basic-numpy

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Run using ipython3 nbconvert --to slides --post serve basic-numpy.ipynb (Now using livereveal)

```
In [1]: %matplotlib nbagg

# For easier python 2 compatibility:
    from __future__ import division, print_function, absolute_import

# Normal imports:
    import numpy as np

In [2]: import numpy as np

# Keep the random numbers identical over runs
    np.random.seed(12345)
```

1 Introduction to the scientific python stack

2 Basic module NumPy

- Basis for scientific computing with Python
- A powerfull N-dimension array object
- Basic and not so basic math operations
- Linear algebra operations
- Normally homogenous data (i.e. numbers)
- random numbers, FFT, sorting, ...

2.1 Convention

```
In [3]: import numpy as np
```

3 Numpy is useful

- Homogenous data:
- Experimental data sets
- Simulations
- ...

For example:

```
[ 0.
     1.8 3.6 5.4 7.2 9.]
In [5]: print(np.sqrt(x)[::200])
[ 0.
              1.34164079 1.8973666
                                       2.32379001 2.68328157 3.
                                                                          ]
  NumPy can be much faster (typically \approx 50 \times):
In [6]: %%timeit
        numpy_result = np.sqrt(x)
100000 loops, best of 3: 3.93 \mu s per loop
In [7]: from math import sqrt
        x = list(x)
In [8]: %%timeit
        python_result = [sqrt(value) for value in x]
10000 loops, best of 3: 86.4 \mu s per loop
  (The actual speedup depends, but it can be much more for simple operations like \times, +)
    Arrays are N-Dimensional (ndarray)
A bit like nested lists:
4.1
     0 Dimensional
In [9]: arr = np.array(5)
        # although O-d arrays are sometimes a bit special :(
        print(arr)
        print('The dimension is:', arr.ndim)
        print('The shape is:', arr.shape)
The dimension is: 0
The shape is: ()
      1 Dimensional
4.2
In [10]: arr = np.array([4, 5, 6])
         print(arr)
         print('The dimension is:', arr.ndim)
         print('The shape is:', arr.shape)
[4 5 6]
The dimension is: 1
The shape is: (3,)
```

4.3 2 Dimensional

4.4 3 Dimensional

5 Array creation

5.1 Homogeneous arrays

5.2 Special one dimensional arrays

Ranges for float and integer arrays

```
In [16]: np.linspace(0, 3, 7)
Out[16]: array([ 0. , 0.5, 1. , 1.5, 2. , 2.5, 3. ])
In [17]: np.arange(10) # much like pythons range
Out[17]: array([0, 1, 2, 3, 4, 5, 6, 7, 8, 9])
```

Note: Please do not use arange for floats!

5.2.1 N-Dimensional versions:

• np.meshgrid; np.ogrid; np.mgrid

5.3 Random arrays

Draw from the interval [0,1]:

```
In [18]: np.random.random((1, 5))
Out[18]: array([[ 0.92961609,  0.31637555,  0.18391881,  0.20456028,  0.56772503]])
```

Draw from a normal distribution with mean 2 and standard deviation 3:

```
In [19]: np.random.normal(loc=2, scale=3, size=(1, 5))
Out[19]: array([[ 3.35166326,  2.27801987,  5.74439852,  4.30430213,  5.74641094]])
```

• And many more, check np.random.<tab>!

Note: np.random.seed() makes sure you get the same numbers. Using np.random.RandomState is often even better.

5.4 Special arrays

And many many more...

6 Lets do math!

```
• Math is elementwise (unlike lists)
In [22]: arr = np.linspace(-1, 1, 5)
        # 5 steps from -1 to 1 (including both)
        print(arr)
[-1. -0.5 0.
                0.5 1.]
In [23]: print(arr + 1)
[ 0. 0.5 1.
                1.5 2.]
    Unary functions
6.1
In [24]: np.sin(arr)
Out[24]: array([-0.84147098, -0.47942554, 0. , 0.47942554, 0.84147098])
In [25]: arr**2
Out[25]: array([ 1. , 0.25, 0. , 0.25, 1. ])
In [26]: abs(arr)
Out[26]: array([ 1. , 0.5, 0. , 0.5, 1. ])
In [27]: -arr
Out[27]: array([ 1. , 0.5, -0. , -0.5, -1. ])
    Binary functions
In [28]: arr + arr # also np.add(arr, arr)
Out[28]: array([-2., -1., 0., 1., 2.])
In [29]: arr * 2
Out[29]: array([-2., -1., 0., 1., 2.])
In [30]: arr + 3
Out[30]: array([ 2. , 2.5, 3. , 3.5, 4. ])
In [31]: arr == -1
Out[31]: array([ True, False, False, False, False], dtype=bool)
```

6.3 Reductions

Many reductions are available either through ndarray attributes or as numpy functions:

```
In [32]: np.sum(arr) # or
    arr.sum()
Out[32]: 0.0
```

Warning: Usual sum(arr) is not correct since it is a python function and not an operator.

6.4 Other reductions

```
In [33]: np.mean(arr)
         arr.mean()
Out[33]: 0.0
In [34]: # Logical:
         arr.all(); arr.any()
         # Minimum/Maximum:
         arr.min(); arr.max(); arr.argmin(); arr.argmax()
         # Standard deviation:
         arr.std(ddof=1); arr.var()
         np.median(arr); # not arr.median here
Out[34]: 0.0
6.5
     Recutions – axis
Most reduction (-like) functions accept an axis argument:
In [35]: arr = np.random.random((50, 3))
         arr.sum(0)
Out[35]: array([ 28.31967429, 24.8259124 , 26.06089517])
In [36]: arr.sum(0, keepdims=True)
Out[36]: array([[ 28.31967429, 24.8259124 , 26.06089517]])
  You can specify multiple axes (its still called "axis"):
In [37]: arr.sum(axis=(0, 1))
Out[37]: 79.206481864020247
```

7 (Master) Reductions

All binary usuncs (simple elementwise math functions from above) allow reductions. For example arr.sum() is actually a thin wrapper around np.add.reduce(arr)!

8 All Available functions

All available unary (math/ufunc) functions:

```
In [38]: for obj_string in dir(np):
    obj = getattr(np, obj_string)
    if (isinstance(obj, np.ufunc)
        and obj.nin == 1 and obj.nout == 1):
        print(obj_string, end=', ')
```

All available binary (math/ufunc) functions:

abs, absolute, arccos, arccosh, arcsin, arcsinh, arctan, arctanh, bitwise_not, ceil, conj, conjugate, co

```
In [39]: for obj_string in dir(np):
                                        obj = getattr(np, obj_string)
                                        if (isinstance(obj, np.ufunc)
                                                                 and obj.nin == 2 and obj.nout == 1):
                                                     print(obj_string, end=', ')
add, arctan2, bitwise_and, bitwise_or, bitwise_xor, copysign, divide, equal, floor_divide, fmax, fmin, fmin,
         Other (math/ufunc) functions:
In [40]: for obj_string in dir(np):
                                        obj = getattr(np, obj_string)
                                        if (isinstance(obj, np.ufunc)
                                                                 and (obj.nin > 2 or obj.nout != 1)):
                                                     print(obj_string, end=', ')
frexp, modf,
9
              Broadcasting
Implicite repetition of arrays.
         We have already done this:
In [41]: arr = np.array([1, 2, 3, 4])
                            arr + 3
Out[41]: array([4, 5, 6, 7])
        Is actually:
In [42]: threes = np.array([3, 3, 3, 3])
                            arr + threes
Out[42]: array([4, 5, 6, 7])
        This happens (more efficiently):
In [43]: three = np.array(3)
                            three = three.reshape(1)
                            print('Shape:', three.shape)
                            threes = three.repeat(len(arr))
                            print('Threes shape:', threes.shape)
Shape: (1,)
Threes shape: (4,)
In [44]: result = arr + threes
```

In [45]: red = np.arange(8)

(4, 3, 8)

green = np.ones((4, 3, 1))

blue = red * green
print(blue.shape)

```
9.1 Example:
```

10 Container manipulation

10.1 Reshaping

You can reshape arrays (more in the exercizes)

10.2 Other manipulations

```
In [51]: np.arange(3).repeat(2)
Out[51]: array([0, 0, 1, 1, 2, 2])
In [52]: np.concatenate((np.arange(2), np.arange(3)))
Out[52]: array([0, 1, 0, 1, 2])
```

• Concatenate has many friends (hstack, see "See Also")

There are more to explorer for specific tasks.

In []:

11 Indexing

- Indexing is very powerfull in NumPy
- There are different types of indexing:
 - 1. Picking a single element
 - 2. Slicing
 - 3. Advanced indexing:
 - picking many elements at once
 - 4. (Advanced) Boolean indexing:
 - Selecting based on logical expressions

Note: Advanced indexing is often also called fancy indexing

11.1 Picking an element

Picking a single element from an array requires an integer along each dimension

12 Incomplete index

12.1 Slicing

- You already know: (slice) from lists
- We can do it in arbitrary dimensions
- NumPy also has ... (Ellipsis)
- NumPy also has np.newaxis (identical to None)

12.1.1 Simple slicing

- Just like slicing of lists list[start:stop:step]
- For many dimensions each is sliced seperatly

13 Small exercise, weather in Göttingen

- Monthly weather data for Göttingen (From the DWD)
- Preprocess the data (we will do this together):
- Use np.genfromtxt to read the data
- Extract interesting columns (mostly temperature)
- Reshape the temp and snow arrays so that they have the year in the first and dimension and the month in the second. We have years 1947 to 2014 (68 years total).
- Do some data analysis

Please open the exercise Notebook

```
In [62]: # Load the data using genfromtxt. names=True, will load the header into a structured
         # array, so that the dictionary like access below works, you may ignore it for now.
         # invalid_raise=False is necessary because of an extra character at the end of the file.
         data = np.genfromtxt(
             "goe_monthly_1947_2015/produkt_monat_Monatswerte_19470101_20141231_01691.txt",
            delimiter=";", names=True, invalid_raise=False)
         # All data starts January 1947 and ends with (including) December 2014:
         temp = data["LUFTTEMPERATUR"] # Mean °C
         sun = data["SONNENSCHEINDAUER"] # sum of Hours
         precipitation = data["NIEDERSCHLAGSHOEHE"] # Sum of precipitation in mm
         print("Mean temperature from Jan. 1947 to Dec. 1949:")
         print(temp[:24])
Mean temperature from Jan. 1947 to Dec. 1949:
Γ-4.4 -8.6
                   9.5 14.6 17.5 18.4 18.3 16.2
              2.8
                                                        7.1
                                                              5.7
                                                                    2 1
   4.
         0.2
              5.7 10.5 13.9 16.1 16.3 16.1 13.6
                                                        8.5
```

```
/usr/lib/python3/dist-packages/numpy/lib/npyio.py:1670: ConversionWarning: Some errors were detected !
Line #818 (got 1 columns instead of 17)
warnings.warn(errmsg, ConversionWarning)
```

14 Continue with the following things

- 1. Reshape the temp, sun, and rain arrays so that the first dimension is the year and the second the month. Hint: Use the np.reshape command or arr.reshape method.
- Now you will have much either access to the data.
- 2. Find the mean sunshine duration when Python was released (January 1994).
- 3. Calculate the mean and the median temperature for each month. Hint: Use the axis argument
- Which one is the coldest month?
- Calculate the difference of the monthly mean to the whole year round mean.
- 3. Find the year with the coldest mean temperature. Hint: Use np.argmin
- 4. Which year had the sunniest summer months (June, July, and August)? Hint: Use slicing
- 5. ONLY if you are quick:
- Calculate the coefficient of correlation for the precipitation, the amount of sunshine, and the temperature. (Use np.corrcoef and possibly the stacking functions)
- Explorer the data, e.g.:
 - The winter in 1946-1947 just after WW II, was very harsh can you confirm?
 - Calculate the standard deviations
 - Did the average temperature in Göttingen rise in the last 30 years?

- ..

```
In [63]: # 1. Reshape the arrays:
         temp = temp.reshape(-1, 12)
         sun = sun.reshape(-1, 12)
         precipitation = precipitation.reshape(-1, 12)
         print("The new shape is correctly 68 years by 12 months:")
         print(temp.shape)
The new shape is correctly 68 years by 12 months:
(68, 12)
In [64]: # 2. Python release made the sun shine?
         print("When Python was first released, the total sunshine hours of the month was:")
         print(sun[1994-1947, 0])
When Python was first released, the total sunshine hours of the month was:
27.0
In [65]: # 3. a) Mean monthly temperatures
         print()
         print("Mean temperature in January:", temp[:, 0].mean())
         print("Mean temperature for all months:")
         print(temp.mean(0))
         print("Median temperature:")
         print(np.median(temp, 0))
```

```
Mean temperature in January: 0.627941176471
Mean temperature for all months:
Γ 0.62794118
              0.99705882
                           4.34558824 8.40882353 12.71911765
  15.66911765 17.39264706 17.00588235 13.62352941
  4.91176471
              1.79558824]
Median temperature:
                       8.3 12.75 15.85 17.3 16.9
         1.1
                 4.65
[1.1]
                                                          13.5
                                                                  9.35
   4.8
         2.051
In [66]: # 3. b) Coldest and warmest months:
         print("Which one is the coldest and warmest month:?")
         mean_monthly_temp = temp.mean(0)
         print(np.argmin(mean_monthly_temp), "(means January)") # January
         print(np.argmax(mean_monthly_temp), "(means July)") # July
        print()
         print("What is the difference of the monthly mean to the all year mean?")
         print(mean_monthly_temp - mean_monthly_temp.mean())
Which one is the coldest and warmest month:?
0 (means January)
6 (means July)
What is the difference of the monthly mean to the all year mean?
 \begin{bmatrix} -8.27426471 & -7.90514706 & -4.55661765 & -0.49338235 & 3.81691176 & 6.76691176 \end{bmatrix} 
  8.49044118 8.10367647 4.72132353 0.42720588 -3.99044118 -7.10661765]
In [67]: # 4. The coldest year:
         print()
         print("Which year is was the coldest?")
         yearly_mean = temp.mean(axis=1)
         print("Coldest was the year {}.".format(np.argmin(yearly_mean) + 1947))
Which year is was the coldest?
Coldest was the year 1963.
In [68]: # 5. Finding the sunniest summers:
         # pick all years, and slice summer months 5, 6, and 7:
         sun_summer = sun[:, 5:8]
                all years-^ ^^^-months 5 to 7 (8 not included)
         sunny_summer_days = sun_summer.sum(axis=1) # Sum of all summer months
         print("Sun hours during summer for all years:")
         print(sunny_summer_days)
         print("The sunniest Summer was:")
        print(np.argmax(sunny_summer_days) + 1947)
Sun hours during summer for all years:
[ 859.5 575. 686.6 744.3 606.9 639.9 616.5 487.7 506.2 444.5
  631.3 551.9 737.1 524.6 503.2 476. 548.9 676.8 478.6 507.9
```

```
606.7 547.4 592.3 636.5 647.2 513.8 684.8 515.
 411.4 479.7 435.5 477.
                             395.9 647.1 635.4 503.4 534.3 570.4
 416.9 531.4 640.7 559.4 600.7 628.7 547.2 669.1 679.2 509.5
 647.7 -663.9 599.9 519.4 633.2 531.9 793.7 587.4 600.2 710.7
 506.6 635.7 593.4 689.3 499.9 524.4 660.2 562.3]
The sunniest Summer was:
1947
In [69]: # 6. Correlations only
        print("The correlation matrix for the three is:")
        # Make the arrays flat again (do not care about the year vs. month):
        sun_ravel = sun.ravel()
        temp_ravel = temp.ravel()
        precipitation_ravel = precipitation.ravel()
        combined_array = np.vstack([sun_ravel, temp_ravel, precipitation_ravel])
        print(np.corrcoef(combined_array))
        print("There is a correlation between sun hours and temperature")
        print("(It is sunnier and warmer in the summer)")
The correlation matrix for the three is:
[[ 1.
              0.60989432 0.01320833
[ 0.60989432 1.
                          0.26277117]
 [ 0.01320833  0.26277117  1.
                                    ]]
There is a correlation between sun hours and temperature
(It is sunnier and warmer in the summer)
      Continued Indexing
15
15.0.1 Ellipsis
... replaces an arbitray number of:
In [70]: print(arr[1, ...]) # identical to arr[1]
        print(repr(arr[1, 0, ...])) # never a scalar
        print(repr(arr[1, 0])) # is a scalar (immutable)
[5 6 7 8 9]
array(5)
In [71]: high_dimensional = np.ones((5, 4, 3, 2))
        high_dimensional[..., :1].shape
Out[71]: (5, 4, 3, 1)
In [72]: high_dimensional[0, ..., 1].shape
```

Out[72]: (4, 3)

15.0.2 Newaxis

```
Inserts a new axis of size 1 (increases dimension)
In [73]: arr.shape
Out[73]: (2, 5)
In [74]: arr[:, np.newaxis, :, np.newaxis].shape
Out[74]: (2, 1, 5, 1)
In [75]: arr[..., None].shape
Out[75]: (2, 5, 1)
In [76]: np.newaxis is None
Out [76]: True
15.1
     Advanced (integer) Indexing
Create a new array selecting many elements
In [77]: arr = np.arange(1, 6)
In [78]: indx = np.array([0, 4, 2], dtype=np.intp)
         arr[indx]
Out[78]: array([1, 5, 3])
In [79]: arr[0], arr[4], arr[2]
Out[79]: (1, 5, 3)
In [80]: arr[[0, 4, 2]] # But nested lists do not!
         # intp is safest, but please do not worry about it generally:
         arr[np.array([0, 4, 2], dtype=np.uint16)]
Out[80]: array([1, 5, 3])
15.2
     Weather Example
Find the mean temperature for the combined years 1947, 1972, and 2014:
In [81]: years = np.array([1947, 1972, 2014], dtype=np.intp) - 1947
         temp[years, :].mean()
Out[81]: 9.030555555555555
15.2.1 Can be combined with other indexing
In [82]: arr = np.arange(6).reshape(2, 3)
         arr
Out[82]: array([[0, 1, 2],
                [3, 4, 5]])
In [83]: arr[[1, 0], :2]
Out[83]: array([[3, 4],
                [0, 1]])
```

Slicing happens first, then the rest (actually it is more the other way around)

15.2.2 Can have arbitrary shapes

15.2.3 Two advanced indexes are iterated together

This is *not* like slicing (or matlab)!

The output has the same shapes as the (broadcasted) input!

15.2.4 Example: Make use of multiple advanced indices

Select the "corners" with advanced indexing

15.3 Boolean indexing

- Filter an array
- Can work on the full arrays or some axes
- Result is always one dimensional

```
In [91]: arr > 3
Out[91]: array([[False, False, False],
               [False, True, True]], dtype=bool)
In [92]: arr[arr > 3]
Out[92]: array([4, 5])
15.3.1 Use it on part of the array only
In [93]: arr
Out[93]: array([[0, 1, 2],
               [3, 4, 5]])
In [94]: print('Every column starting >=1:', repr(arr[0] >= 1))
        arr[:, arr[0] >= 1] # Every column starting >= 1
Every column starting >=1: array([False, True, True], dtype=bool)
Out[94]: array([[1, 2],
               [4, 5]])
In [95]: print('Every row starting >1:', repr(arr[:, 0] > 1))
        arr[arr[:, 0] > 1]
Every row starting >1: array([False, True], dtype=bool)
Out[95]: array([[3, 4, 5]])
15.4 Weather Example
Find the mean temperature in June when January was below or above 0 °C
In [96]: below_zero = temp[:, 0] < 0</pre>
        print(below_zero)
        print()
        print("Mean temp June when it was below zero:", temp[below_zero, 5].mean())
        print("Mean temp June when it was below zero:", temp[~below_zero, 5].mean())
[ True False False True False False True True False False False
False False True False True False True False True False True
False True False False False False False True True True True
False False True False False False False False False False False
False True True False False False False False False False True
False False True True False False False False]
Mean temp June when it was below zero: 15.8636363636
Mean temp June when it was below zero: 15.5760869565
```

15.5 Assignments

Indexing can also be used for assignments:

15.6 Some notes

- All of these can be combined
- But combination can be very complicating in some cases
 - for example arr[index_array, :, index_array].
- Indexing is best with the np.intp type (others may be slower or in principle unsafe)

16 Memory and Views

- 1. Numpy arrays are of course mutable objects.
- 2. Slices create **views** into the same memory.

```
In [100]: arr = np.arange(10)
    # Take the first half:
    view = arr[:5]
    # Set it to 0:
    view[...] = 0
    print(arr)
[0 0 0 0 0 5 6 7 8 9]
```

Note: Advanced indexing always creates a copy, slicing never creates a copy.

16.1 Take care about views

- Some functions will return a view if possible i.e.:
 - np.reshapenp.ravel
- A functions $reads \rightarrow views$ are great.
- A function $writes \rightarrow no \text{ view unless out argument.}$

16.2 Optimizing memory usage

- Many numpy functions provide an out argument (all ufuncs): arr += 1 is the same as np.add(arr, 1, out=arr)
- **Be careful** when using the out. *Only* use out when this is **not** the same data. A common pitfall for example is:

```
arr += arr.T
```

Since arr.T is a view, it is changed during the operation \rightarrow unpredictable results (it might even work)

• A small view into a large array will keep the large array alive.

16.3 Datatypes

- Unlike lists, arrays have a specific element type.
- Be careful with integers:

17 SciPy

Scipy is a collection of many packages such as:

- integrate: Integration and ordinary differential equation solvers
- interpolate: Interpolation and smoothing splines
- linalg: Linear algebra
- ndimage: N-dimensional image processing
- optimize: Optimization and root-finding routines
- signal: Signal processing
- spatial: Spatial data structures and algorithms
- stats: Statistical distributions and functions
- ...

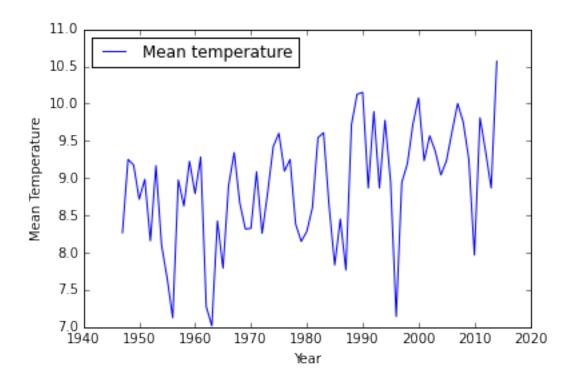
17.1 Usage

- Import a subpackage directly for example:
- from scipy import integrate
- from scipy.spatial import KDTree
- Documentation available at (also numpy): http://scipy.org
- Main namespace is (basically) just numpy \rightarrow do not use it.

17.2 Other packages

- 1. pandas (pandas.pydata.org):
- "data structures and data analysis tools for the Python programming language."
- Very useful for structured data (i.e. the weather data)
- 2. Some packages to keep in mind are for example:
- scikits-learn (sklearn as a package)
- scikits-image (skimage)
- \bullet networkx
- astropy
- statsmodels
- . . .
- 3. The ecosystem is constantly growing.
- Check if there are packages doing what you need to do
- Do not hesitate to ask e.g. on the SciPy user list

18 Later: plotting



18.1 More Examples

- Many, many very good examples at the **Gallery**: http://matplotlib.org/gallery
- Examples for animations, Graphical User Interface: http://matplotlib.org/examples/index.html

18.2 Conclusions

We have seen: 1. How to do convenient, fast math in **NumPy** 2. Where to find many useful tools with **SciPy and friends** 3. Later more information on how to plot with **matplotlib**

Last point: 1. Do not reinvent the wheel 2. Algorithms matter 3. "Premature optimization is the root of all evil" – Donald Knuth