Programming in Python[1]

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Lecture XIII: Using Third-party libraries

Third-party libraries

Python is "sold" *batteries included* (with many useful built-in libraries). Moreover, like many modern programming environments, it has standard online package directories that list libraries produced by independent developers.

https://pypi.org/

The Python package index currently lists almost 300K libraries!

Installing a library

The details are explained here: https://packaging.python.org/tutorials/installing-packages/

- In most cases it is very easy, the `pip` program does all the magic
- It is very important to understand the difference between a system-wide and a project-specific installation.

System-wide vs. Project-specific

If you don't take special precautions, a package is installed in a way that makes it available to your Python system: every Python interpreter you launch sees them.

- In many cases, this is not what you want
- Different projects/programs might depend on different versions of the libraries
- Libraries themselves depend on other libraries, you want to understand exactly which packages your program is using in order to reproduce the settings on other machines

Virtual environments

Python provides the idea of virtual development environments (venv)

- You can create one with: `python -m venv CHOOSE_A_NAME`
- You must activate it (syntax depends on your OS): `CHOOSE_A_NAME\Scripts \activate`
- In an active virtual environment all the installation are confined to it
- You can get the list of installed packages with `pip freeze`

Simplified venv administration

Virtual environments are key to avoid messing up your system. Many tools simplify their administration.

- `pipenv` (my preferred one, we will use this)
- `poetry` (similar to `pipenv`, currently less popular, but it has a better dependency control, a bit more complex)
- `conda` (uses its own package index, great flexibility and complexity, manage different python versions)

Virtual environments caveats

When you are working in a Python virtual environment, remember to launch all your development tools "inside" the virtual space.

For example, to use IDLE don't click on the main application launcher, instead: `python -m idlelib`.

NumPy

`NumPy` is a third-party library very popular for scientific/numerical programming (`https://numpy.org/`).

- Features familiar to `matlab`, R, Julia programmers
- The key data structure is the array
  - 1-dimension arrays: vectors
  - 2-dimension arrays: matrices
  - n-dimension arrays

In some languages array is more or less synonym of list: Python distinguishes: lists (mutable, arbitrary elements), arrays (mutable, all elements have the same type), tuples (immutable, fixed length, arbitrary elements).

Lecture XIV: NumPy arrays

NumPy arrays

The most important data structure in `NumPy` is `ndarray`: a (usually fixed-size) sequence of same type elements, organized in one or more dimensions.

`https://numpy.org/doc/stable/reference/arrays.ndarray.html`

Implementation is based on byte arrays: accessing an element (all of the same byte-size) is virtually just the computation of an 'address'.

Why?

- using NumPy arrays is often more compact, especially when there's more than one dimension
- faster than lists when the operation can be vectorized
- (slower than lists when you append elements to the end)
- can be used with element of different types but this is less efficient

A `ndarray` has a `dtype` (the type of elements) and a `shape` (the length of the array on each dimensional axis). (Note the jargon: slightly different from linear algebra)

- Since appending is costly, normally they are pre-allocated (`zeros`, `ones`, `arange`, `linspace`, ...)
- vectorized operations can simplify code (no need for loops) and they are faster with big arrays
- vector indexing syntax (similar to R): very convenient (but you need to learn something new)

All the elements must have the same size

This is actually a big limitation: the faster access comes with a price in flexibility.

```
>>> np.array(['','',''])
array(['', '', ''], dtype='<U1')
>>> np.array(['a','bb','ccc'])
array(['a', 'bb', 'ccc'], dtype='<U3')
>>> np.array(['a','bb','cccxxxxxxxxxxxxxxxxxx'])
array(['a', 'bb', 'cccxxxxxxxxxxxxxxxxxx'], dtype='<U21')
```

Usually the length is not changed

The best use of arrays is to avoid a change in their length, that can be costly. Thus, they are normally preallocated at creation:

- `np.array([1,2,3])`
- `np.zeros(2)`, `np.zeros(2, float)`, `np.ones(2)`
- `np.empty((2,3))` six not meaningful float values
- `np.arange(1, 5)` be careful with floats:

  ```
  >>> np.arange(0.4, 0.8, 0.1)
  array([0.4, 0.5, 0.6, 0.7])
  >>> np.arange(0.5, 0.8, 0.1)
  array([0.5, 0.6, 0.7, 0.8])
  ```
- `np.linspace(0.5, 0.8, 3)` with this the length is easier to predict

You can concatenate arrays with `np.concatenate` (be careful with the shapes!)

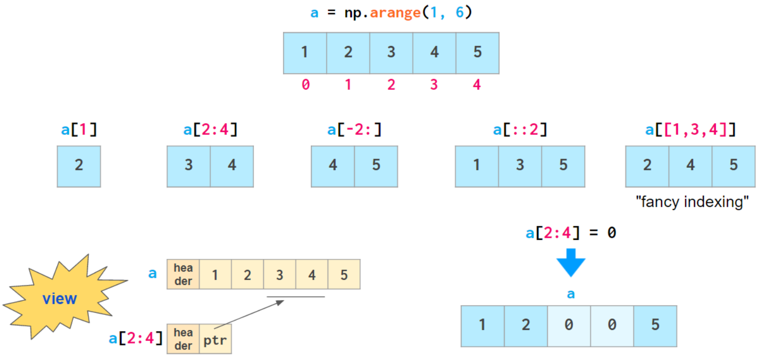
Don't remove, select

In general you don't remove elements but select them. Be careful: if you don't make an explicit copy you get a "view" and possibly side-effects.

```
>>> a = np.ones((2,3))
>>> a
array([[1., 1., 1.],
       [1., 1., 1.]])
>>> x = a[:, 1]
>>> x
array([1., 1.])
>>> x[0] = 0
>>> x
array([0., 1.])
>>> a
array([[1., 0., 1.],
       [1., 1., 1.]])
```

```
>>> x = a[:, 1].copy()
>>> x[1] = 100
>>> x
array([  0., 100.])
>>> a
array([[1., 0., 1.],
       [1., 1., 1.]])
```

Indexing is powerful



Picture from "NumPy Illustrated: The Visual Guide to NumPy", highly recommended

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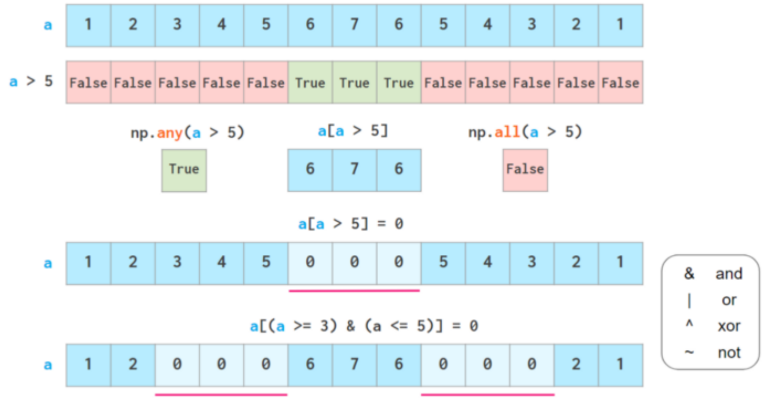

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The highest power: vectorization

Most of the basic mathematical function are vectorized: no need for loops! This is both convenient and faster!

```
>>> a = np.array([1,2,3,4])
>>> a + 1
array([2, 3, 4, 5])
>>> a ** 2
array([ 1,  4,  9, 16])
>>> np.exp(a)
array([ 2.71828183,  7.3890561 , 20.08553692,
↪  54.59815003])
```

Array operations

On arrays you have many "aggregate" operations.

```
>>> a
array([1, 2, 3, 4])
>>> a.sum()
10
>>> a.max()
4
>>> a.argmin()
0
>>> a.mean()
2.5
```

Remember to look at `dir` or the online documentation.