

3. The libraries NumPy and SciPy

Markus REINERT¹

Leibniz Institute of Baltic Sea Research Warnemünde (IOW)

30 April 2021

¹ ✉ markus.reinert@io-warnemuende.de

Python course 3

Installation of NumPy and SciPy

Overview of NumPy and SciPy

Comparison of lists and arrays

Creation of arrays

Usage of arrays (see the course notebook)

- ▶ If you are on conda: already installed.
- ▶ Otherwise, run in a terminal:

```
$ python -m pip install numpy scipy
```

(You might need to write python3 instead of python.)
- ▶ More information: <https://scipy.org/install.html>

Write at the beginning of every script where you use NumPy:

```
import numpy as np
```

and if you use anything from SciPy:

```
from scipy import stats, optimize, special, ...
```

(import only what you need)

NumPy

<https://numpy.org/doc/stable/reference/>

- ▶ common mathematical functions:
`np.sqrt(x)`, `np.sin(x)`, `np.cos(x)`,
`np.exp(x)`, ...
- ▶ basic statistics:
`np.mean(a)`, `np.std(a)`
- ▶ random numbers with simple
distributions: `np.random.randint(n)`
(random integer from $\{0, 1, \dots, n-1\}$)
- ▶ basic linear algebra
- ▶ solving linear or polynomial
equations
- ▶ arrays (→ next slide)

SciPy

<https://docs.scipy.org/doc/scipy/reference/>

- ▶ less common functions:
`special.gamma(x)`, Bessel functions,
...
- ▶ advanced statistics:
`stats.skew(x)`, `stats.norm.pdf(x)`
- ▶ random numbers from complicated
distributions:
`stats.poisson.rvs(mu)`
- ▶ advanced linear algebra
- ▶ solving “any” equation
(for example with `optimize.newton`)

Lists

- ▶ one-dimensional
(but can contain other lists)
- ▶ can be extended
- ▶ can contain any data
- ▶ data access with indices

- ▶ list-operations (count, index, ...)

Arrays

- ▶ zero-, one-, two-, ..., n -dimensional
- ▶ have a fixed length / shape
- ▶ can contain only one data type
- ▶ data access with indices
or conditions
- ▶ mathematical operations
(efficiently)

1. from a list (or similar): `np.array(l)`
- 2a. filled with 0s or 1s: `np.zeros(shape)`, `np.ones(shape)`
- 2b. filled with 0s or 1s, but with shape and data type of another array:
`np.zeros_like(a)`, `np.ones_like(a)`
- 3a. numerical 1D-ranges:
`np.arange(start, stop, step)`, `np.linspace(start, stop, num)`
- 3b. to go from 1D-ranges to 2D: `X, Y = np.meshgrid(x, y)`
4. from a text file: `np.loadtxt(file_name)`

- ▶ determine size, shape, and number of dimensions
- ▶ selection of single and multiple entries, rows, columns
- ▶ mathematics
- ▶ broadcasting
- ▶ selection by conditions