HPSC 101 — Lecture 6

This lecture:

- NumPy arrays and functions
- “Pythonic” ways to do things

- Python: main programs and private variables
- Timing Python execution

Lists aren’t good as numerical arrays

Lists in Python are quite general, can have arbitrary objects as elements.

Addition and scalar multiplication are defined for lists, but not what we want for numerical computation, e.g.

Multiplication repeats:

```
>>> x = [2., 3.]
>>> 2*x
[2.0, 3.0, 2.0, 3.0]
```

Addition concatenates:

```
>>> y = [5., 6.]
>>> x+y
[2.0, 3.0, 5.0, 6.0]
```

NumPy module

Instead, use NumPy arrays:

```
>>> import numpy as np

>>> x = np.array([2., 3.])
>>> 2*x
array([ 4.,  6.])

Try x*y where both x and y are
arrays of the same size.
```

Other operations also apply component-wise:

```
>>> np.sqrt(x) * np.cos(x) * x**3
array([ -4.708164  , -46.29736719])
```

Note: `*` is component-wise multiply

NumPy arrays

Unlike lists, all elements of an `np.array` have the same type

```
>>> np.array([1, 2, 3])     # all integers
array([1, 2, 3])

>>> np.array([1, 2, 3.])    # one float
array([ 1.,  2.,  3.])      # they're all floats!
```

Can explicitly state desired data type:

```
>>> x = np.array([1, 2, 3], dtype=complex)
>>> print x
[ 1.+0.j,  2.+0.j,  3.+0.j]

>>> (x + 1.j) * 2.j
array([-2.+2.j, -2.+4.j, -2.+6.j])
```

NumPy arrays for vectors and matrices

```
>>> A = np.array([[1.,2], [3,4], [5,6]])
>>> A
array([[ 1.,  2.],
       [ 3.,  4.],
       [ 5.,  6.]])

>>> A.shape
(3, 2)

>>> A.T
array([[ 1.,  3.,  5.],
       [ 2.,  4.,  6.]])

>>> x = np.array([1., 1.])
>>> x.T
array([ 1.,  1.])
```

NumPy arrays for vectors and matrices

```
>>> A
array([[ 1.,  2.],
       [ 3.,  4.],
       [ 5.,  6.]])

>>> x
array([ 1.,  1.])

>>> np.dot(A,x)     # matrix-vector product
array([  3.,   7.,  11.])

>>> np.dot(A.T, A)    # matrix-matrix product
array([[ 35.,  44.],
       [ 44.,  56.]])
```

NumPy matrices for vectors and matrices

For Linear algebra, may instead want to use numpy.matrix:

```
>>> A = np.matrix([[1.,2], [3,4], [5,6]])
>>> A
matrix([[ 1.,  2.],
        [ 3.,  4.],
        [ 5.,  6.]])
```

Or, Matlab style (as a string that is converted):

```
>>> A = np.matrix("1.,2; 3,4; 5,6")
>>> A
matrix([[ 1.,  2.],
        [ 3.,  4.],
        [ 5.,  6.]])
```

NumPy matrices for vectors and matrices

Note: vectors are handled as matrices with 1 row or column:

```
>>> x = np.matrix("4.;5.")
>>> x
matrix([[ 4.],
        [ 5.]])
>>> x.T
matrix([[ 4.,  5.]])
>>> A*x
matrix([[ 14.],
        [ 32.],
        [ 50.]])
```

But note that indexing into *x* requires two indices:

```
>>> print x[0,0], x[1,0]
4.0 5.0
Try x[:]
```

Which to use, array or matrix?

For linear algebra matrix may be easier (and more like Matlab), but vectors need two subscripts!

For most other uses, arrays more natural, e.g.

```
>>> x = np.linspace(0., 3., 100)   # 100 points
>>> y = x**5 - 2.*sqrt(x)*cos(x)   # 100 values
>>> plot(x,y)
```

np.linspace returns an array, which is what is needed here.

We will always use arrays.

See **http://www.scipy.org/NumPy_for_Matlab_Users**

Rank of an array

The rank of an array is the number of subscripts it takes:

```
>>> A = np.ones((4,4))

>>> A
array([[ 1.,  1.,  1.,  1.],
       [ 1.,  1.,  1.,  1.],
       [ 1.,  1.,  1.,  1.],
       [ 1.,  1.,  1.,  1.]])

>>> np.rank(A)
2
```

Warning: This is not the rank of the matrix in the linear algebra sense (dimension of the column space)!

Rank of an array

Scalars have rank 0:

```
>>> z = np.array(7.)
>>> z
array(7.0)
```

NumPy arrays of any dimension are supported, e.g. rank 3:

```
>>> T = np.ones((2,2,2))
>>> T
array([[[ 1.,  1.],
        [ 1.,  1.]],

       [[ 1.,  1.],
        [ 1.,  1.]]])
>>> T[0,0,0]
1.0
```

Linear algebra with NumPy

```
>>> A = np.array([[1., 2.], [3, 4]])
>>> A
array([[ 1.,  2.],
       [ 3.,  4.]])

>>> b = np.dot(A, np.array([8., 9.]))
>>> b
array([ 26.,  60.])
```

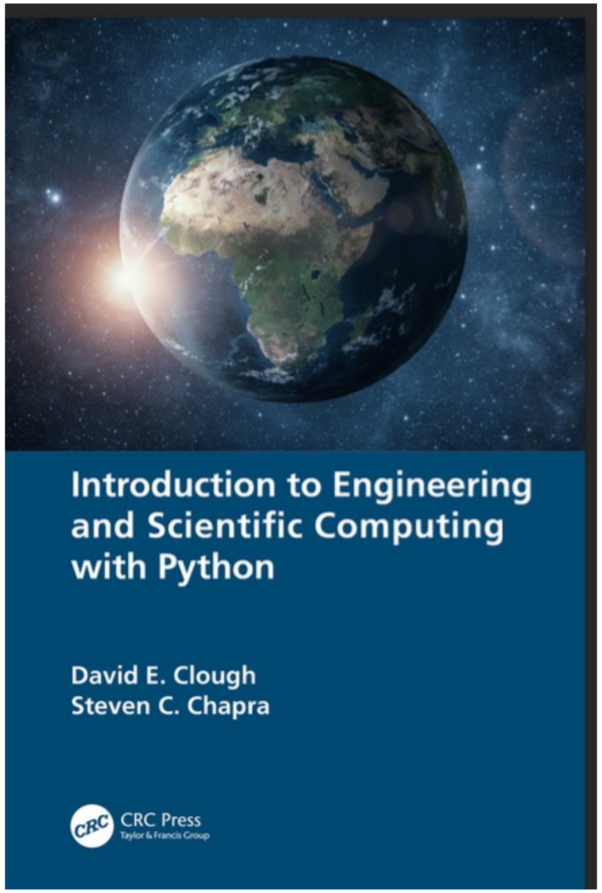
Now solve $Ax = b$:

```
>>> from numpy.linalg import solve
>>> solve(A,b)
array([ 8.,  9.])
```

Eigenvalues

```
>>> from numpy.linalg import eig

>>> eig(A)  # returns a tuple (evals,evecs)

(array([-0.37228132,  5.37228132]),
       array([[-0.82456484, -0.41597356],
              [ 0.56576746, -0.90937671]]))

>>> evals, evecs = eig(A)  # unpacks tuple

>>> evals
array([-0.37228132,  5.37228132])

>>> evecs
array([[-0.82456484, -0.41597356],
       [ 0.56576746, -0.90937671]])
```

Reference


Introduction to Engineering and Scientific Computing with Python
David E. Clough
Steven C. Chapra
CRC Press
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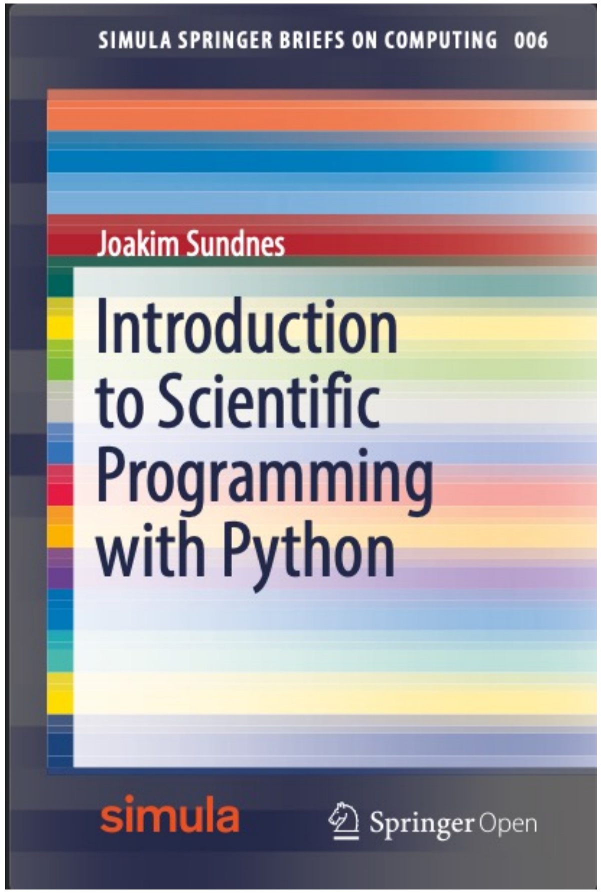
SIMULA SPRINGER BRIEFS ON COMPUTING 006
Joakim Sundnes
Introduction to Scientific Programming with Python
simula
Springer Open

https://link.springer.com/book/10.1007/978-3-030-50356-7

Pythonic ways

- f-string format (since Python 3.6)

```
print("At iteration number %s, s= %20.15f" %(k,s))
print(f"At iteration number {k}, s= {s}")
print(f"At iteration number {k}, s= {s:10.15f}")

t = 1.234567
print(f"Default output gives t = {t}.")
print(f"We can set the precision: t = {t:.2}.")
print(f"Or control the number of decimals: t = {t:.2f}.")

Default output gives t = 1.234567.
We can set the precision: t = 1.2.
Or control the number of decimals: t = 1.23.
```

- Zip function

```
for low, high in zip(A_low, A_high):
    print(low, high)
```

Python ways - continued

- List slicing

```
>>> a = [2, 3.5, 8, 10]
>>> a[2:] # from index 2 to end of list [8, 10]
>>> a[1:3] # from index 1 up to, but not incl.,
index 3 [3.5, 8]
>>> a[:3] # from start up to, but not incl., index
3 [2, 3.5, 8]
>>> a[1:-1] # from index 1 to next last element
[3.5, 8]
>>> a[:] # the whole list [2, 3.5, 8, 10]

b = a[:] will make a copy of the entire list a, and
any subsequent changes to b will not change a
```

- Membership

```
List1=[1,2,3,"hello"]
2 in List1 - True
4 in List1 - False
"hello" in List1 - True
```

Quadrature (numerical integration)

Estimate $\int_0^2 x^2 \, \mathrm{d}x = \frac{8}{3}$:

```
>>> from scipy.integrate import quad

>>> def f(x):
...     return x**2
...
>>> quad(f, 0., 2.)
(2.6666666666666667, 2.960594732333751e-14)
```

returns (value, error estimate).

Other keyword arguments to set error tolerance, for example.

Lambda functions

In the last example, f is so simple we might want to just include its definition directly in the call to quad.

We can do this with a lambda function:

```
>>> f = lambda x: x**2
>>> f(4)
16
```

This defines the same f as before. But instead we could do:

```
>>> quad(lambda x: x**2, 0., 2.)
(2.6666666666666667, 2.960594732333751e-14)
```

“Main program” in a Python module

Python modules often end with a section that looks like:

```
if __name__ == "__main__":

    # some code
```

This code is **not** executed if the file is imported as a module, only if it is run as a script, e.g. by...

```
    $ python filename.py

    >>> execfile("filename.py")

    In[1]: run filename.py
```

Exercise

- Write a function to calculate the exponential using the exponential series
    - The function should take the number of terms of the series as an argument, use default of 100
    - Check the convergence of the series
- Plot y=exp(x) for 1000 points between 0 and 100, using the built-in numpy exp() function and your_exp() function
- Compare the execution time of the two functions using the timeit command of Ipython
- All work should be done in Jupyter online and the notebook saved back into your local machine and pushed into your fork