.axis('off')
plt.subplot(3, 3, 9)
plt.imshow(gray, cmap='gray')
plt.title(f'Original image {gray.shape[0]} x {gray.shape[1]}')
plt.show()
```



... and in color

image-reconstruction-color.py

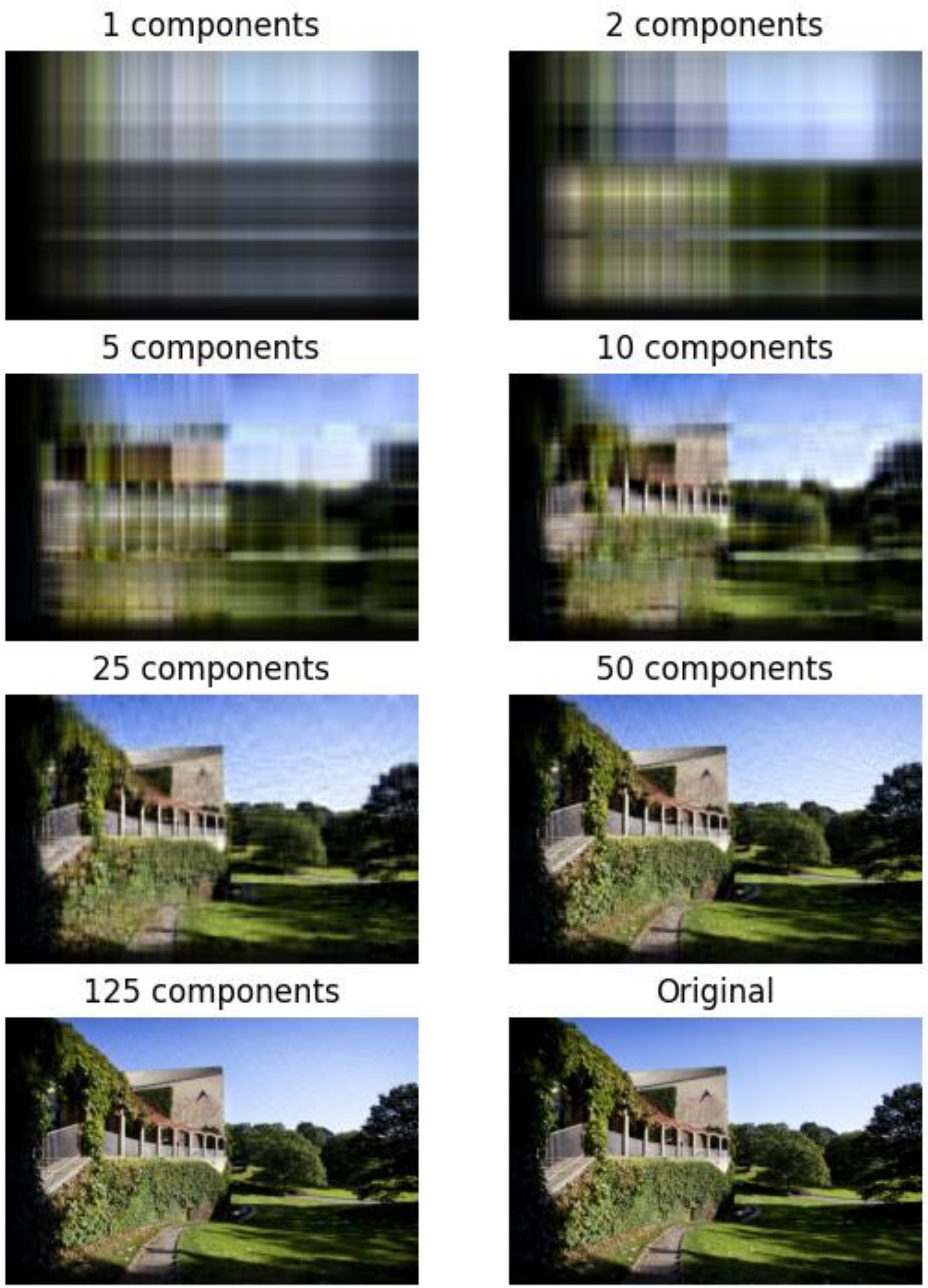
```
import numpy as np
import matplotlib.pyplot as plt
from matplotlib.image import imread

color = imread('university.jpg')
color = color / 255   # convert integers 0..255 to floats 0..1

plt.subplot(4, 2, 8)
plt.imshow(color)
plt.axis('off')
plt.title(f'Original')

height, width, colors = color.shape

u, s, v = np.linalg.svd(color.reshape((height, width * colors)),
                        full_matrices=False)

for i, r in enumerate([1, 2, 5, 10, 25, 50, 125], start=1):
    rank_r = u[:, :r] @ np.diag(s[:r]) @ v[:r, :]
    plt.subplot(4, 2, i)
    plt.imshow(rank_r.reshape((height, width, colors)))
    plt.title(f'{r} components')
    plt.axis('off')
plt.show()
```

shape=(520, 800, 3)
3 = (red, blue, green)

shape=(520, 2400)

shape=(520, 800, 3)

v shape=(520, 2400)
instead of (2400, 2400)



... and in color (stacked)

image-reconstruction-color-stacked.py

```python
import numpy as np
import matplotlib.pyplot as plt
from matplotlib.image import imread

color = imread('university.jpg')
color = color / 255  # convert integers 0..255 to floats 0..1

plt.subplot(4, 2, 8)
plt.imshow(color)
plt.axis('off')
plt.title(f'Original')

u, s, v = np.linalg.svd(color.transpose(2, 0, 1), full_matrices=False)

print(f'{u.shape=} {s.shape=} {v.shape=}')

for i, r in enumerate([1, 2, 5, 10, 25, 50, 125], start=1):
    rank_r = (u[:, :, :r] * s[:, None, :r]) @ v[:, :r, :]
    plt.subplot(4, 2, i)
    plt.imshow(rank_r.transpose(1, 2, 0))
    plt.title(f'{r} components')
    plt.axis('off')
plt.show()
```

shape = (520, 800, 3)

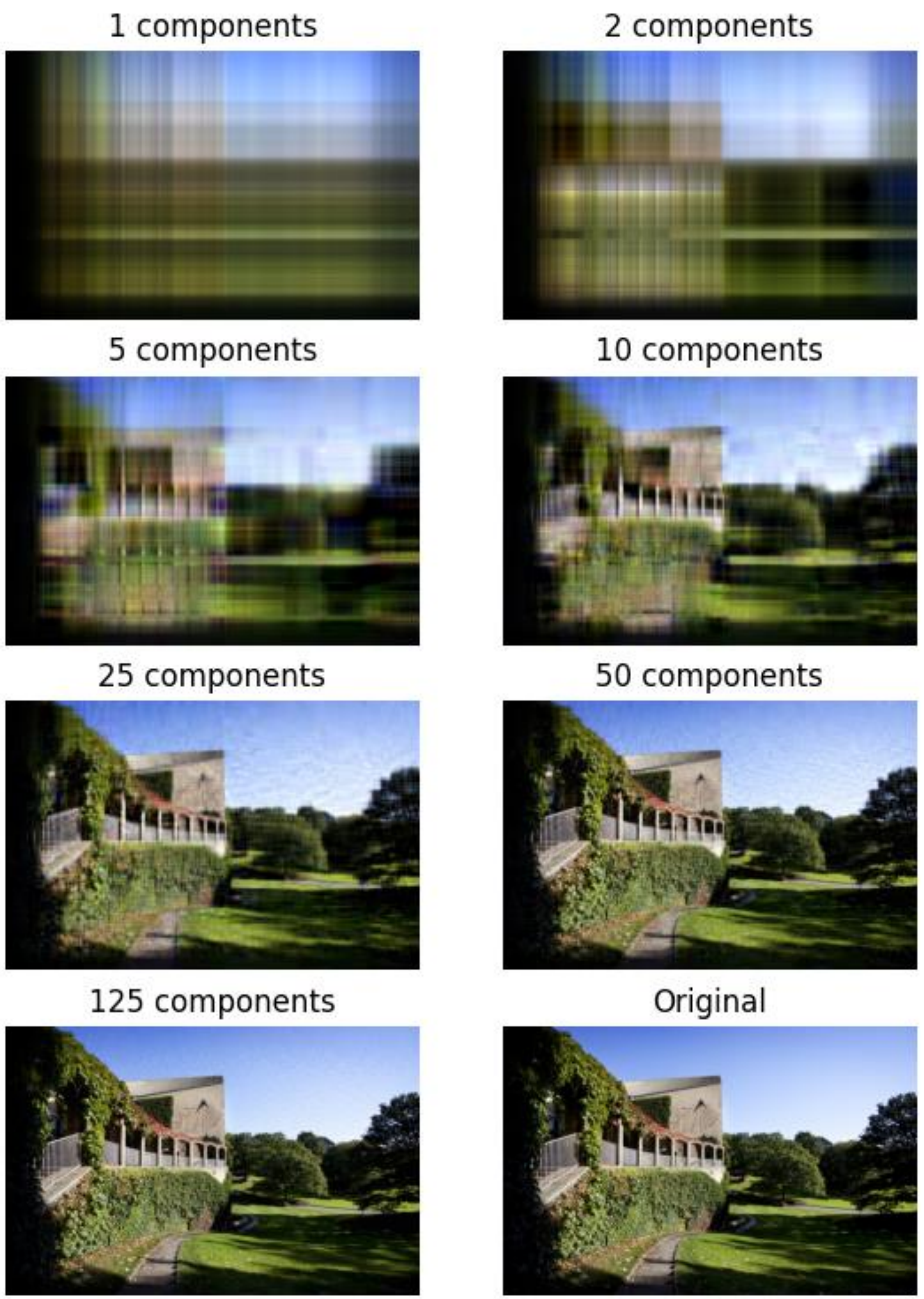
shape = (3, 520, 800)

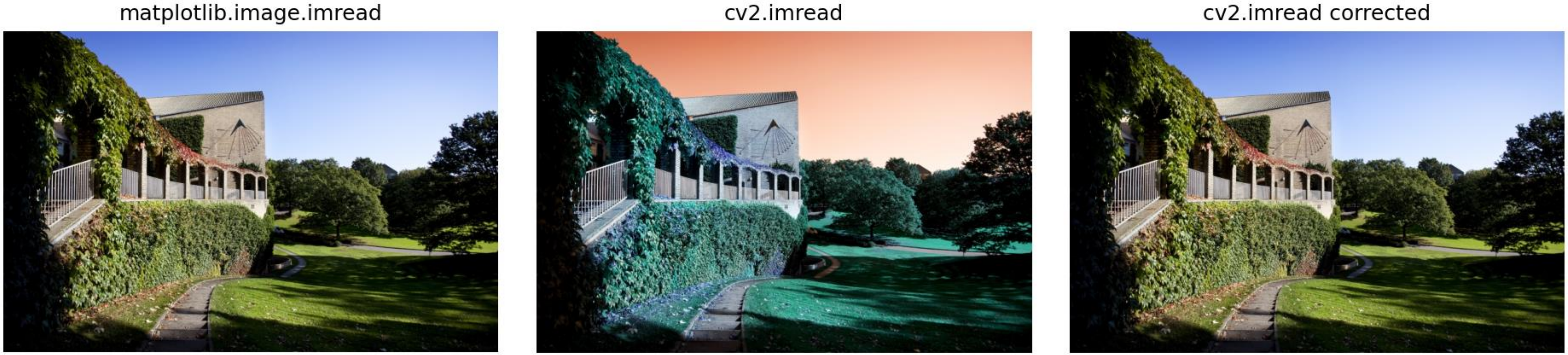
element-wise multiplication (*), broadcasting (None), stacked for each color (:)

shape = (520, 800, 3)

Python shell

```
| u.shape=(3, 520, 520) s.shape=(3, 520) v.shape=(3, 520, 800)
```

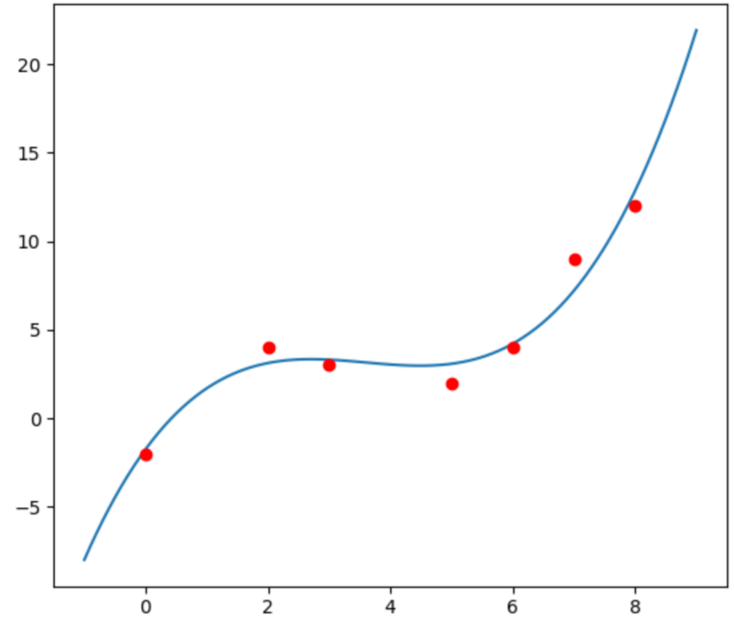




color-image.py

```
import matplotlib.pyplot as plt
import matplotlib.image
import cv2

img1 = matplotlib.image.imread('university.jpg')
img2 = cv2.imread('university.jpg')   # cv2 uses BGR instead of RGB
img3 = img2[:, :, ::-1]               # change color order BGR to RGB

Images = [(img1, 'matplotlib.image.imread'), (img2, 'cv2.imread'), (img3, 'cv2.imread corrected')]

for i, (img, title) in enumerate(images, start=1):
    plt.subplot(1, 3, i)
    plt.imshow(img)
    plt.axis('off')
    plt.title(title)

plt.show()
```

numpy.polyfit



- Given n points with $(x_0, y_0), \ldots, (x_{n-1}, y_{n-1})$
- Find polynomial p of degree d that minimizes

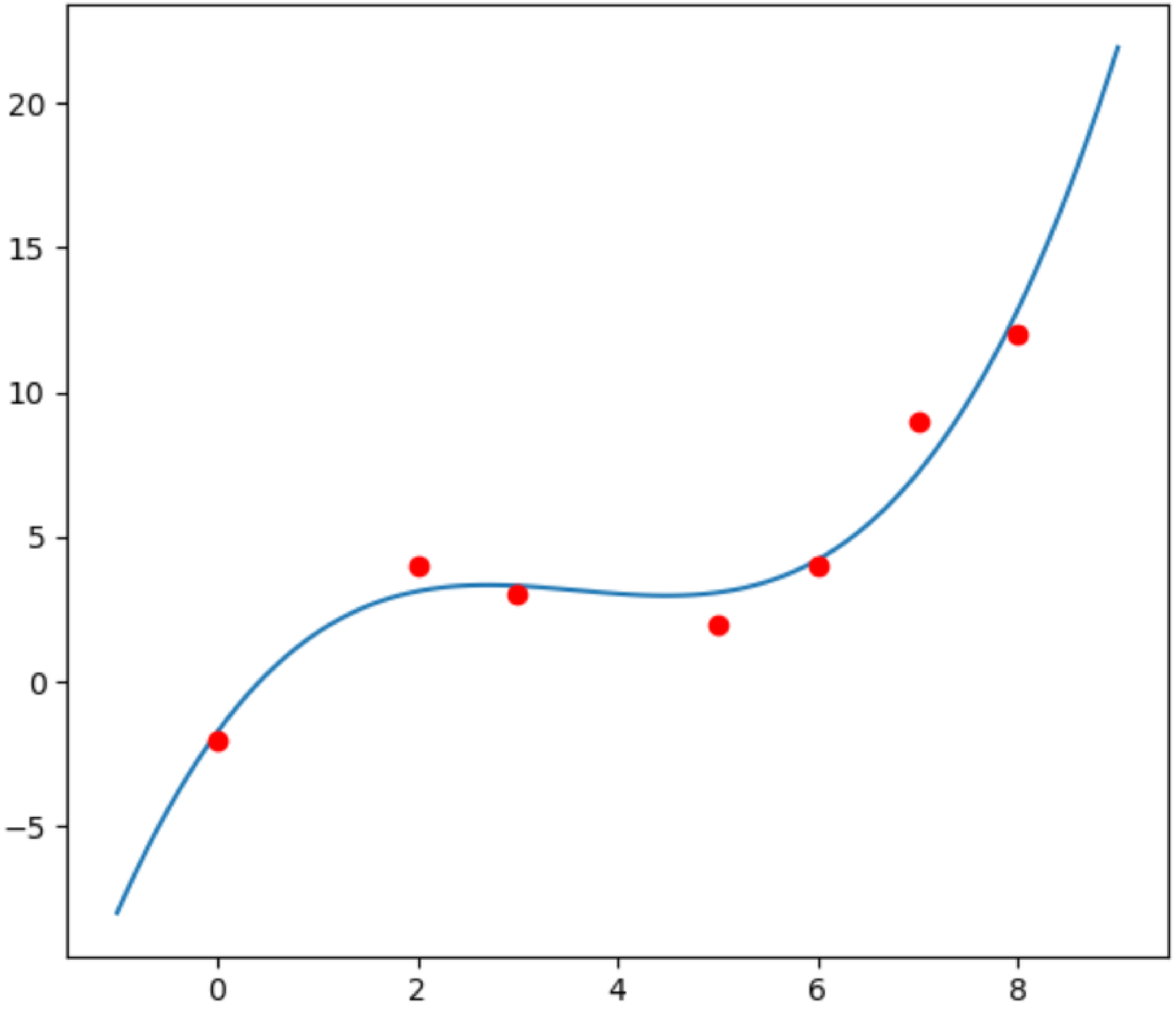
$$\sum_{i=0}^{n-1} (y_i - p(x_i))^2$$

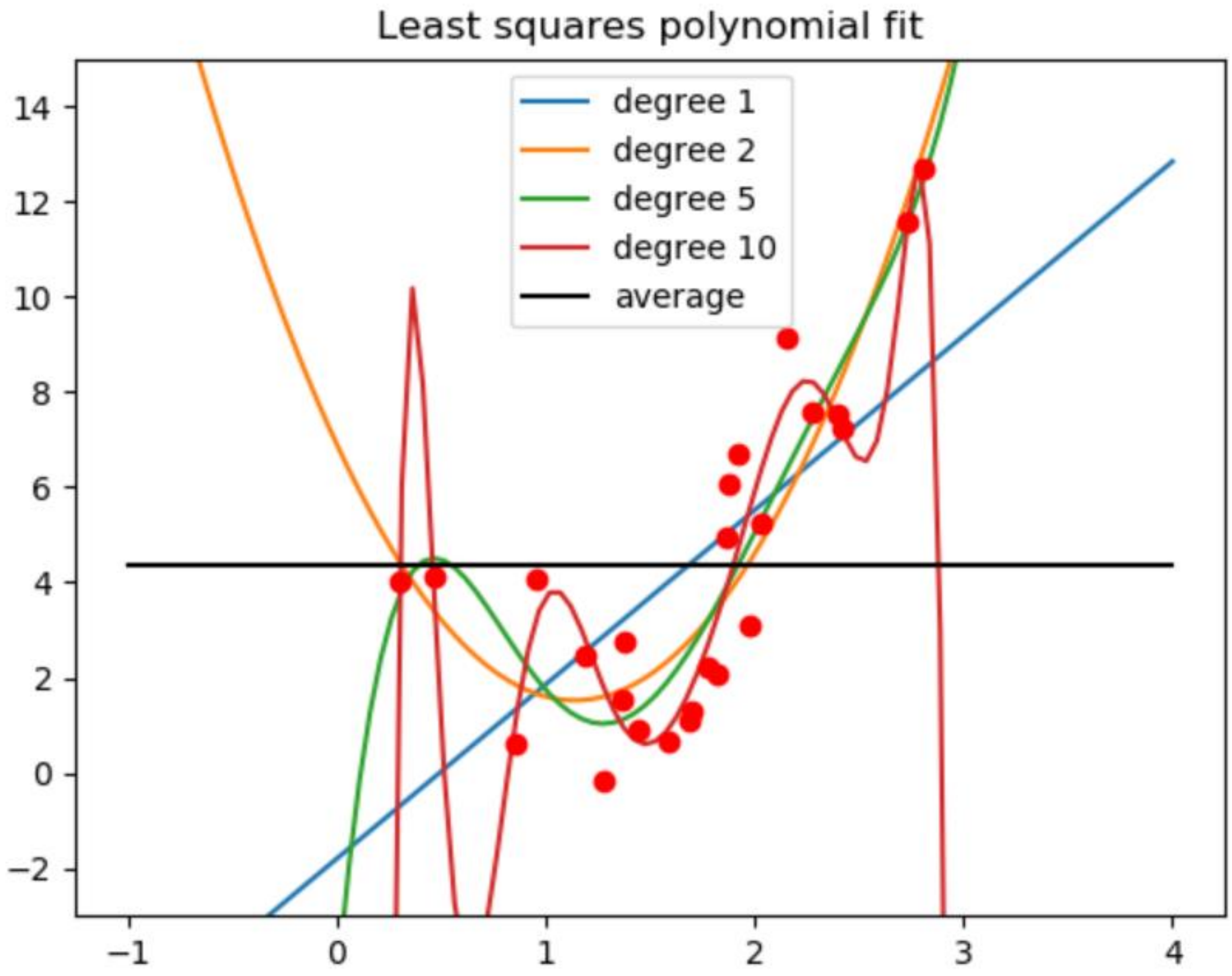
- know as least squares fit / linear regression / polynomial regression

docs.scipy.org/doc/numpy/reference/generated/numpy.polyfit.html

```
fit.py
import matplotlib.pyplot as plt
import numpy as np

x = [0, 2, 3, 5, 6, 7, 8]
y = [-2, 4, 3, 2, 4, 9, 12]

coefficients = np.polyfit(x, y, 3)

fx = np.linspace(-1, 9, 100)
fy = np.polyval(coefficients, fx)

plt.plot(fx, fy, '-')
plt.plot(x, y, 'ro')

plt.show()
```

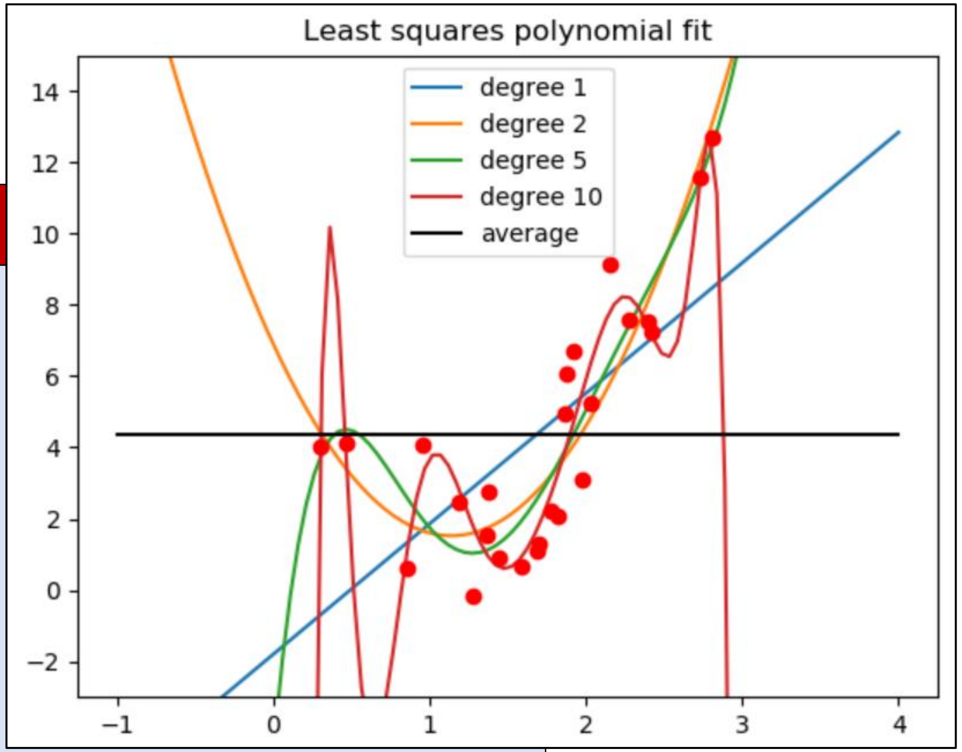
degree




Least squares polynomial fit
degree 1
degree 2
degree 5
degree 10
average
14
12
10
8
6
4
2
0
−2
−1
0
1
2
3
4

polyfit.py

```
import matplotlib.pyplot as plt
import numpy as np

x = 3 * np.random.random(25)
noise = np.random.random(x.size) ** 2
y = 5 * x ** 2 - 12 * x + 7 + 5 * noise

for degree in [1, 2, 5, 10]:
    coefficients = np.polyfit(x, y, degree)
    fx = np.linspace(-1, 4, 100)
    fy = np.polyval(coefficients, fx)
    plt.plot(fx, fy, '-', label="degree %s" % degree)

avg = np.average(y)
plt.plot(x, y, 'ro')
plt.plot([-1, 4], [avg, avg], 'k-', label="average")
plt.ylim(-3, 15)
plt.title('Least squares polynomial fit')
plt.legend()
plt.show()
```

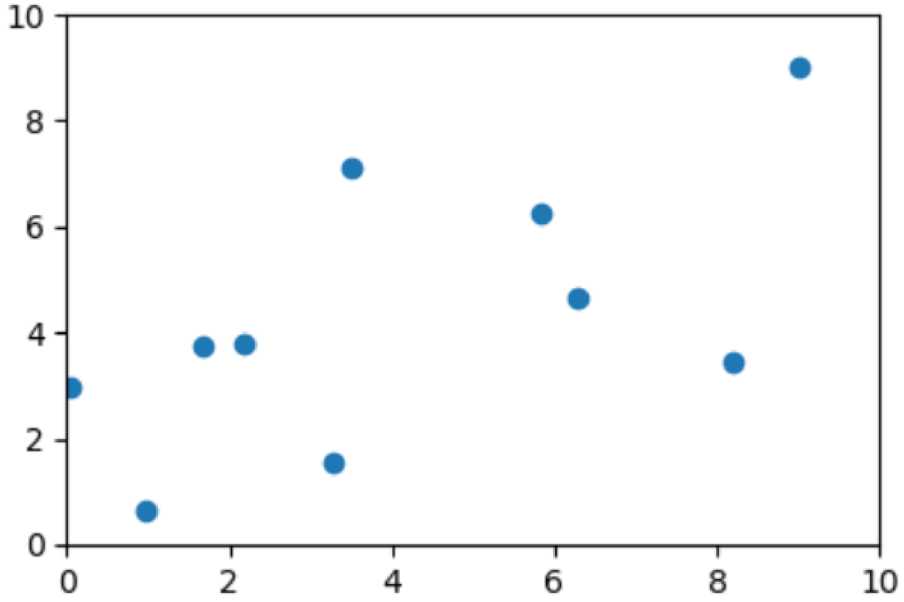


Animating bouncing balls

- matplotlib figures can be animated using

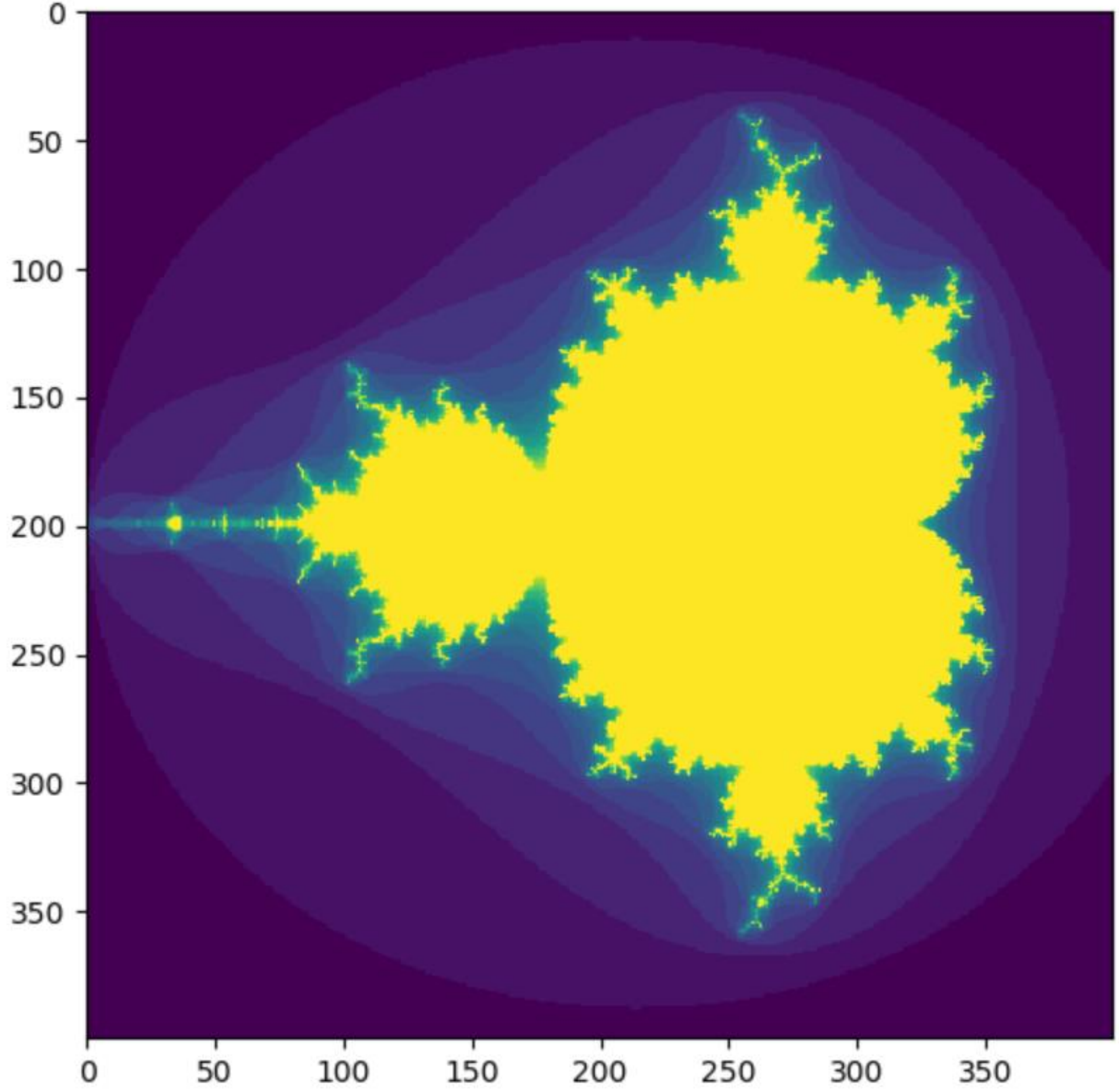
  `matplotlib.animation.FuncAnimation`

  that as arguments takes the figure to be updated/ redrawn, a function to call for each update, and an interval in milliseconds between updates

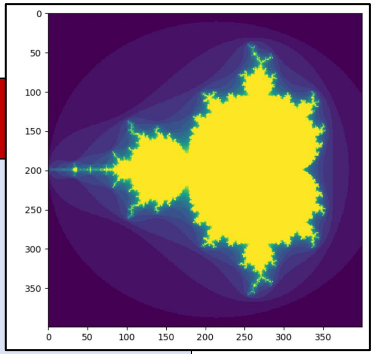


balls.py

```python
import matplotlib.pyplot as plt
from matplotlib.animation import FuncAnimation
from numpy import zeros, maximum, minimum
from numpy.random import random

g = 0.01
N = 10
x, y = 10.0 * random(N), 1.0 + 9.0 * random(N)
dx, dy = random(N) / 5, zeros(N)

fig = plt.figure()
plt.xlim(0, 10)
plt.ylim(0, 10)
balls, = plt.plot(x, y, 'o') # returns Line2D obj

def move(frame):
    global x, y, dx, dy

    x += dx
    bounce = (x > 10.0) | (x < 0.0) # numpy mask
    dx[bounce] = -dx[bounce]
    x = minimum(10.0, maximum(0.0, x))

    y += dy
    bounce = y < 0.0  # numpy mask
    y[bounce] -= dy[bounce]
    dy[bounce] = -dy[bounce]
    dy -= g

    balls.set_data(x, y)  # update positions

# removing 'ani =' causes program to fail...
ani = FuncAnimation(fig, move, interval=25)
plt.show()
```


0
50
100
150
200
250
300
350
0
50
100
150
200
250
300
350

mandelbrot.py




```python
import numpy as np
import matplotlib.pyplot as plt
def mandelbrot(h, w, maxit=20):
    '''Returns an image of the Mandelbrot fractal of size (h, w).'''
    x = np.linspace(-2.0, 0.8, w).reshape(1, w)    # row vector
    y = np.linspace(-1.4, 1.4, h).reshape(h, 1)    # column vector
    c = x + y * 1j                                 # broadcast & complex
    z = c
    divtime = np.full(z.shape, maxit, dtype=int)   # all values = maxit
    for i in range(maxit):
        z = z * z + c                              # elementwise
        diverge = z * np.conj(z) > 4               # who is diverging
        div_now = diverge & (divtime == maxit)     # who is diverging now
        divtime[div_now] = i                       # note when
        z[diverge] = 0                             # limit divergence
    return divtime                                 #   (avoids overflows)
plt.imshow(mandelbrot(400, 400))
plt.show()
```

code from docs.scipy.org/doc/numpy/user/quickstart.html