



NUMERICAL PYTHON

EE 541 – UNIT 2B



SCIENTIFIC PROGRAMMING LANGUAGES

	Fortran	C	C++	MATLAB	Python
Performance	+	+	+	0	0
Object Oriented	-	-	+	-	+
Exceptions	-	-	+	-	+
Open Source	+	+	+	-	+
Easy to Learn	0+	0	0-	+	+

- Python provides a robust platform for most possible tasks
- Strategy
 - write parts of the code that take computational cycles in C/Fortran
 - write other parts in high-level language (visualization, I/O, preprocessing)
 - Note: for heavy computational programs, 99% of CPU time on small % of code



MATLAB VS PYTHON

- MATLAB and Python share (good ideas)
 - higher level scripting (but slow)
 - fast compiled libraries
- Differences are important
 - MATLAB intended for Engineering and Computational Science tasks and combines powerful computation with visualization
 - MATLAB is commercial
 - Python is a modern general-purpose language and is easier to extend
 - For *large* projects usually best to use Python for program “glue”



PYTHON MODULES

- Bundle functions, classes, and code into a reusable package (a “library”)
- Can import any Python file as a module
- Optional `__main__` program to run on import

```
# mymod.py

def afunction():
    pass

print(f"Name is {__name__}")

# python3 mymod.py, prints: Name is __main__

# program.py
import mymod

# print: Name is mymod
```



CONDITIONAL LIBRARY

```
def afunction():
    pass

def test_for_afunction():
    print("Running test...")

if __name__ == "__main__":
    test_for_afunction()
else
    print("Setting up")
    # code to prepare if imported as a library
```



ADVANCED TECHNIQUE: LIST COMPREHENSION

- List comprehension
 - uses “set builder notation”
 - convenient to map from one list to another

```
>>> [ 2**k for k in range(10) ]  
# [1, 2, 4, 8, 16, 32, 64, 128, 256, 512, 1024]
```

```
>>> import math  
>>> xs = [0.1 * j for j in range(5)]  
>>> ys = [math.exp(x) for x in xs]
```



LIST COMPREHENSION

- Conditional List Comprehension
 - map with filter

```
>>> [k for k in range(10)]  
# [0, 1, 2, 3, 4, 5, 6, 7, 8, 9]
```

```
>>> [2*k for k in range(10) if k ** 2 > 16]  
# [10, 12, 14, 16, 18]
```



ADVANCED TECHNIQUES: RECURSION

- program where function calls itself
- conditional terminate at “base” or “terminal” case

```
def factorial(n):  
    if n == 0:  
        return 1  
    else:  
        return n * factorial(n-1)  
  
>>> factorial(6)  
720  
>>> factorial(0)  
1
```

```
def fib(n):  
    if n == 1:  
        return 1  
    elif n == 2:  
        return 1  
    else:  
        return fib(n-2) + fib(n-1)  
  
>>> fib(6)  
8
```



Random Numbers and Python



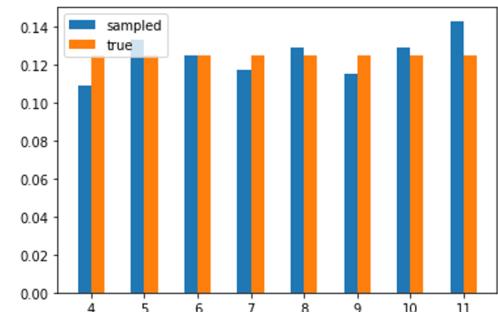
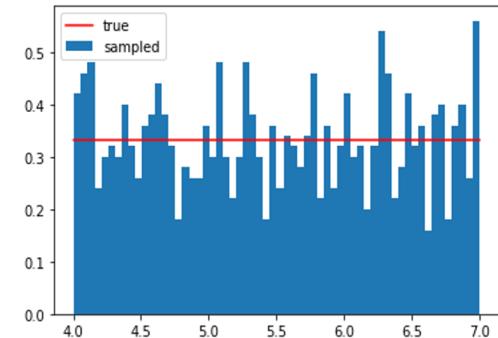
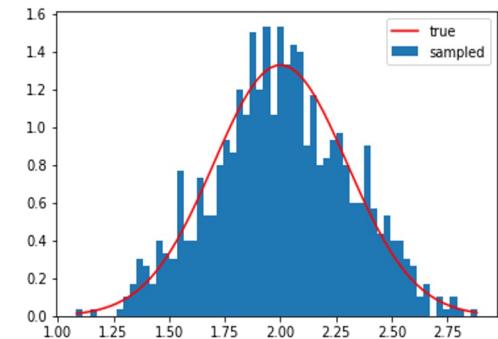
Built in python random module

- random module
- Sample (uniformly) integers, between 1-6:
 - random.randint(1, 6)
- Sample (uniformly) from a list of objects:
 - random.choice(["heads", "tails"])
- Sample from list with probability values:
 - random.choices(["rainy", "cloudy", "sunny", "foggy"], [0.1, 0.3, 0.5, 0.1])
- Shuffle a list:
 - random.shuffle(["heads", "tails", "monkey"])



Randomness with numpy, sampling

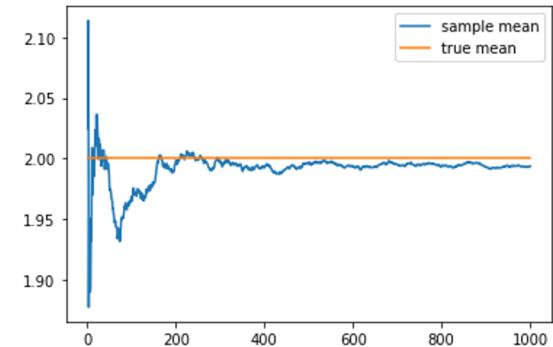
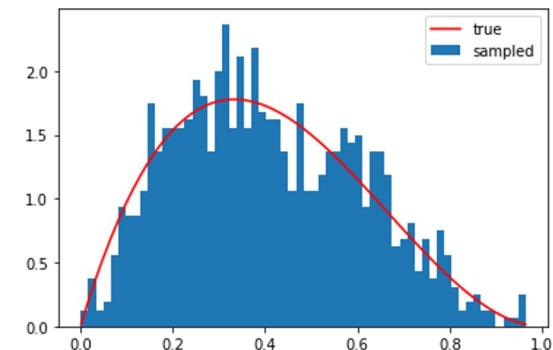
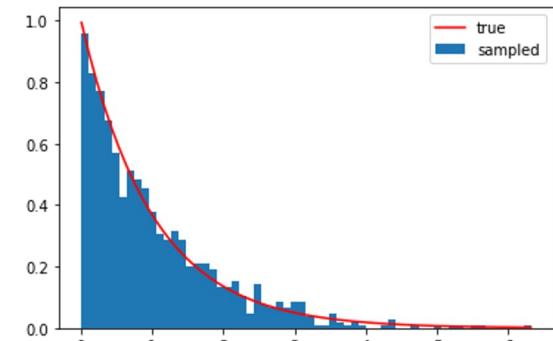
- Sample from list with probability:
 - `numpy.random.choice(["rainy", "cloudy", "sunny", "foggy"], p = [0.1, 0.3, 0.5, 0.1])`
- Sampling 1000 points from a Normal distribution, $\mu = 2$, $\sigma = 0.3$:
 - `numpy.random.normal(2, 0.3, 1000)`
- Sample 1000 points from a continuous uniformly distribution, $a = 4$, $b = 7$:
 - `numpy.random.uniform(4, 7, 1000)`
- Sample 1000 points from a discrete uniform distribution, $a = 4$, $b = 12$
 - `numpy.random.randint(4, 12, 1000)`





Randomness with numpy, sampling(cont.)

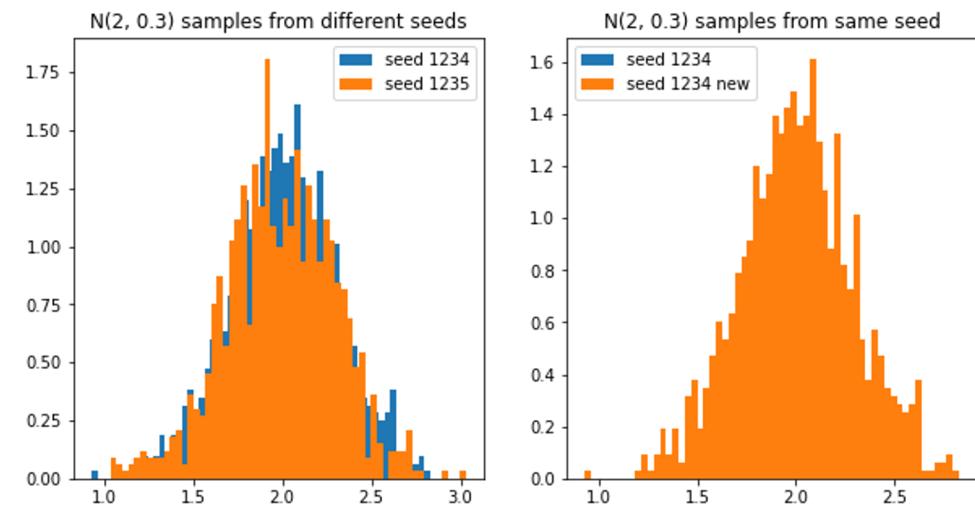
- Sampling 1000 points from an exponential distribution, $\text{lam} = 1$:
 - `numpy.random.exponential(1, 1000)`
- Sampling 1000 points from a Beta distribution, $a = 2, b = 3$:
 - `numpy.random.beta(2, 3, 1000)`
- Weak law of large numbers: Sample mean → Population mean:
 - `samples = np.random.normal(2, 0.3, 1000)`
 - `sample_means = sample.cumsum()/np.arange(1,1001)`





Randomness with numpy, seeds

- Can set seed to reproduce randomness:
 - `np.random.seed(1234)`
- Can set it on the built-in random module too:
 - `random.seed(1234)`
- Same seed generates same samples:
 - `numpy.random.normal(2, 0.3, 1000)`





NUMERIC COMPUTING



COMPUTATIONAL TASKS

- Processing data file, python and numpy (`array`)
- Generate random numbers (`numpy`)
- Linear algebra (`numpy`)
- Interpolation (`scipy.interpolate.interp`)
- Regression and curve-fit (`scipy.optimize.curve_fit`)
- Numerical integration (`scipy.integrate.quad`)
- Numerical ODE integration (`scipy.integrate.odeint`)



COMPUTATIONAL TASKS

- Root finding
 - (`scipy.optimize.fsolve`, `scipy.optimize.brentq`)
- Function minimization (`scipy.optimize.fmin`)
- Symbolic math, integration, differentiation, and generators (`sympy`)
- Analytics and data frames (`pandas`)



EXAMPLE: ROOT FINDING

- Find x_0 such that $f(x_0) = 0$.
- HW #1 - secant method
- Bisection algorithm
- Assumptions
 - Input, a and b float
 - Input f continuous with a single root in $[a, b]$, $f(a)f(b) < 0$
 - Input tol for termination tolerance (allowed error)
 - i.e., $|f(\hat{x}_0)| < tol$



BISECTION ALGORITHM

```
def (f, a, b, tol):  
    x = (a+b)/2  
    while abs(f(x)) > tol:  
        if f(x)*f(a) > 0:  
            a = x  
        else:  
            b = x  
        x = (a+b)/2  
    return x
```

```
f(cos, 1.5, 1.6, 10E-6)
```



BISECTION ALGORITHM USING SCIPY

- `scipy.optimize.bisect(f, a, b [, xtol])`
 - bisect until $|a - b| < xtol$, default $x_{tol} = 10^{-12}$

```
from scipy.optimize import bisect
```

```
def f(x):  
    return x ** 3 - 2 * x ** 2
```

```
x = bisect(f, a=1.5, b=3, xtol=1e-6)  
print(f"Root found approx x={x:14.12g}")  
# Root found approx x=2.000000023842
```



SCIPY FSOLVE ALGORITHM

```
from scipy.optimize import fsolve
# fsolve is multidimensional

def f(x):
    return x ** 3 - 2 * x ** 2

x = fsolve(f, x0=[1.6])
print(f"Root found approx x={x}")
# Root found approx x=[2.]
```



CALCULUS: DERIVATIVES

- Deep neural networks rely on robust derivative
 - But most of these have closed form and easy evaluation
- Need generic numeric methods for functions without analytic representations
- Two common methods that use a finite-difference technique
 - forward difference
 - backward difference



NUMERICAL DIFFERENTIATION

- Recall: $\frac{df}{dx}(x) = \lim_{h \rightarrow 0} \frac{f(x+h)-f(x)}{h}$
- Approximate with *forward difference* operator:

$$f'(x) \approx \frac{f(x + h) - f(x)}{h}$$

Does not require knowledge of analytic derivative, only $f(x)$

Forward difference uses $f(x)$ and $f(x + h)$

Error: $E_{fw}(h) = -h \frac{f''(x)}{2!} - \frac{h^2 f'''(x)}{3!} + \dots$

$$f'(x) \approx \frac{f(x + h) - f(x)}{h} + \textcolor{red}{\epsilon(h)}$$



IMPROVING NUMERICAL DIFFERENTIATION

- Consider *backward difference* operator:

$$f'(x) \approx \frac{f(x) - f(x - h)}{h}$$

Forward difference uses $f(x)$ and $f(x - h)$.

Similar behavior to forward.

Improve by (symmetric) combination, forward + backward (central)

$$f'(x) = \frac{f(x + h) - f(x - h)}{2h} + \sigma(h^2)$$



NUMPY



NUMPY

- numpy is an interface to high performance linear algebra libraries
 - ATLAS, LAPACK, BLAS
- Numpy's big contribution: the array object
 - very fast mathematical operations with arrays
 - linear algebra
 - fourier transforms
 - generating random numbers
- Numpy is an EXTERNAL module, not part of Python standard library



NUMPY ARRAYS ARE A SEQUENCE OF OBJECTS

- Think as vector - all objects in array must be same type

```
>>> import numpy as np
>>> a = np.array([1, 4, 16])
>>> type(a)
<class 'numpy.ndarray'>
>>> a.shape
(3,)
>>> np.sqrt(a)
array([1., 2., 4.])
>>> a > 3
array([False, True, True], dtype=bool)
```



Numpy - Datatypes

- `a = np.array([1, 2, 3, 4])`
 - `a.dtype = int64`
- `a = a.astype(np.float32)`
 - `a = [1. 2. 3. 4.]`
- `a = a.astype(np.complex64)`
 - `a = [1.+0.j 2.+0.j 3.+0.j 4.+0.j]`
- `a = a.astype(bool)`
 - `a = [True True True True]`
- `a = a.astype(str)`
 - `a = ['True' 'True' 'True' 'True']`
- `a=np.random.rand(1000000).astype(np.float64)`
 - Memory size of a = 8000000 bytes
- `b = a.astype(np.float32)`
 - Memory size of b = 4000000 bytes
- Precision loss
 - `np.sum(a - b)`
 - `8.81246785733314e-06`



CREATE ARRAYS FROM ITERABLES

```
>>> from numpy import array  
# 1Dim (vector)  
>>> a = array([1, 4, 10])  
>>> print(a)  
[1, 4, 10]  
# 2Dim (matrix)  
>>> B = array([[0, 2.5], [11, 12]])  
>>> B  
array([[0., 2.5],  
       [11., 12.]])
```



ARRAY SHAPE TUPLE: DIMENSION AND SIZE

```
>>> a.shape  
(3, )      # 1d with 3 elements  
  
>>> B.shape  
(2, 2)      # 2d with 2 x 2 = 4 elements  
  
# array.shape is mutable  
  
>>> B.shape = (4, )  
  
>>> B  
array([0., 2.5, 11., 12.])
```



ARRAY SHAPE TUPLE: DIMENSION AND SIZE

- Array shape - array.shape
- Array size - array.size
- Array dimension - array.dimension

```
mu_vector = np.array([2, 3, 4])
sigma_vector = np.array([0.3, 0.5, 0.7])
num_samples = 1000
samples = np.random.normal(mu_vector, sigma_vector, (num_samples, 3))
```

```
# inspect size, dimensions,
print("\n Multivariate normal samples shapes")
print(f"Sample shape: {samples.shape}")
print(f"Sample size: {samples.size}")
print(f"Sample dimensions: {samples.ndim}")
```

-----output-----

```
Multivariate normal samples shapes
Sample shape: (1000, 3)
Sample size: 3000
Sample dimensions: 2
```



Numpy “Empty” dimensions

- Difference between an array of shape [5,1] and [5]
- `array.T` - transpose of the array

```
# create an array with empty dimensions
d1 = np.array([1,2,3,4,5])
d2 = np.array([[1,2,3,4,5]])
d3 = np.array([[1],[2],[3],[4],[5]])
print("\n Original arrays shapes")
print(f"d1 shape: {d1.shape}")
print(f"d2 shape: {d2.shape}")
print(f"d3 shape: {d3.shape}")

# Note: d2.T is the same as
print("\n Transpose of d2 is same as d3")
print(f"d2.T = \n {d2.T}")
print(f"d3 = \n {d3}")
```

-----output-----

```
Original arrays shapes
d1 shape: (5,)
d2 shape: (1, 5)
d3 shape: (5, 1)
```

Transpose of d2 is same as d3

```
d2.T :[[1]
        [2]
        [3]
        [4]
        [5]]
```

```
d3 = [[1]
       [2]
       [3]
       [4]
       [5]]
```



Numpy - add/remove “Empty” dimensions

- original array d1: [1 2 3 4 5]
- Add an empty dimension to 0st axis using
np.newaxis
d1[np.newaxis, :] : [[1 2 3 4 5]]
- Add an empty dimension to 1th axis using
np.newaxis
d1[:, np.newaxis] : [[1
[2]
[3]
[4]
[5]]]
- Add an empty dimension to 0th axis using
np.expand_dims
np.expand_dims(d1, axis=0) : [[1 2 3 4 5]]
- Add an empty dimension to 1th axis using
np.expand_dims
np.expand_dims(d1, axis=1) : [[1
[2]
[3]
[4]
[5]]]
- Remove an empty dimension using squeeze
- Original array d2: [[1 2 3 4 5]]
- **np.squeeze(d2)** : [1 2 3 4 5]
- Original array d3: [[1
[2]
[3]
[4]
[5]]]
- np.squeeze(d3) : [1 2 3 4 5]



ARRAY LENGTH AND MEMORY ALLOCATION

```
>>> a.size
```

```
3
```

```
>>> B.size
```

```
4
```

```
>>> a.nbytes
```

```
12
```

```
>>> B.nbytes
```

```
32
```



ARRAY ELEMENTS MUST ALL BE SAME TYPE

```
>>> a.dtype  
dtype('int64')  
>>> B.dtype  
dtype('float64')  
  
# type assignable on create  
>>> a2 = array([1, 4, 10], numpy.float)  
>>> a2.dtype  
dtype('float64')
```



CREATE FIXED SIZE ARRAY – FILL WITH 0 OR 1

```
>>> numpy.zeros( (3, 3) )    # tuple  
array([[0., 0., 0.],  
       [0., 0., 0.],  
       [0., 0., 0.]])  
  
>>> numpy.zeros( (4, ) )      # same:  
numpy.zeros(4)  
array([0., 0., 0., 0.])  
  
>>> numpy.ones( (2, 4) )  
array([[1., 1., 1., 1.],  
       [1., 1., 1., 1.]])
```



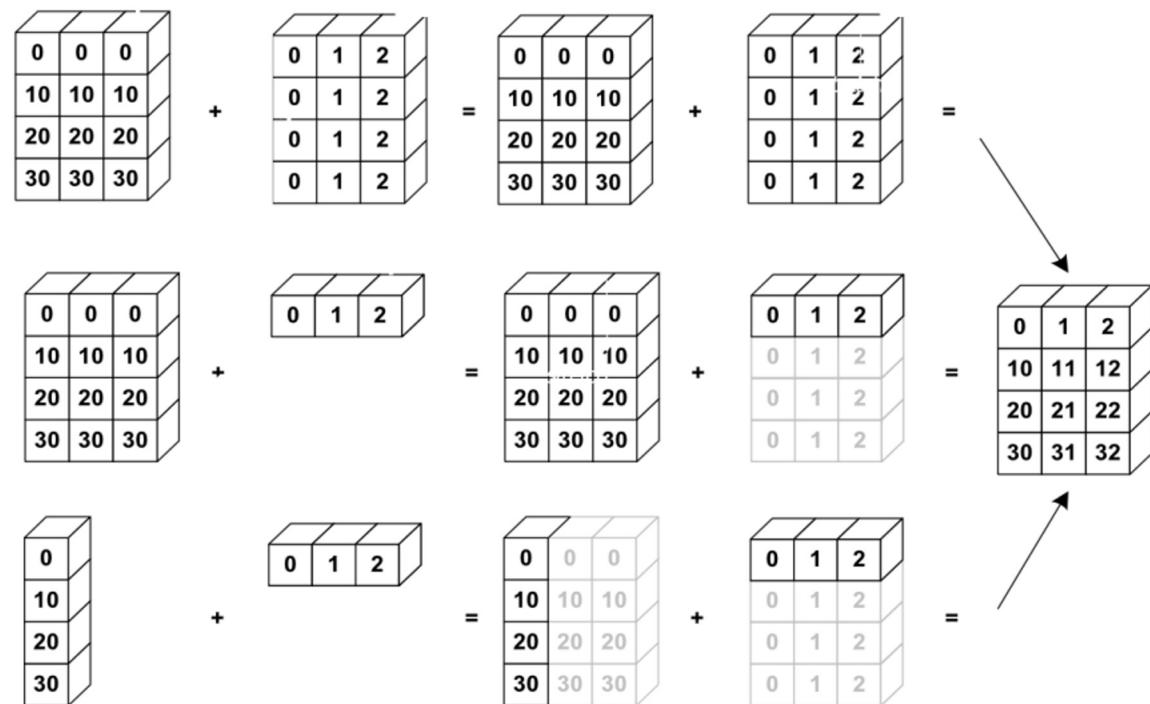
ARRAY INDEXING

```
>>> x = numpy.array(range(0, 10, 2))          # length 5
>>> x[4]                                     # 8
>>> len(x)                                    # 5
>>> x.shape                                   # (5, )
>>> C = numpy.arange(12)
>>> C.shape = (3,4)
array([[0, 1, 2, 3],
       [4, 5, 6, 7],
       [8, 9, 10, 11]])
>>> C[0, 0]                                    # 0
>>> C[2, -1]                                   # 11
>>> C[-1, -1]                                  # 11
```



ARRAY BROADCASTING

- NumPy compares shapes when operating on multiple shapes.
- Two dimensions are compatible if:
 1. Equal size, or
 2. One size = 1





Array Operations

$a = [1 2 3 4]$

$b = [5 6 7 8]$

- Element-wise addition/subtraction:
 - $a + b = [6 8 10 12]$
- Element-wise multiplication/division:
 - $a * b = [5 12 21 32]$
- Element-wise exponent
 - $a^{**} b = [1 64 2187 65536]$
- Scalar Operations
 - $a + 1 = [2 3 4 5]$



VECTOR OPERATIONS

- Inner product
- Outer product
- Dot product (matrix multiplication)

```
>>> u = [1, 2, 3]
>>> v = [1, 1, 1]
>>> np.inner(u, v)
6
>>> np.outer(u, v)
array([[1, 1, 1], [2, 2, 2], [3, 3, 3]])
>>> np.dot(u, v)
6
```



NP.DOT

`numpy.dot(a, b, out=None)`

Dot product of two arrays. Specifically,

- If both a and b are 1-D arrays, it is inner product of vectors (without complex conjugation).
- If both a and b are 2-D arrays, it is matrix multiplication, but using `matmul` or $a @ b$ is preferred.
- If either a or b is 0-D (scalar), it is equivalent to `multiply` and using `numpy.multiply(a, b)` or $a * b$ is preferred.
- If a is an N-D array and b is a 1-D array, it is a sum product over the last axis of a and b .
- If a is an N-D array and b is an M-D array (where $M \geq 2$), it is a sum product over the last axis of a and the second-to-last axis of b :

```
dot(a, b)[i,j,k,m] = sum(a[i,j,:] * b[k,:,:m])
```

<https://numpy.org/doc/stable/reference/generated/numpy.dot.html>



OPERATIONS OVER AXES

```
a = np.random.random((2,3))
# array([[ 0.9190687 ,  0.36497813,  0.75644216],
       [ 0.91938241,  0.08599547,  0.49544003]])
a.sum()
# 3.5413068994445549
a.sum(axis=0) # column sum (aggregate over rows)
# array([ 1.83845111,  0.4509736 ,  1.25188219])
a.cumsum(axis=1) # cumulative row sum
# array([[0.9190687, 1.28404683, 2.04048899],
       [0.91938241, 1.00537788, 1.50081791]])
a.min()
# 0.0859954690403677
a.max(axis=0)
# array([ 0.91938241,  0.36497813,  0.75644216])
```



COPY AND RESHAPING ARRAY

```
>>> copy_x = x[:]                      # or copy_x = x[::]  
>>> rev_x = x[::-1]  
>>> zero_x = numpy.zeros(x.shape)
```

- Reshape arrays with `np.reshape()`
 - “Total” size must remain the same (number of elements)
- Reshape arrays with `np.resize()`
 - Always works
 - Chops or appends zero
 - First dimension(s) have fill priority
 - Can lead to unexpected results



Numpy - Reshape/Resize

- original array d1: [1 2 3 4 5]
- Resize an array using **np.resize**
- `np.resize(d1, (5, 1))` : [[1]
[2]
[3]
[4]
[5]]
- Reshape an array using **np.reshape**
- `np.reshape(d1, (5, 1))` : [[1]
[2]
[3]
[4]
[5]]
- Original array d4: [[[1 2 0 7]
[4 1 4 5]
[3 1 8 1]]]
[[9 9 2 3]
[0 2 9 7]
[9 8 1 8]]]
- `np.reshape(d4, (6, 4))` : [[1 2 0 7]
[4 1 4 5]
[3 1 8 1]
[9 9 2 3]
[0 2 9 7]
[9 8 1 8]]]



HIGHER DIMENSIONAL ARRAY SLICING

- Identical to 1-D but applied per component

```
>>> C  
array([0, 1, 2, 3],  
      [4, 5, 6, 7],  
      [8, 9, 10, 11]])  
>>> C[0, :]          # row 0  
array([0, 1, 2, 3])  
>>> C[:, 1]         # col 1  
array([1, 5, 9])
```



USEFUL LINEAR ALGEBRA OPERATIONS

```
>>> import numpy.linalg
```

- `pinv`
 - **matrix pseudo-inverse**
- `svd`
 - **singular value decomposition**
- `det`
 - **matrix determinant**
- `eig`
 - **eigenvalue and eigenvector pairs**



Numpy - Matrix Operations

- $a =$
[[1 2 3]
[4 5 6]
[7 8 9]]
- $b =$
[[1 2 4]
[4 2 6]
[1 8 9]]
- Matrix multiplication
 - $a @ b =$
[[12 30 43]
[30 66 100]
[48 102 157]]
- Note this is different from element-wise multiplication
 - $a * b =$
[[1 4 12]
[16 10 36]
[7 64 81]]
- Matrix transpose
 - $a.T =$
[[1 4 7]
[2 5 8]
[3 6 9]]
- Matrix inverse (if matrix is invertible)
 - a is not invertible
 - $b^{-1} = \underline{\text{np.linalg.inv}}(b) =$
[[-1. 0.46666667 0.13333333]
[-1. 0.16666667 0.33333333]
[1. -0.2 -0.2]]
- Matrix determinant
 - $\det(a) = \underline{\text{np.linalg.det}}(a) = 0.0$
 - $\det(b) = \text{np.linalg.det}(b) = 30.0$



SOLVING A LINEAR SYSTEM OF EQUATIONS

- `numpy.linalg.solve(A, b)` solves $Ax = b$ for square matrix A and vector b . Return solution vector x as an array.

```
>>> A = numpy.array([[1, 0], [0, 2]])  
>>> b = numpy.array([1, 4])  
>>> from numpy import linalg as LA  
>>> x = LA.solve(A, b)  
array([1., 2.])  
>>> numpy.dot(A, x) # verify = b  
array([1., 4.])
```



MATPLOTLIB



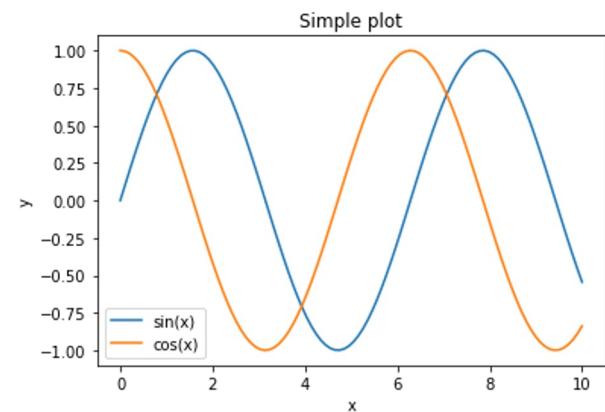
PLOTTING WITH MATPLOTLIB

- Matplotlib is the de facto plotting library
 - keep easy tasks easy, and hard tasks possible
- Full 2D+3D plotting library
 - publication quality figures
- Can run fully scripted
 - or Interactive
- Jupyter/IPython configurations
 - `%matplotlib inline`
 - `%matplotlib qt`
 - `%matplotlib notebook`



Line Plot

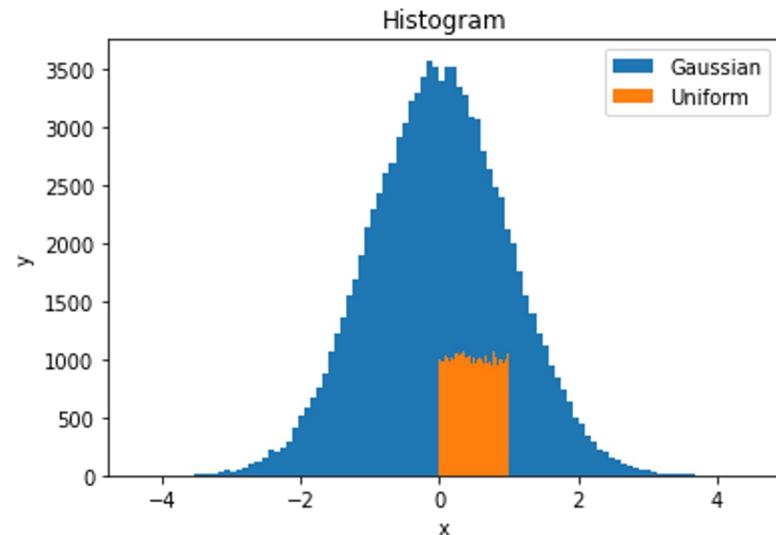
```
x = np.linspace(0, 10, 100)
y = np.sin(x)
z = np.cos(x)
plt.plot(x, y, label="sin(x)")
plt.plot(x, z, label="cos(x)")
plt.xlabel("x")
plt.ylabel("y")
plt.title("Simple plot")
plt.legend()
plt.show()
```



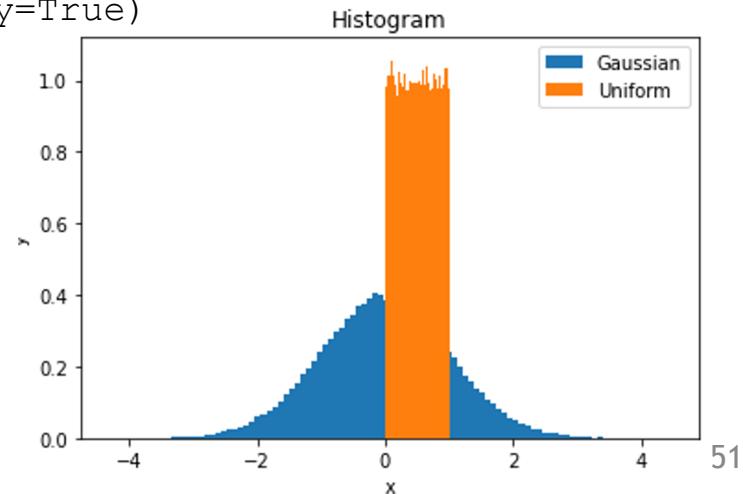


Histogram

```
x = np.random.randn(100000)
y = np.random.uniform(0, 1, 100000)
plt.hist(x, bins=100, label="Gaussian")
plt.hist(y, bins=100, label="Uniform")
plt.xlabel("x")
plt.ylabel("y")
plt.title("Histogram")
plt.legend()
plt.show()
```



```
plt.hist(x, bins=100, label="Gaussian", density=True)
plt.hist(y, bins=100, label="Uniform", density=True)
plt.xlabel("x")
plt.ylabel("y")
plt.title("Histogram")
plt.legend()
plt.show()
```



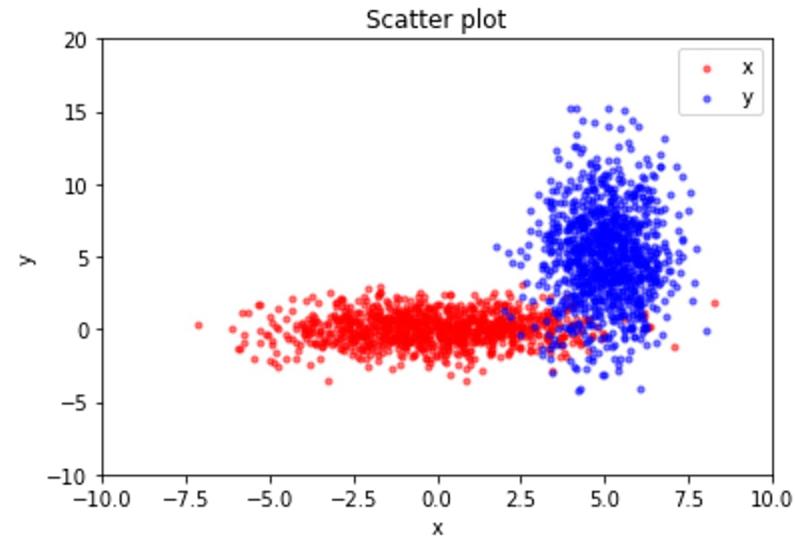


Scatter plots

```
# scatter plots
# generate two 2D gaussian samples
x = np.random.multivariate_normal([0, 0], [[5, 0], [0, 1]], 1000)
y = np.random.multivariate_normal([5, 5], [[1, 0], [0, 10]], 1000)

# plot the samples
plt.scatter(x[:, 0], x[:, 1], label="x", color="red", alpha=0.5, s=10)
plt.scatter(y[:, 0], y[:, 1], label="y", color="blue", alpha=0.5, s=10)
plt.xlabel("x")
plt.ylabel("y")
plt.title("Scatter plot")
# set axis limits
plt.xlim(-10, 10)
plt.ylim(-10, 20)

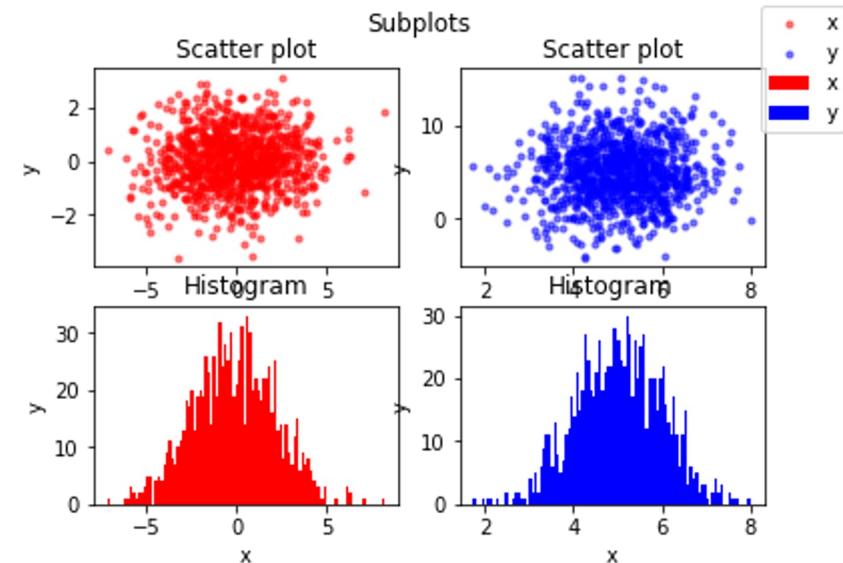
plt.legend()
plt.show()
```





Subplots

```
fig, ax = plt.subplots(2, 2)
ax[0, 0].scatter(x[:, 0], x[:, 1], label="x", color="red", alpha=0.5, s=10)
ax[0, 1].scatter(y[:, 0], y[:, 1], label="y", color="blue", alpha=0.5, s=10)
ax[1, 0].hist(x[:, 0], bins=100, label="x", color="red")
ax[1, 1].hist(y[:, 0], bins=100, label="y", color="blue")
# set labels for all subplots
for i in range(2):
    for j in range(2):
        ax[i, j].set_xlabel("x")
        ax[i, j].set_ylabel("y")
# set titles for each subplot
ax[0, 0].set_title("Scatter plot")
ax[0, 1].set_title("Scatter plot")
ax[1, 0].set_title("Histogram")
ax[1, 1].set_title("Histogram")
# set title for the whole figure
fig.suptitle("Subplots")
# set legend for the whole figure
fig.legend()
# increase space between upper and lower subplots
fig.subplots_adjust(hspace=0.5)
plt.show()
```



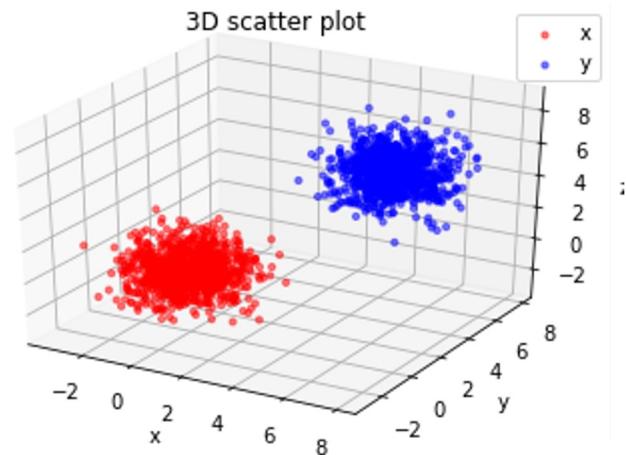


3D scatter

```
# create a simple 3d figure
fig = plt.figure()
ax = fig.add_subplot(111, projection="3d")

# generate 3D gaussian samples
x = np.random.multivariate_normal([0, 0, 0], [[1, 0, 0], [0, 1, 0], [0, 0, 1]], 1000)
y = np.random.multivariate_normal([5, 5, 5], [[1, 0, 0], [0, 1, 0], [0, 0, 1]], 1000)

# plot the samples
ax.scatter(x[:, 0], x[:, 1], x[:, 2], label="x", color="red", alpha=0.5, s=10)
ax.scatter(y[:, 0], y[:, 1], y[:, 2], label="y", color="blue", alpha=0.5, s=10)
ax.set_xlabel("x")
ax.set_ylabel("y")
ax.set_zlabel("z")
ax.set_title("3D scatter plot")
ax.legend()
plt.show()
```

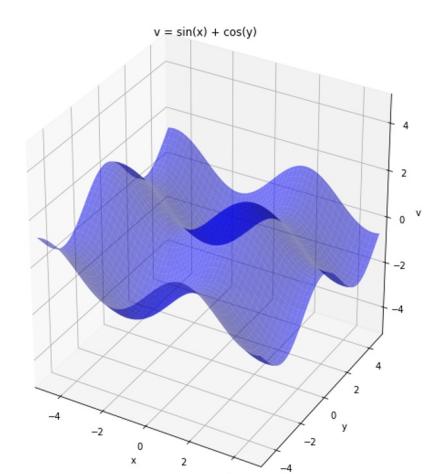
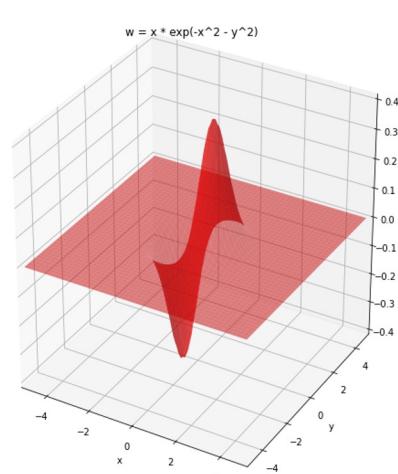




3D Mesh

```
x = np.linspace(-5, 5, 100)
y = np.linspace(-5, 5, 100)
x, y = np.meshgrid(x, y)
v = np.sin(x) + np.cos(y)
w = x*np.exp(-x**2 - y**2)
fig = plt.figure(figsize=(20, 10))
ax1 = fig.add_subplot(121, projection="3d")
ax1.plot_surface(x, y, w, label="w", color="red", alpha=0.5)
ax2 = fig.add_subplot(122, projection="3d")
ax2.plot_surface(x, y, v, label="v", color="blue", alpha=0.5)
ax1.set_xlabel("x")
ax1.set_ylabel("y")
ax1.set_zlabel("w")
ax1.set_title("w = x * exp(-x^2 - y^2)")
ax2.set_xlabel("x")
ax2.set_ylabel("y")
ax2.set_zlabel("v")
ax2.set_title("v = sin(x) + cos(y)")
ax1.set_xlim(-5, 5)
ax1.set_ylim(-5, 5)
ax1.set_zlim(-0.4, 0.4)
ax2.set_xlim(-5, 5)
ax2.set_ylim(-5, 5)
ax2.set_zlim(-5, 5)
fig.suptitle("3D Subplots")
```

3D Subplots





MATPLOTLIB.PYTHON

- `Matplotlib.pyplot` is object-oriented plotting interface
 - fine grained control over all aspects of plotting
- Impressive demo gallery

<https://matplotlib.org/2.0.2/gallery.html>

- Instructive demo notebook

<https://www.desy.de/~fangohr/teaching/csds2019/notebooks/Matplotlib.html>



FUNCTIONAL PROGRAMMING



FUNCTIONAL TOOLS

- List processing is a common pattern
- `for`-loops are conceptually simple
 - not compact and not always performant
- Other options:
 - list comprehension
 - map, filter, and reduce (lambda functions)



LAMBDA FUNCTIONS ARE ANONYMOUS FUNCTIONS

Useful to define small *helper* functions - usually single purpose use

```
>>> lambda a: a
<function <lambda> at 0x319c60>
>>> lambda a: 2 * a
<function <lambda> at 0x319ce0>
>>> (lambda a: 2 * a)(10)
20
>>> (lambda x, y, z: (x + y) * z)(10, 20, 2)
60
>>> type(lambda x, y: x + y)
<type 'function'>
```



LAMBDA VS DECLARED FUNCTION

```
from scipy.integrate import quad
def f(x):
    return x * x    # x^2
y, abserr = quad(f, a=0, b=2)
print(f"Int f(x)=x^2 from 0 to 2 = {y} +/- {abserr}")
```

```
from scipy.integrate import quad
y, abserr = quad(lambda x: x * x, a=0, b=2)
print(f"Int f(x)=x^2 from 0 to 2 = {y} +/- {abserr}")
```



HIGHER ORDER FUNCTIONS

- functions that take or return functions
- `map(function, iterable) → iterable`
 - apply function each element in iterable, returns a new iterable
- `filter(function, iterable) → iterable`
 - return new iterable containing only elements with `function(item)` is true
- `reduce(function, iterable, initial) → value`
 - apply `function(x, y)` from left to right - reduces iterable to single value



MAPPING ITERABLES

```
>>> def f(x): return x ** 2
>>> map(f, [0, 1, 2, 3, 4])
<map object at 0x1026a52e0>
>>> list(map(f, [0, 1, 2, 3, 4]))
[0, 1, 4, 9, 16]
>>> list(map(lambda x: x ** x, [0, 1, 2, 3, 4]))
>>> [x ** 2 for x in [0, 1, 2, 3, 4]]
```



```
>>> import math
>>> list(map(math.exp, [0, 0.1, 1.]))
```



FILTERING ITERABLES

```
>>> c = "The quick brown fox jumps".split()  
['The', 'quick', 'brown', 'fox', 'jumps']  
>>> list(map(lambda s: len(s) > 4, c))  
[False, True, True, False, True]  
>>> list(filter(lambda s: len(s) > 4, c))  
['quick', 'brown', 'jumps']  
  
# compare  

```



REDUCE AN ITERABLE TO A VALUE

```
>>> from functools import reduce
>>> def f(x, y):
...     print(f"Called with x={x}, y={y}")
...     return x + y
>>> reduce(f, [1, 3, 5], 0)
9
>>> reduce(f, [1, 3, 5], 100)
109
```



FUNCTIONAL PROGRAMMING

- map, reduce, and filter are common across language
 - allows consistent patterns to deal with lists and iterables
- they functionally abstract common loop tasks
- Recommendation: use these instead of loops (or list comprehension)
 - loops are tedious (and error prone)
 - these functional equivalents often clearer to read
 - resulting code *can* be faster (lambda functions can be slower)
 - if you need to use lambda. often better off with list comprehension



SCIPY



SCIENTIFIC PYTHON (SCIPY)

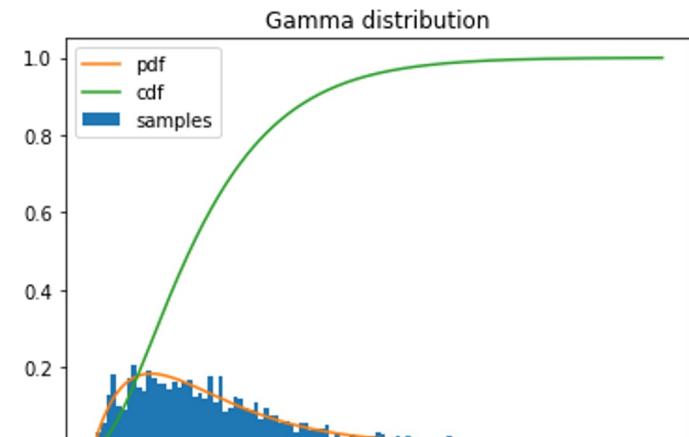
- > stats Statistical functions
- > sparse Sparse matrices
- > linalg Linear algebra
- > signal Signal processing
- > interpolate Interpolation
- > optimize Optimization
- > cluster Vector quantization / K-means
- > fftpack Discrete Fourier Transforms
- > Integrate Integration



SCIPY - stats

```
# with stats we have access to a lot of statistical distributions, their pdfs, cdfs, their moments, tests, etc.
```

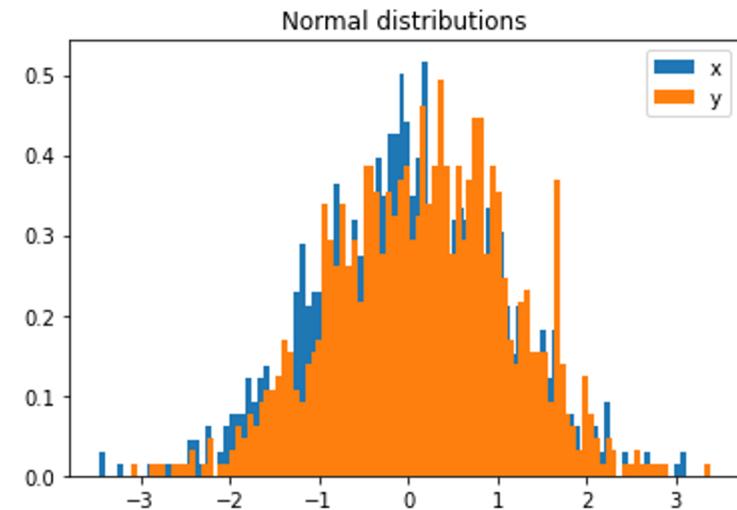
```
x = stats.gamma.rvs(2, scale=2, size=1000)
plt.hist(x, bins=100, density=True, label="samples")
x = np.linspace(0, 20, 1000)
plt.plot(x, stats.gamma.pdf(x, 2, scale=2), label="pdf")
plt.plot(x, stats.gamma.cdf(x, 2, scale=2), label="cdf")
```



```
# statistical tests
```

```
x = stats.norm.rvs(0, 1, size=1000)
y = stats.norm.rvs(0.15, 1, size=1000)
plt.hist(x, bins=100, density=True, label="x")
plt.hist(y, bins=100, density=True, label="y")
print(stats.ttest_ind(x, y))

#Ttest_indResult(statistic=-3.357944448803533,
pvalue=0.0007999795533366586)
```





SCIPY - sparse

```
# with sparse we can work with sparse matrices, to save memory and speed up computations
# example: create a 1000x1000 matrix with 1s on the diagonal and 0s everywhere else
x = sparse.eye(1000, 1000)

# create corresponding dense matrix
x_dense = x.todense()

# print the memory usage of the sparse and dense matrices
print(x.data.nbytes, x_dense.nbytes)
# 8000 8000000

# perform matrix multiplication
%timeit x_dense.dot(x_dense)
%timeit x.dot(x)
# 82.4 ms ± 23.3 ms per loop (mean ± std. dev. of 7 runs, 10 loops each)
# 507 µs ± 23.3 µs per loop (mean ± std. dev. of 7 runs, 1000 loops each)
```



SCIPY - linalg

```
from scipy import linalg
# with linalg we can perform linear algebra operations like matrix
multiplication, solving linear systems, singular value
decomposition, get eigenvalues and eigenvectors, etc.

# SVD
x = np.array([[1, 4, 2], [6, 3, 0], [5, 2, 1], [2, 1, 3], [4, 5,
2]])
u, s, vh = linalg.svd(x)

# solve a linear system
# create a 3x3 matrix with random values, non singular
A = np.array([[1, 2, 3], [6, 3, 0], [5, 2, 1]])
# create a 3x1 vector with random values
b = np.array([1, 2, 3])
x = linalg.solve(A, b)

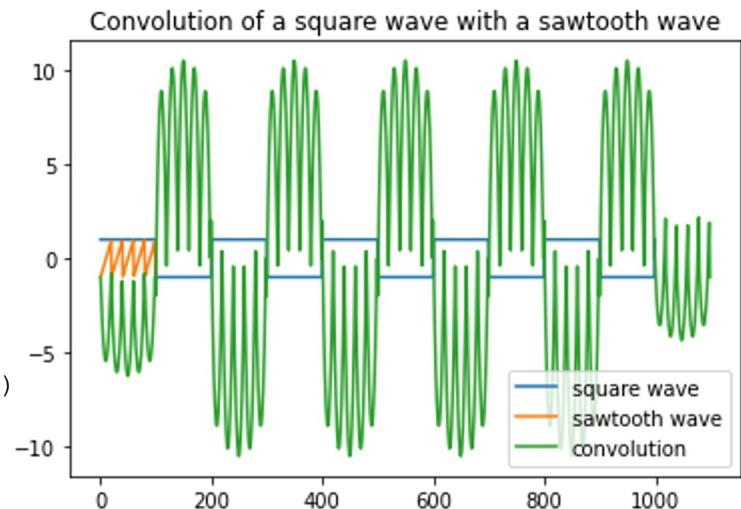
# get the eigenvalues and eigenvectors of a matrix
A = np.array([[1, 2, 3], [6, 3, 0], [5, 2, 1]])
eigenvalues, eigenvectors = linalg.eig(A)
```



SCIPY - signal

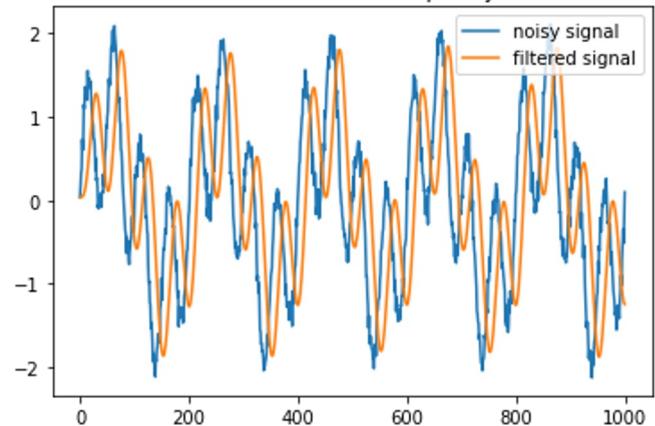
```
# signal processing from scipy
from scipy import signal
# with signal we can perform signal processing operations
# like filtering, convolution, etc.

# create a 1000x1 vector with square wave values
x = signal.square(2 * np.pi * 5 * np.linspace(0, 1, 1000))
# create a 100x1 vector with a sawtooth wave
h = signal.sawtooth(2 * np.pi * 5 * np.linspace(0, 1, 100))
# perform convolution
y = signal.convolve(x, h)
```



```
# filter a signal
# create a 1000x1 vector with sine wave values with frequency
# component 5 and 20
base = np.linspace(0, 1, 1000)
x = np.sin(2 * np.pi * 5 * base) + np.sin(2 * np.pi * 20 * base)
# add some noise
x += np.random.randn(len(x)) * 0.1
# create a butterworth filter
b, a = signal.butter(3, 0.05)
# apply the filter
zi = signal.lfilter_zi(b, a)
z, _ = signal.lfilter(b, a, x, zi=zi*x[0])
```

Filtering a noisy signal with a butterworth filter of order 3 and cutoff frequency 0.05





SCIPY - INTERPOLATION EXAMPLE

```
import numpy as np
import scipy.interpolate
import pylab

def create_data(n):
    """Given integer n return n data points x and y values"""
    xmax = 5.
    x = np.linspace(0, xmax, n)
    y = -x ** 2
    y += 1.5 * np.random.normal(size=len(x))      # additive
    Gaussian noise
    return x, y

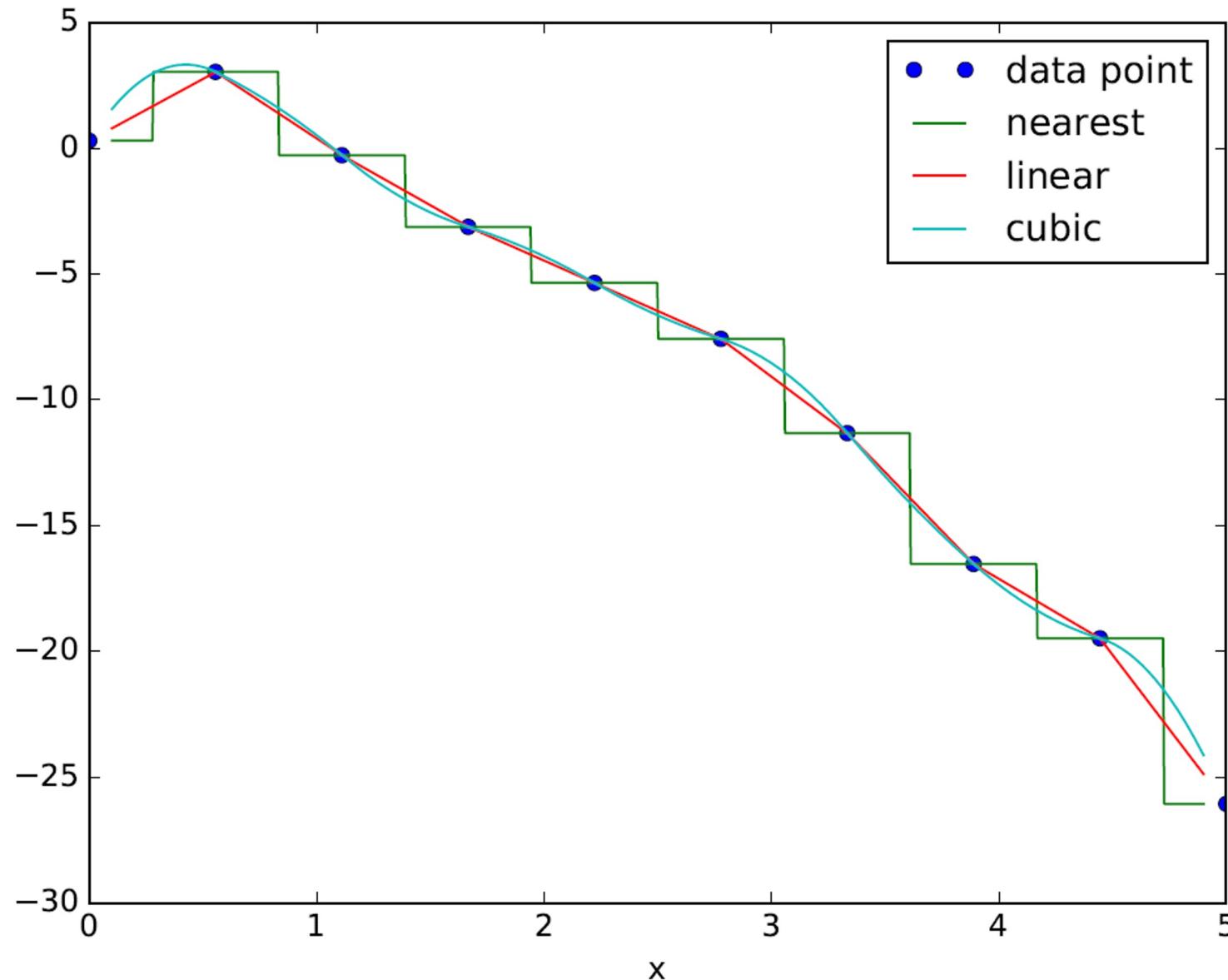
[...]
```



```
n = 10
x, y = create_data(n)
# plot mesh
xf = np.linspace(0.1, 4.9, n * 100)
# piecewise const, linear, quadratic
y0 = scipy.interpolate.interp1d(x, y, kind="nearest")
y1 = scipy.interpolate.interp1d(x, y, kind="linear")
y2 = scipy.interpolate.interp1d(x, y, kind="quadratic")

pylab.plot(x, y, 'o', label='data')
pylab.plot(xf, y0(xf), label='nearest')
pylab.plot(xf, y1(xf), label='linear')
pylab.plot(xf, y2(xf), label='quadratic')

pylab.legend()
pylab.xlabel('x')
pylab.show()
```





SCIPY - optimize CURVE FITTING EXAMPLE

```
import numpy as np
import scipy.optimize
import pylab

def create_data(n):
    """Given integer n return n data points x and y values"""
    xmax = 5.
    x = np.linspace(0, xmax, n)
    y = -x ** 2
    y += 1.5 * np.random.normal(size=len(x))      # additive Gaussian noise
    return x, y

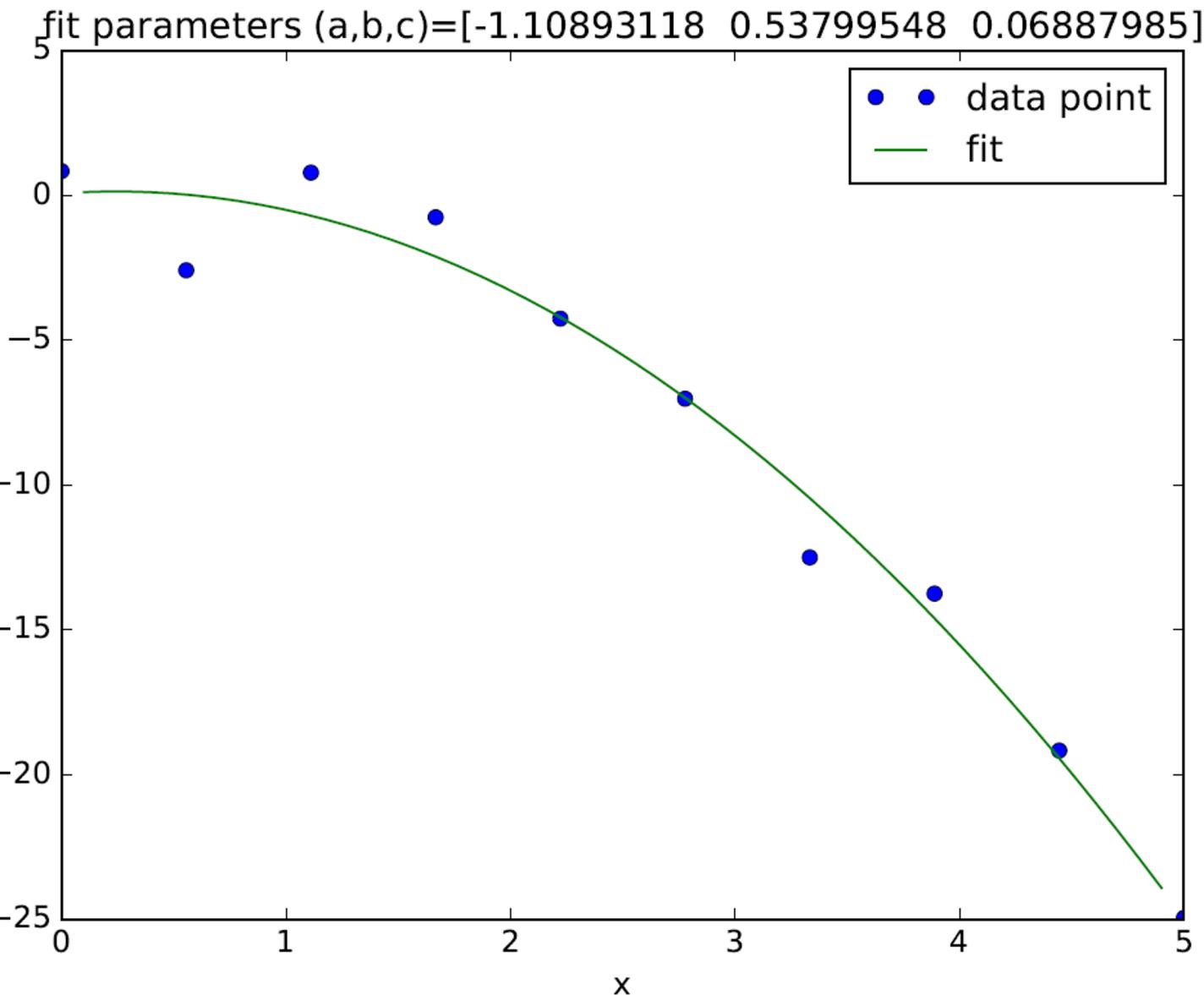
def model(x, a, b, c):
    return a * x ** 2 + b * x + c
```



```
n = 10
x, y = create_data(n)
# fit
p, pcov = scipy.optimize.curve_fit(model, x, y)
a, b, c = p
# plot mesh
xf = np.linspace(0.1, 4.9, n * 100)

pylab.plot(x, y, 'o', label='data')
pylab.plot(xf, model(xf, a, b, c), label='fit')

pylab.title(f"fit parameters (a,b,c)=({{a}},{ {b}},{ {c}}) ")
pylab.legend()
pylab.xlabel('x')
pylab.show()
```





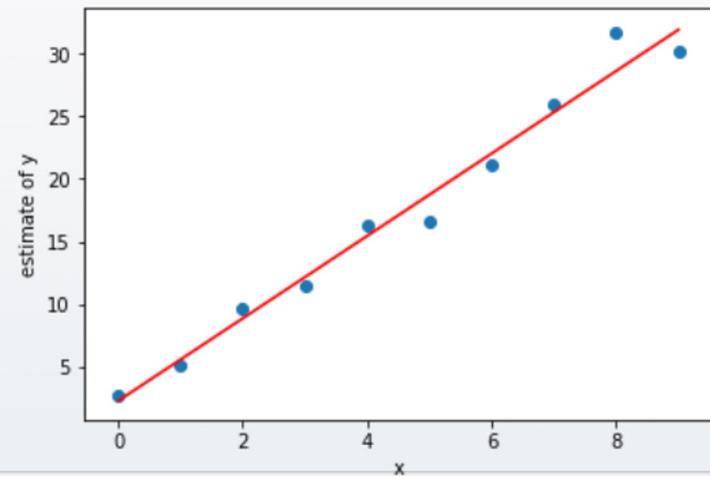
REGRESSION (CURVE-FITTING) FROM DATA

- Assume: data generated with known model + noise
- Guess: at model in practice (e.g., linear)
- Choose: parameters to minimize error

```
from scipy import stats
import numpy as np
import matplotlib.pyplot as plt

x = np.arange(10)
y = 3*x+4
y = y + np.random.normal(0,2,10)
slope, intercept, r_value, p_value, std_err = stats.linregress(x,y)
y_hat = intercept + slope * x

fig = plt.figure()
plt.plot(x,y_hat, color='r')
plt.scatter(x,y)
plt.xlabel("x")
plt.ylabel("estimate of y")
#axes = plt.gca()
#axes.set_xlim([-1, 4])
```





DEFINITE INTEGRAL EXAMPLE

```
from math import cos, exp, pi
from scipy.integrate import quad

def f(x):
    return exp(cos(-2 * x * pi)) + 3.2

# integrate [-2, 2]
res, err = quad(f, -2, 2)

print(f"Result is: {res} +/- {err}")
# The numerical result is 17.864264 (+-1.55117e-11)
```



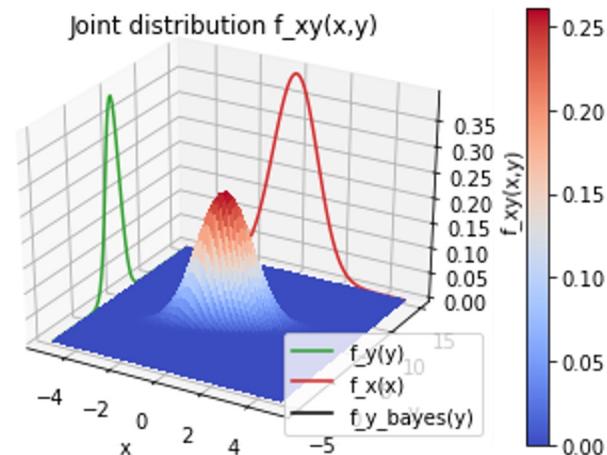
DEFINITE INTEGRAL EXAMPLE (Bayesian partition integral)

```
from scipy import integrate
import scipy
```

```
mu = np.array([0, 4])
sigma = np.array([[1, 0.8], [0.8, 1]])
```

```
f_xy = lambda x,y: scipy.stats.multivariate_normal.pdf([x,y], mean=mu, cov=sigma)
f_x = lambda x: integrate.quad(lambda y: f_xy(x, y), -np.inf, np.inf)[0]
f_y = lambda y: integrate.quad(lambda x: f_xy(x, y), -np.inf, np.inf)[0]
```

```
def conditional_distribution(x, f_xy, f_x):
    return lambda y: f_xy(x, y)/ f_x(x)
```



```
f_y_given_x = lambda x: conditional_distribution(x, f_xy, f_x)
f_y_bayes = lambda y: integrate.quad(lambda x: f_y_given_x(x)(y)*f_x(x), -np.inf, np.inf)[0]
```



EE 541: OPTIMIZATION / MINIMIZATION

- Given a function $f(x)$ find x_m so that $f(x_m) < f(x)$ for $\forall x$.
 - Usually have to accept a local minimum (i.e., not global minimum)
 - $f(x_m) < f(x)$ for $\forall x: |x - x_m| < \epsilon$
- Maximization of $f(x)$ is minimization of $-f(x)$
 - does not require separate routines
- Most algorithms require a starting point(s) x_0 - “guesses”
 - “better” guesses usually closer to x_m



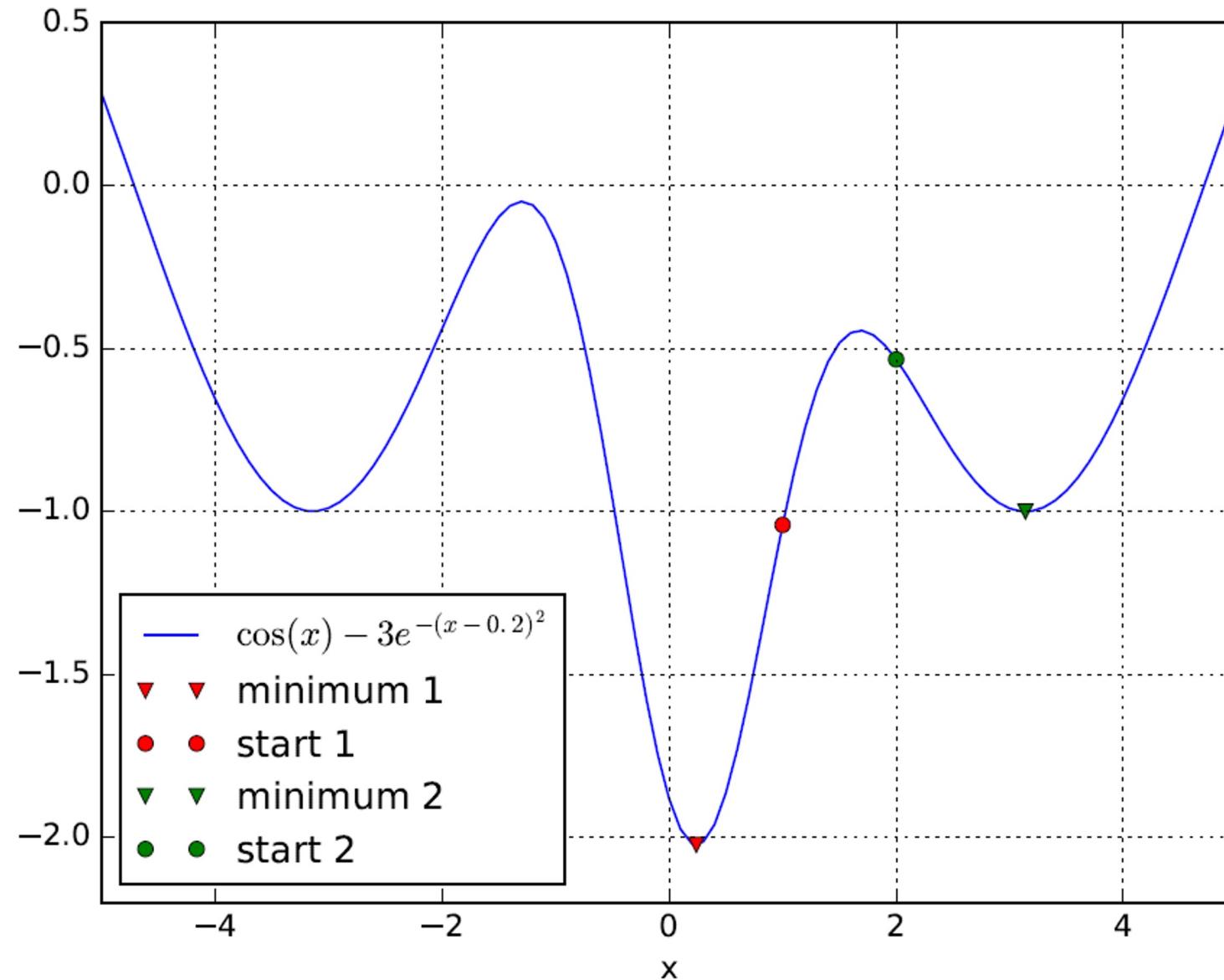
OPTIMIZATION EXAMPLE

```
from scipy import arange, cos, exp
from scipy.optimize import fmin
import pylab

def f(x):
    return cos(x) - 3 * exp( -(x - 0.2) ** 2
)
# find minima using 2 different x0
min1 = fmin(f, 1.0)                      # [0.23964844]
min2 = fmin(f, 2.0)                      # [3.13847656]
```



```
x = arrange(-10, 10, 0.1)
y = f(x)
pylab.plot(x, y, label, '$\cos(x) - 3 e^{- (x - 0.2)^2}$')
pylab.xlabel('x')
pylab.grid()
pylab.axis([-5, 5, -2.2, 0.5])
# add initial guess and min to plot
pylab.plot(min1, f(min1), 'vr', label='minimum 1')
pylab.plot(1.0, f(1.0), 'or', label='start 1')
pylab.plot(min2, f(min2), 'vg', label='minimum 2')
pylab.plot(2.0, f(2.0), 'og', label='start 2')
pylab.legend(loc='lower left')
pylab.show()
```

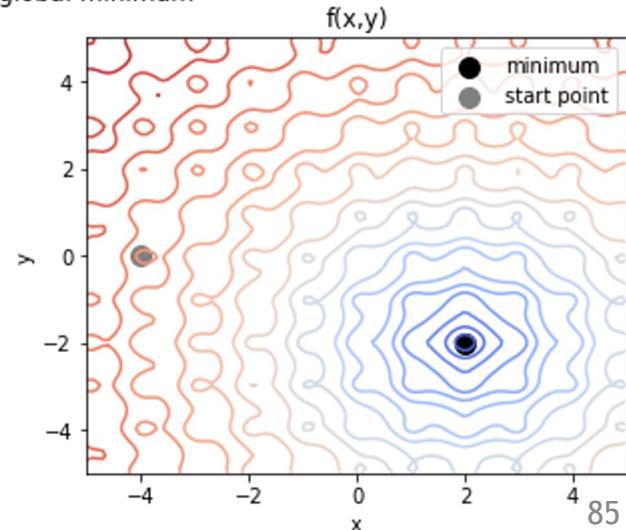
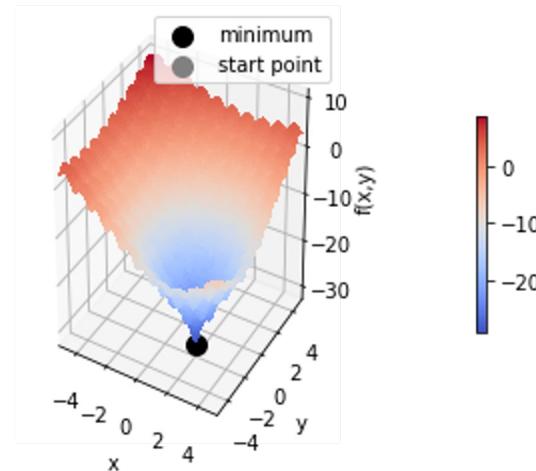




2D Optimization

```
def f(x, y, x_0, y_0): #x_0, y_0 is the mean (and minimum) here
    return -50.0 * np.exp(-0.2 * np.sqrt(0.5 * ((x-x_0)**2 + (y-y_0)**2))) - \
        np.exp(0.5 * (np.cos(2 * np.pi * (x-x_0)) + np.cos(2 * np.pi * (y-y_0)))) + \
        np.e + \
        20
x0 = np.array([-4, 0]) # starting point
res = scipy.optimize.minimize(lambda x: f(x[0], x[1], x_0, y_0), x0, method='BFGS') #res.x - solution
```

Complicated function with multiple local minima and a global minimum





SKLEARN



SciKit - Learn(`sklearn`)

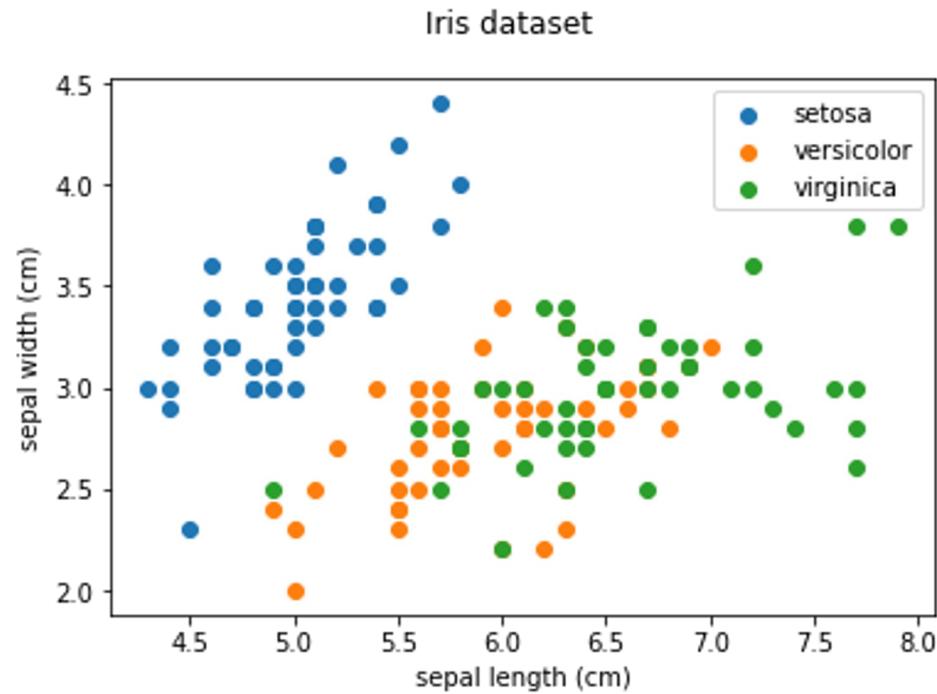
- > datasets
benchmarking datasets
 - > clustering
KMeans
 - > linear_model
 - > decomposition
 - > model_selection
 - > neural_network
- Few lightweight
- Clustering models like
- Linear Regression models
- PCA
- Grid search and test_train_split
- MLP models



Sklearn - Datasets

Eg, Iris Dataset:
3 classes of 50 instances each,
each class refers to a type of iris plant
4 features: sepal length, sepal width, petal length and petal width

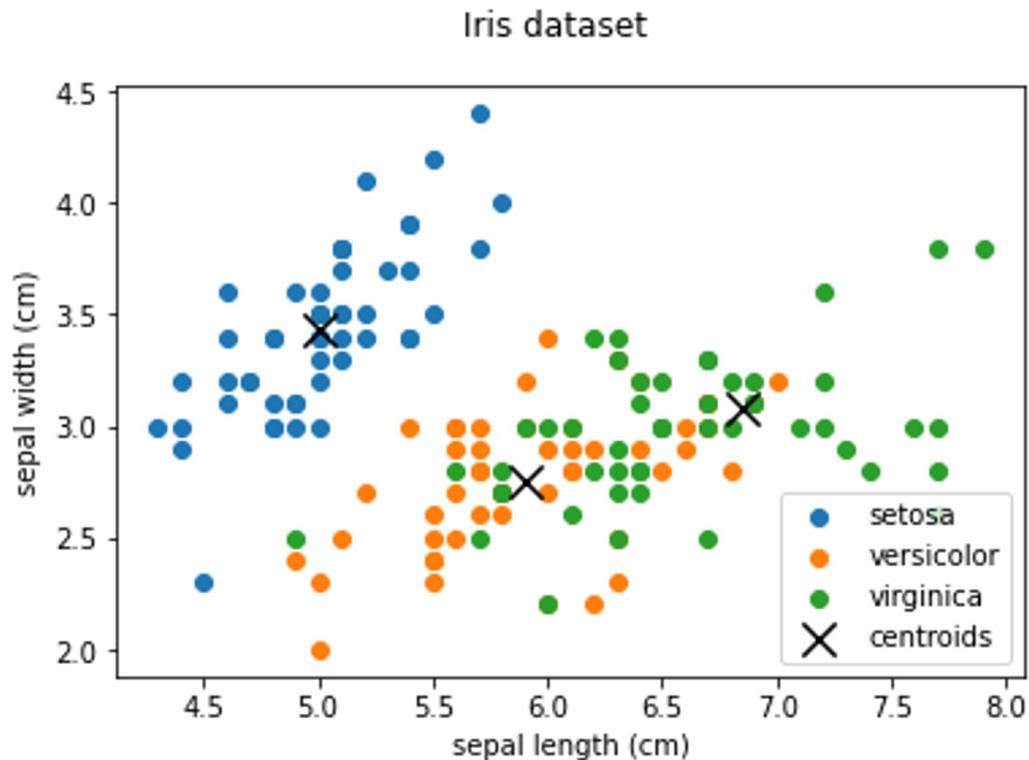
```
iris = sklearn.datasets.load_iris()  
X = iris.data  
y = iris.target
```





Sklearn - cluster

```
#clustering the iris dataset  
kmeans = sklearn.KMeans(n_clusters=3)  
kmeans.fit(X)  
C = kmeans.cluster_centers_
```



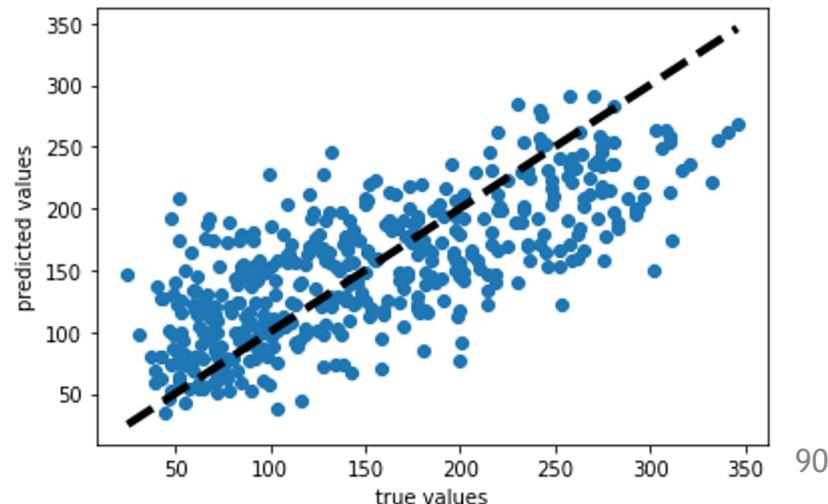
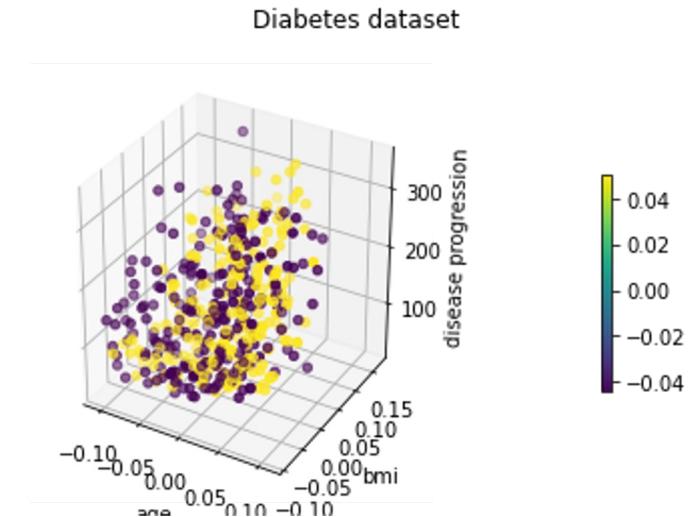


Sklearn - linear_model

```
# train a linear regression model on the diabetes dataset
diabetes = datasets.load_diabetes()
X_orig = diabetes.data
y_orig = diabetes.target
# plot first 3 features vs target
```

```
regr = sklearn.linear_model.LinearRegression()
regr.fit(X_orig, y_orig)
y_pred = regr.predict(X_orig)
```

```
# plot predicted target values vs true target values
# should ideally be on the straight line
```



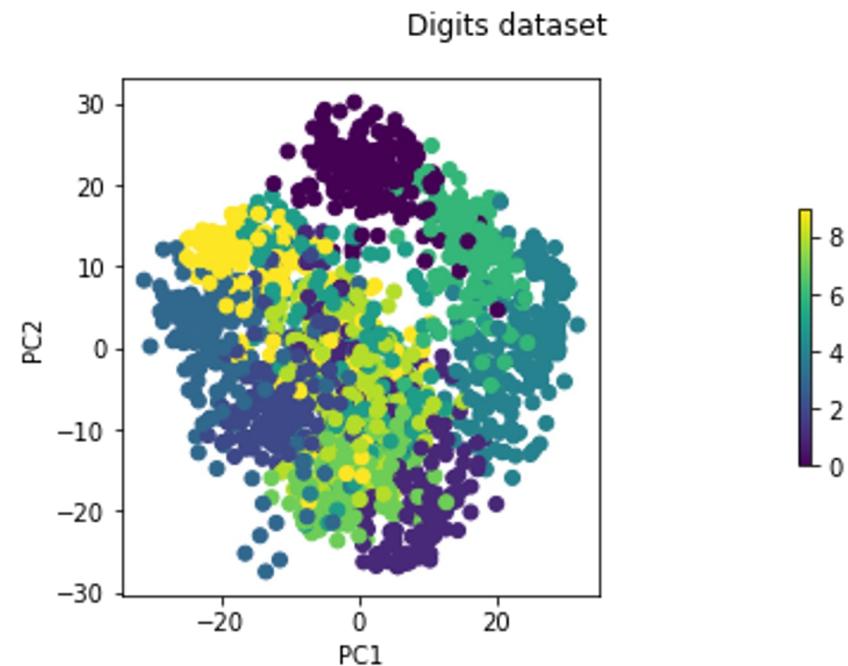


Sklearn - decomposition

```
# PCA on the digits dataset  
# 10 classes of 1797 instances  
# Each class is a digit  
# 64 features: 8x8 pixel values
```

```
digits = datasets.load_digits()  
X = digits.data  
y = digits.target
```

```
pca = sklearn.decomposition.PCA(n_components=2)  
pca.fit(X)  
X_pca = pca.transform(X)
```





Sklearn - neural_network

```
# on the digit dataset, we train an MLP classifier
```

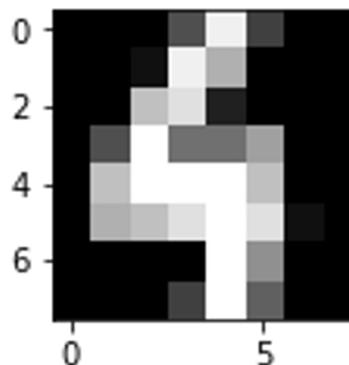
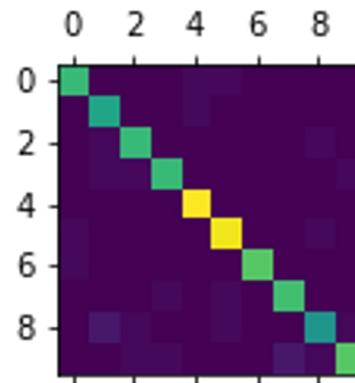
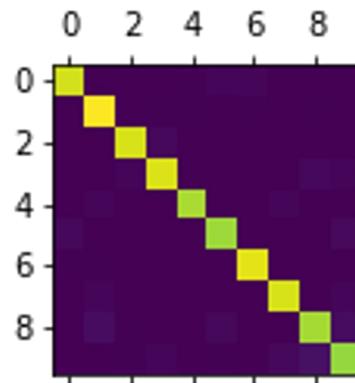
```
clf = sklearn.neural_network.MLPClassifier(hidden_layer_sizes=(8, 8), solver='adam',
learning_rate_init=0.0001, alpha=0.0001, max_iter=1000, activation='relu')
```

```
# split dataset into train and test
```

```
X_train, X_test, y_train, y_test = sklearn.model_selection.train_test_split(X, y,
test_size=0.2, random_state=42)
clf.fit(X_train, y_train)
```

Training image. true label: 4, predicted label: 4.

Train accuracy: 0.9554627696590118, test accuracy: 0.9305555555555556





Sklearn - model_selection

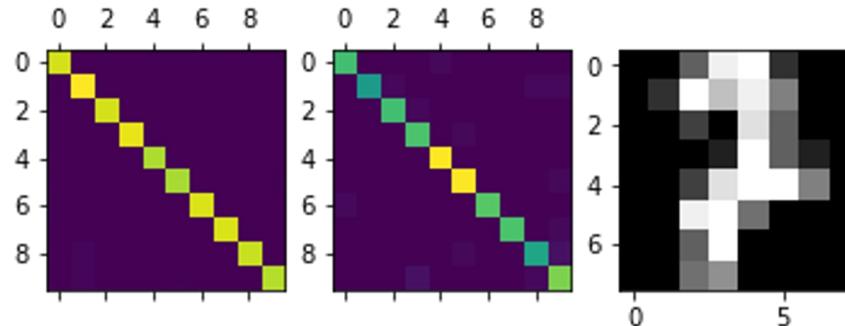
```
# run a grid search to find the best parameters for the MLP classifier
from sklearn.model_selection import GridSearchCV
from sklearn.neural_network import MLPClassifier

clf = MLPClassifier(hidden_layer_sizes=(8, 8), solver='adam', learning_rate_init=0.0001, alpha=0.0001,
max_iter=1000, activation='relu')
```

```
gs = GridSearchCV(clf, param_grid={'hidden_layer_sizes': [(8, 8), (16, 16)], 'learning_rate_init': [0.0001, 0.001], 'alpha': [0.0001, 0.001]}, cv=5, n_jobs=-1, verbose=2)
```

```
gs.fit(X_train, y_train)
best_params = gs.best_params_
best_clf = gs.best_estimator_
```

```
Training image. true label: 7, predicted label: 7.
Train accuracy: 0.9937369519832986, test accuracy: 0.9583333333333334.
Best parameters: {'alpha': 0.001, 'hidden_layer_sizes': (16, 16), 'learning_rate_init': 0.0001}
```





Pytorch



Pytorch - Tensors, randomness

- Just like numpy arrays
- Can be stored/operated on on GPU

```
x = torch.tensor([1,2,3,4,5]) #instead of numpy.array([1,2,3,4,5])
```

- Checking if cuda is available:
 - `torch.cuda.is_available()`
- Moving a tensor to GPU:
 - `x = x.cuda()`
- Moving back to CPU:
 - `x = x.cpu()`
- Randomness:
 - Can be controlled by setting seed:
 - `torch.manual_seed(0)`
 - Can create random numbers/vectors just like numpy:
 - `torch.randn(2, 2)`



Pytorch - Operations

- Perform operations similar to numpy arrays, Eg:
 - Element-wise addition $a + b$
 - Element-wise multiplication $a * b$
 - Matrix multiplication `torch.mm(a, b.t())`
- Operations can be performed on tensors on GPU
- NOTE: operations can be done only if the tensors are on the same device



Pytorch - From numpy arrays

```
x = np.array([1,2,3,4,5])
y = torch.from_numpy(x)
z = y.numpy()
```

NOTE: both the numpy array and torch tensor share the same memory location!

```
# change the array x
x[0] = 100
# This also changes y
print(y)
# tensor([100,2,3,4,5])
```



Pytorch - copy vs Inplace, Reshape, transpose, resize, etc

- `y = x.add(1)`
- `x.add_(1)`

- Just Like Numpy:
 - `x.view()`
 - `x.reshape()`
 - `x.transpose()`
 - `x.squeeze()`
 - `x.unsqueeze()`
 - `x.resize()`

