



Scientific Programming: Data Structures – NumPy, Pandas & beyond

Scientific Programming with Python
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Based partially on a talk by Stéfan van der Walt

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The Ecosystem of Homo Python Scientificus



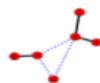
IPython



SymPy



pandas



NetworkX

[Ondřej Čertík/LANL]



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NumPy – the Fundamental Container for Scientific Computing





```
import numpy as np
```

<https://www.numpy.org>

NumPy offers memory-efficient data containers for fast numerical operations, *i.e.* in data manipulation and also in typical linear algebra calculations

Standard Python

```
>>> L = list(range(1000))  
>>> [i**2 for i in L]
```

NumPy

```
>>> import numpy as np  
>>> a = np.arange(1000)  
>>> a**2
```

⇒ Speed up by a factor of ~ 100



Creating NumPy Arrays

There are several ways to do so

Creating arrays

```
>>> a = np.array([1,2,4]) # [1,2,4]
>>> b = np.arange(1,15,2) # [1,3,5,7,9,11,13,15]
>>> c = np.linspace(0,1,6) # [0.0,0.2,0.4,0.6,0.8,1.0]
>>> d = np.empty((1,3)) # empty 1x3 array
>>> e = np.zeros((2,5,3)) # 2x5x3 array of zeros
>>> f = np.ones((3,3)) # 3x3 array of ones
>>> g = np.eye(4) # 4x4 unit matrix
>>> h = np.identity(4) # 4x4 unit matrix
>>> i = np.diag(np.array([1,2,3,4])) # diagonal matrix
>>> l = np.diag(np.array([1,2,3,4]),k=-1) # values just below the main diagonal
>>> m = np.diag(np.array([1,2,3,4]),k=2) # values 2 rows above the main diagonal
```



NumPy Arrays of Random Numbers

Again, several possibilities

Creating arrays

```
>>> a = np.random.rand(4)           # 4-elements array from [0,1)
>>> b = np.random.rand(4,3)        # 4x3 array from [0,1)
>>> c = np.random.randint(1,3,(2,3)) # 2x3 array from [1,3)
>>> d = np.random.randn(4,5)       # 4x5 array (norm. dist)
>>> e = np.random.poisson(3,5)     # 5-element array (Poisson dist of mean 3)
```

Random seed can be set with `np.random.seed(<integer>)`, useful for reproducibility of results



Details about NumPy

`np.__version__` indicates version, `np.show_config()` reveals information about LinAlg Calculus

NumPy's C API

```
ndarray typedef struct PyArrayObject {
    PyObject_HEAD
    char *data;
    int nd;
    npy_intp *dimensions;
    npy_intp *strides;
    PyObject *base;
    PyArray_Descr *descr;
    int flags;
    PyObject *weakreflist;
} PyArrayObject ;
```



Basic Operations

Many basic functions/operators can be applied on NumPy arrays

Examples

```
>>> a = np.random.rand(3,4)
>>> b = np.random.rand(3,4)

>>> a+b
>>> a-b
>>> a*b # Which product? See exercise in this lecture
>>> a/b
>>> a+3.0

>>> a>b
```



Basic Operations - more

Many basic functions/operators can be applied on NumPy arrays

Examples

```
>>> a = np.random.rand(3,4)
>>> b = np.random.rand(3,4)

>>> a.min()
>>> a.min(axis=0)
>>> a.min(axis=1)

>>> np.exp(b)
>>> np.cos(b)
```

All element-wise operations including dedicated functions, called universal functions (ufunc)

`math.exp(b)` \Rightarrow failure as it expects scalar



Data Representation

Data type accessible via dtype variable

Datatype

```
»»» a = np.array([1,0,-2],dtype=np.int64)    #[1,0,-2]
»»» b = np.array([1,0,-2],dtype=np.float64) #[1.0,0.0,-2.0]
»»» c = np.array([1,0,-2],dtype=np.bool)    #[True,False,True]
»»» c.dtype # dtype('bool')
```



Data Structure

Information via attributes accessible:

<code>ndim</code>	number of dimensions (axes)
<code>shape</code>	size of the different dimensions (as a tuple, <code>ndim</code> elements)
<code>size</code>	total number of elements
<code>itemsize</code>	size of one element
<code>nbytes</code>	data size
<code>data</code>	memoryview of the data (<code>tobytes()</code> returns the byte representation)
<code>strides</code>	number of bytes to jump to in-/decrement index by one (as a tuple)
<code>flags</code>	among other things if the memory “belongs” to this array

Transpose of arrays can be called by `<array name>.T` \Rightarrow inverts shape and strides (*i.e.* C-contiguous \leftrightarrow F-contiguous)

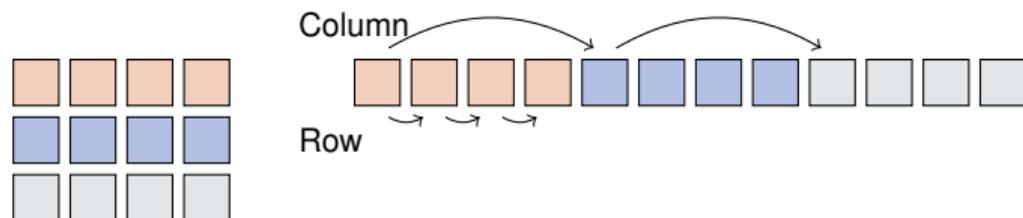
Be aware that many manipulations do not lead to memory duplications. You can force it by the `copy` method.



Data Structure

Strides

Problem of one-dimensional memory to store multi-dimensional arrays:



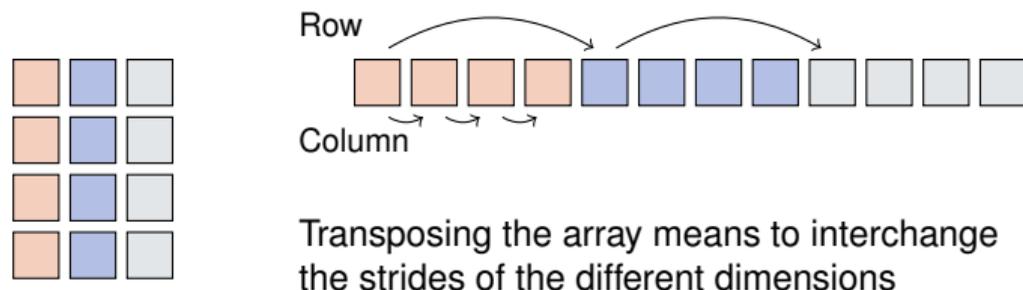
Strides describe the logical alignment of the data within the memory



Data Structure

Strides

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Strides describe the logical alignment of the data within the memory



Data Structure

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Shape Manipulation

Possible to manipulate the shape of existing arrays

Examples

```
>>> a = np.random.randn(3,4)
>>> b = np.random.randn(4)
>>> c = np.random.randn(4,1)

>>> a.reshape(1,12)
>>> a.resize(1,12) # Modify existing array
>>> a.ravel()
>>> a.T
>>> b.shape #(4,) wrong way
>>> b.T # no changes
>>> c.shape #(4,1) right way
>>> c.T # expected behaviour
```



Get the Data

Reading data from txt/csv/etc. files can be sometimes very painful, especially with complicated/mixed data structure

NumPy offers an easy way to read in data from text files

- ▶ function `loadtxt(fname, dtype, comments, delimiter, skiprows, usecols, ...)`
 - ▶ `delimiter` for columns separation, `comments` for the string indicating comments in the text file
- ▶ function `genfromtxt(..., missing_values, filling_values)`
 - ▶ more advanced options for missing data

Binary files as well as text files are also readable via the function `fromfile`



Get the Data

Complicated data structure are manageable by defining the data type, e.g.

Solar.txt (Solar system on June 21, 2014)

```
Sun      332946  2.13E-03 -1.60E-03 -1.20E-04  5.01E-06 ...
Mercury  0.0552 1.62E-01  2.64E-01  6.94E-03 -2.97E-02 ...
Venus    0.8149 3.02E-01  6.54E-01 -8.44E-03 -1.85E-02 ...
Earth    1.00    5.66E-01 -8.46E-01 -9.12E-05  1.40E-02 ...
...
```

Datatype

```
>>> dt = np.dtype([('name', '|S7'), ('mass', np.float),
                    ('position', [('x', np.float), ('y', np.float), ('z', np.float)]),
                    ('velocity', [('x', np.float), ('y', np.float), ('z', np.float)])])
>>> data = np.loadtxt('Solar.txt', dtype=dt)
```



Strings in Arrays

Strings in arrays are in principle not a problem (as seen before), but two things to keep in mind

1. Speed reduction due to a different common base type of the objects stored in the array (*i.e.* PyObject)
 2. Memory spoiling since the entry size is defined by the maximal length of the stored strings
- ⇒ if possible, better work with *e.g.* lookup tables

In general you can mix different data types in an array

Mixed datatype

```
>>> na = np.array([2, True, "Hello"], dtype=object)
```

without `dtype=object` the elements would be treated as strings



Broadcasting – Leveraging Vectorisation

Memory-friendly way of combining arrays with different shapes in mathematical operations

Example:

$$\begin{array}{|c|} \hline 1 \\ \hline \end{array} \begin{array}{|c|} \hline 8 \\ \hline \end{array} \begin{array}{|c|} \hline 3 \\ \hline \end{array} \begin{array}{|c|} \hline 7 \\ \hline \end{array} + \begin{array}{|c|} \hline 3 \\ \hline \end{array}$$

Arrays are alignable if the number of elements in the dimensions match (*i.e.* they are equal or there is only one element)

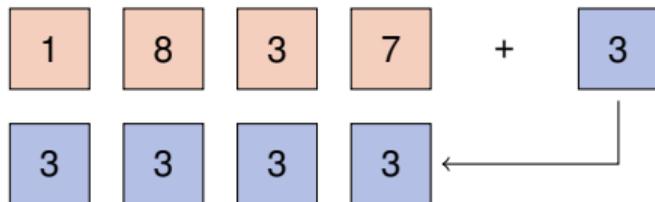
Details can be found in docstrings `np.doc.broadcasting`



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Memory-friendly way of combining arrays with different shapes in mathematical operations

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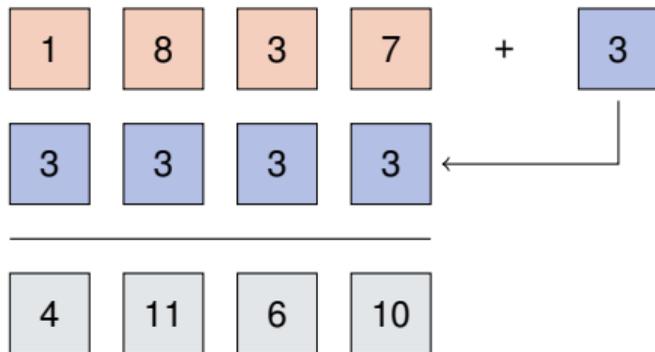
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Broadcasting – Leveraging Vectorisation

Memory-friendly way of combining arrays with different shapes in mathematical operations

Example:



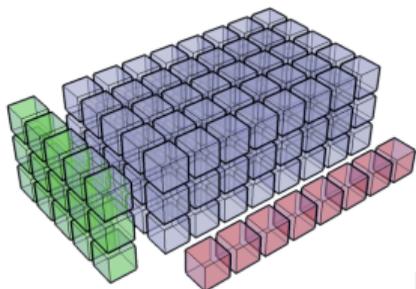
Arrays are alignable if the number of elements in the dimensions match (*i.e.* they are equal or there is only one element)

Details can be found in docstrings `np.doc.broadcasting`



Broadcasting – More complex

Multiplication of a 3×5 -array and a 8-elements array



[S. v. d. Walt]

Broadcasting

```
>>> a = np.random.rand(3,5)
>>> b = np.random.rand(8)
>>> c = a[...,np.newaxis]*b
>>> c.shape # (3,5,8)
```

`np.newaxis` allows to align the dimensions of arrays so that they can be broadcasted, but be careful and make sure the arrays are aligned as you want them.



Broadcasting – Matching Rules

This principle can be expanded to multi-dimensional arrays,

e.g. a 3×4 -array and a 4-elements array

⇒ adding/multiplying/etc. the 1D array to each of the three rows of the 2D array

Rule: Compare dimensions, starting from the last one. Match when either dimension is one or None, or if dimensions are equal.

(3,4)	(4,1,6)	(3,4,1)	(3,2,5)	(4,2,3)	(4,1,3)
(4)	(1,3,6)	(8)	(6)	(4,3)	(4,3)
(3,4)	(4,3,6)	(3,4,8)	not OK	not OK	(4,4,3)

Arrays can be extended further dimensions by

`<array name>[... , np.newaxis]`, *e.g.*

`a.shape` → (3,2)

⇒ `a[... , np.newaxis, np.newaxis].shape` → (3,2,1,1)



Explicit Broadcasting

NumPy has the method `broadcast_arrays` to align two or more arrays

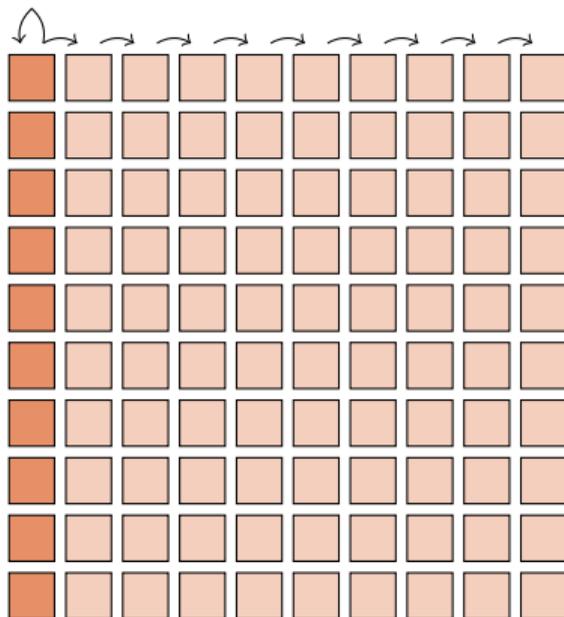
Explicit Broadcasting

```
>>> d = np.random.rand(1,10)
>>> e = np.random.rand(10,1)
>>> dd, ee = np.broadcast_arrays(d,e)
```

`dd` and `ee` are now 10×10 -arrays, but without own data

Broadcasted arrays have a stride of zero \Rightarrow pointer stays while index moves

This concept is a generalisation of the `meshgrid` function in MATLAB





Simple Indexing

NumPy allows to easily select subsets in the array, *e.g.*

Simple indexing

```
>>> a = np.arange(100).reshape(10,10)
>>> a[4:9]           # rows 4 to 8
>>> a[:,3:8]        # columns 3 to 7
>>> a[:, -1]        # the last column
>>> a[-2::-3,1:6:2] # 2nd-to-last row every 3rd and every odd column from 1 to 5
```

Also repetition of rows or columns are possible, *e.g.*

Simple indexing (continued)

```
>>> a[:, [1,3,1]]
```

All these operations do not create additional memory entries!



Fancy Indexing

NumPy also allows to select subsets via arrays of indices, *e.g.*

Fancy indexing

```
>>> a = np.arange(100).reshape(10,10)
>>> i0 = np.random.randint(0,10,(8,1,8))
>>> i1 = np.random.randint(0,10,(2,8))
>>> a[i0,i1] # creates a 8x2x8 array
```

- ▶ First broadcasting of the two index arrays `i0` and `i1`
- ▶ Then selecting the elements in `a` according to the broadcasted arrays

Caution: Mixing of indexing types (*e.g.* `b[5:10,i0,:,i1]`) can lead to unpredictable output shapes (and to barely readable code)



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Pandas





`import pandas as pd` – **and Never use Excel again!**

<https://pandas.pydata.org>

- ▶ Python data analysis library
- ▶ Offering data containers plus corresponding functionality
 - ▶ DataFrame object for data manipulation
 - ▶ time series `pd.Series` and their notorious functions (*i.e.* rolling-“whatever”-you-want function)
 - ▶ many SQL-like data operations (group, merge, join)
- ▶ Tools for reading and writing data and interface to a large variety of file formats (nobody has heard about all of them!)
- ▶ Data interface/API to many data repositories (Yahoo Finance, FRED)

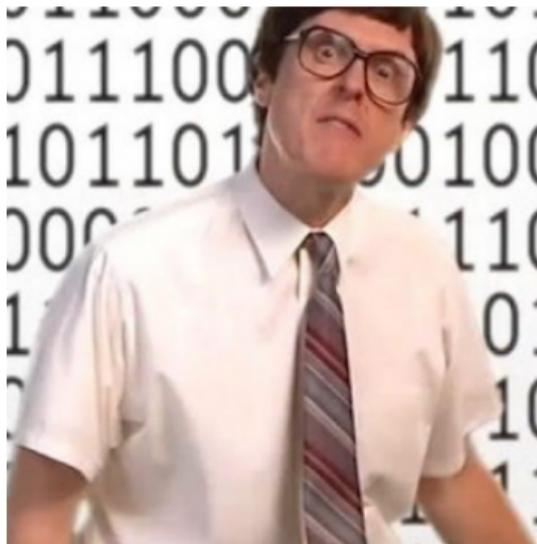
Excel on steroids!

... but particularly helpful tool to transform data (clean-up, aggregation, ...)



numpy **VS.** pandas

NumPy



fast and good with numbers

Pandas



a bit slow and cool with everything



Some Functionalities and Pitfalls

Functionalities

- ▶ Fill missing (NA) values according to different principles
- ▶ Timeseries applications (*e.g.* `resample`)
- ▶ Data aggregation (*e.g.* `groupby`)
- ▶ Merging tools (*e.g.* `append`, `concat`, `merge`, `join`)
- ▶ Derivation of new features via `map` (from Series) or `apply` (from Dataframe)

Pitfalls

- ▶ **Pandas tries to be smart!!!**
- ▶ It accepts data as long as it can derive the lowest common ancestor (almost always the case although ending up with `object`)
- ▶ ... so you should check the data types `dtypes` since your processing code (*e.g.* `groupby`) will work, but not as expected



NumPy and Pandas - Reloaded

If you work with big data, chances are high that at some point you'll encounter a `MemoryError` when loading your data. What next?

- ▶ Dask

<https://dask.pydata.org/en/latest/>

- ▶ flexible parallel computing library for analytics
- ▶ compatible with NumPy, Pandas, Scikit-Learn and many others

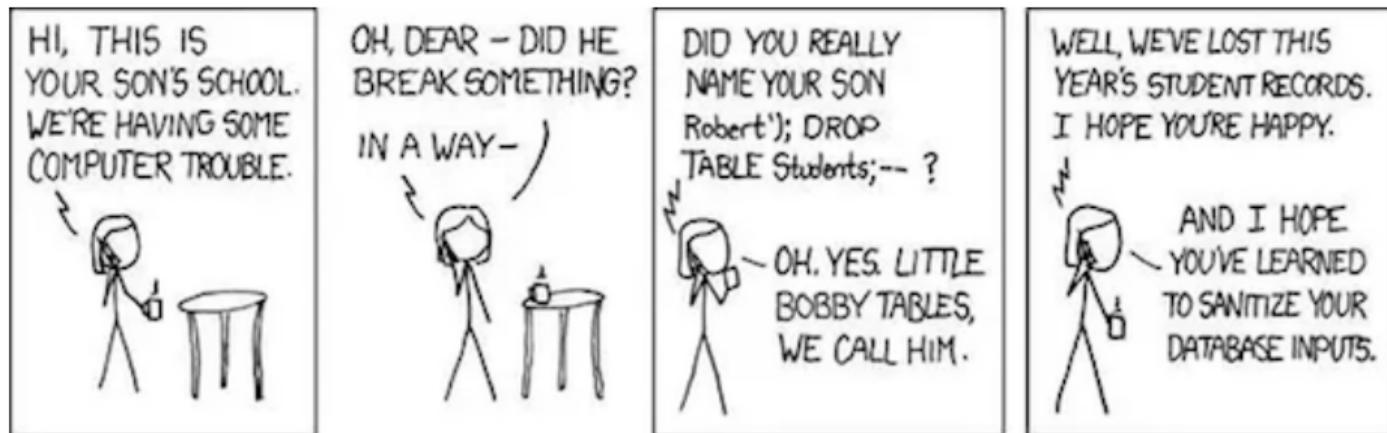
Pandas

```
>>> import pandas as pd
>>> df = pd.read_csv('2018-01-01.csv')
>>> df.groupby(df.user_id).value.mean()
```

Dask

```
>>> import dask.dataframe as dd
>>> df = dd.read_csv('2018-*-.csv')
>>> df.groupby(df.user_id).value.mean()
    .compute()
```

Other Options for Storing Data



- ▶ Pickle, JSON and YAML
- ▶ SQL and NoSQL



Pickle and JSON – Brothers from Other Mothers

Pickle

- ▶ Python proprietary
- ▶ ... thus also Python objects storable
 - class instances
 - NumPy arrays
- ▶ Binary files

Pickle

```
>>> a = dict(...)
>>> with open(<filename>,'wb') as f_o:
>>>     pickle.dump(a,f_o)
>>> with open(<filename>,'rb') as f_i:
>>>     b = pickle.load(f_i)
```

JSON (javascript object notation)

- ▶ Interface to other/web applications
- ▶ Similar structures
 - Python: array → JSON: array
 - Python: dict → JSON: object
- ▶ Some format issues need to be cleared

JSON

```
>>> a = dict(...)
>>> with open(<filename>,'w') as f_o:
>>>     json.dump(a,f_o)
>>> with open(<filename>,'r') as f_i:
>>>     b = json.load(f_i)
```

... also string-wise possible (dumps/loads)



YAML

Improved version of JSON

- ▶ language-portable
- ▶ more human-readable, *e.g.* indentation instead of symbols

Examples

```
data = {  
    'first_data': [1,2,3,4,5],  
    'second_data': 'Just a string.',  
    'third_data': dict(a=1.1,b=1.2,c=1.3)}  
with open('example.yaml','w',default_flow_style=False) as f_o :  
    yaml.dump(data,f_o)  
  
with open('example.yaml','r') as f_i:  
    new_data = yaml.load(f_i)
```



Connection to SQL Databases - `sqlite3`

What is SQLite? (<https://www.sqlite.org>)

- ▶ Lightweight disk-based (= server-less) SQL-type (= spreadsheet-based) database system
- ▶ Does not require a separate server process
- ▶ Understands most of the standard SQL language but omits some features (drop column, rename column)
- ▶ Due to the outsourced write-interlock handling write-intensive programs will suffer

Another option, SQLAlchemy (<http://www.sqlalchemy.org>)

- ▶ Python SQL toolkit that gives developers the full power and flexibility of SQL
- ▶ Probably the most suitable package for a database-type independent approach, with connections to:
 - ▶ MySQL
 - ▶ Microsoft Access
 - ▶ SQLite



A Few Typical (SQL) Commands

<https://www.sqlite.org>

Purpose

Retrieve all data from a table

Retrieve columns (c1,c2) from table t based on condition

Group entries according to values

Add new entry

Delete one or more entries

Command

```
SELECT * FROM <table>
```

```
SELECT c1,c2 FROM t WHERE <cond>
```

```
SELECT SUM(c1),AVG(c2) FROM t GROUP BY c3,c4
```

```
INSERT INTO t (c1,c2) values (v1,v2)
```

```
DELETE FROM t WHERE c1=v1 AND c2=v2
```



sqlite3

<https://docs.python.org/3.6/library/sqlite3.html>

- ▶ Database operations on sqlite3 databases
- ▶ `sqlite3.connect` to get a handler on the database
- ▶ Default output of (part of) a row is a list
 - ⇒ possibility to change the behaviour via the `row_factory` variable of the database
- ▶ Use `?` as placeholder instead of concatenating the SQL command by Python string operations
- ▶ Use `executemany()` to run same SQL command with several parameter sets
- ▶ All executed commands need to be committed before closing the connection
`(<dbvariable>.commit())`

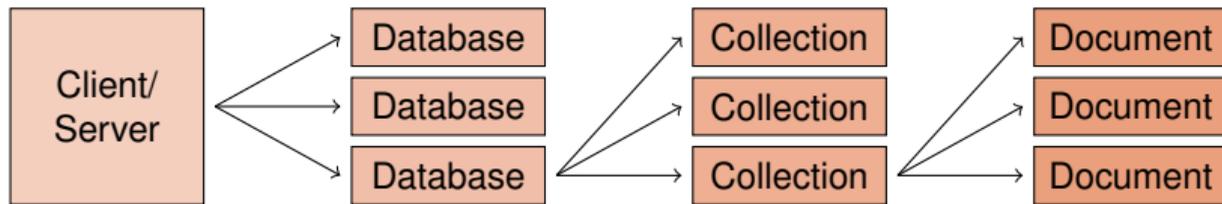


NoSQL Databases and the Flexibility of Data Formats

- ▶ General problem of matching datastructures to a spreadsheet
- ▶ ... on the other hand nice ways to store individual “rows” → JSON

MongoDB as most common NoSQL database <http://www.mongodb.org>

- ▶ It requires a corresponding database server
- ▶ `$ mongod` in the console for start-up



- ▶ Individual documents as special JSON objects (BSON = binary JSON)



pymongo as Python Interface to MongoDB

Basic interface

How to select the collection

```
>>> from pymongo import MongoClient
>>> client = MongoClient(<url>, <port>)
>>> db = client[<database name>]
>>> col = db[<collection name>]
```

Handle to the collection can be used to
insert, get, alter or delete entries

- ▶ `find` method returns iterable cursor
- ▶ MongoDB requires unique identifier `_id` (if not specified given via a hash as `ObjectID`)

Actions

How to read/write/modify

```
>>> col.insert_one(<dict>)
>>> col.insert_many(<list of dict>)
>>> col.delete_one/_many(<query>)
>>> col.find_one/find(<query>)
```

Queries are formulated as dictionaries \implies
{<variable> : <sub-query>} with sub-
query as {<operator> : <value(s)>} or
{‘\$and/\$or’ : <list of sub-queries>}



Summary

- ▶ Python offers various options to handle data suitable for different purposes
 - ▶ NumPy is a very powerful tool for numerical computations and data manipulations
 - ▶ Pandas offers functionalities of the combination of spreadsheet and database processing
 - ▶ Various other options to store data – different formats for different purposes
- ▶ Further leverage with analytics tool (`scipy`) \implies Scientific analysis lecture
- ▶ Very handy tool for data management. . .
- ▶ . . . but, for certain particular tasks, other and more suitable options (*e.g.* large image databases that can be heavily compressed)
- ▶ Try it out, try it out, try it out!



References

1. Stéfán van der Walt, *Diving into NumPy*, Advanced Scientific Programming in Python, 2013 (Zurich)
2. Bartosz Teleńczuk, *Introduction to data visualization*, Advanced Scientific Programming in Python, 2013 (Zurich)
3. Stéfán van der Walt, S. Chris Colbert and Gaël Varoquaux, *The NumPy array: a structure for efficient numerical computation*, Computing in Science and Engineering (IEEE)
4. <http://www.numpy.org>
5. <http://pandas.pydata.org>
6. <http://www.mongodb.com>



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Backup



Data Structure (Advanced)

Further information via the `flags` variable accessible:

<code>C_CONTIGUOUS</code>	dimension ordering C-like
<code>F_CONTIGUOUS</code>	dimension ordering Fortran-like
<code>OWNDATA</code>	responsibility of memory handling
<code>WRITEABLE</code>	data changable
<code>ALIGNED</code>	appropriate hardware alignment
<code>UPDATEIFCOPY</code>	update of base array

C-contiguous:

$a[0, 0], a[0, 1], \dots, a[0, n], a[1, 0], \dots, a[m, n]$

F-contiguous:

$a[0, 0], a[1, 0], \dots, a[m, 0], a[0, 1], \dots, a[m, n]$



Broadcasting (Dimensional)

This principle can be expanded to multi-dimensional arrays, *e.g.* a 3×4 -array and a 1D 4-elements array \Rightarrow adding/multiplying/etc. to each of the three rows the 1D array

Rule: Compare dimensions, starting from the last one. Match when either dimension is one or None, or if dimensions are equal.

(3,4)	(4,1,6)	(3,4,1)	(3,2,5)
(4)	(1,3,6)	(8)	(6)

(3,4)	(4,3,6)	(3,4,8)	not OK
-------	---------	---------	--------

Arrays can be extended to further dimensions by

`<array name>[... , np.newaxis]`, *e.g.*

`a.shape` \rightarrow (3,2)

\Rightarrow `a[... , np.newaxis, np.newaxis].shape` \rightarrow (3,2,1,1)