University of Zurich[UZH]

Department of Physics

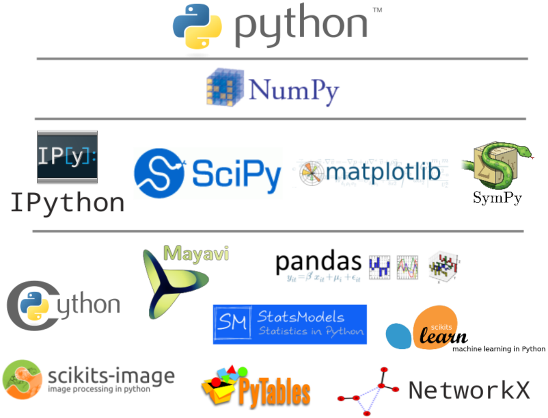
# Scientific Programming: Data Structures – NumPy, Pandas & beyond

Scientific Programming with Python

Federica Lionetto

Based partially on a talk by Stéfan van der Walt

# The Ecosystem of Homo Python Scientificus




[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
```

$\Rightarrow$ Speed up by a factor of $\sim$ 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:

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

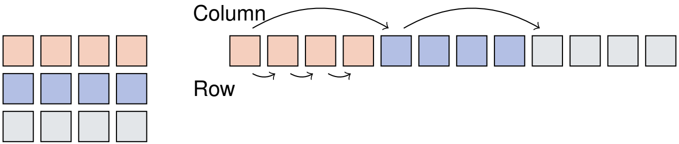
Transpose of arrays can be called by `<array name>.T` $\Rightarrow$ inverts shape and strides (*i.e.* C-contiguous $\leftrightarrow$ F-contiguous)

**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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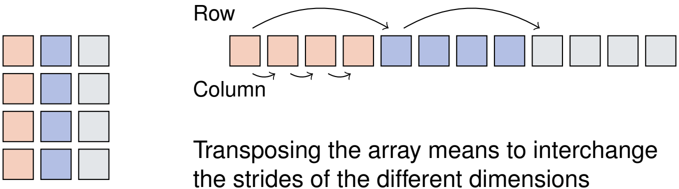


Transposing the array means to interchange the strides of the different dimensions

Strides describe the logical alignment of the data within the memory

# Data Structure

Information via attributes accessible:

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

# 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:**

| | | | | | |
|---|---|---|---|---|---|
| 1 | 8 | 3 | 7 | + | 3 |

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 – Leveraging Vectorisation

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

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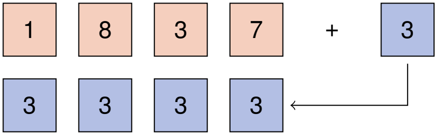


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# Broadcasting – Leveraging Vectorisation

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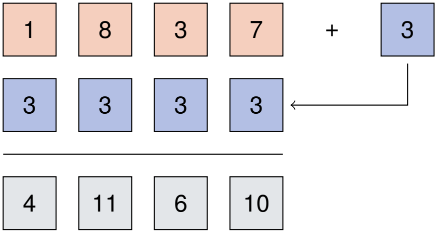
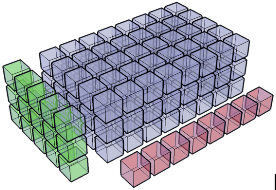



Arrays are alignable if the number of elements in the dimensions match
(*i.e.* they are equal or there is only one element)

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

# Broadcasting – More complex

Multiplication of a 3 $\times$ 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
$\Rightarrow$ 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 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)

# Explicit Broadcasting

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

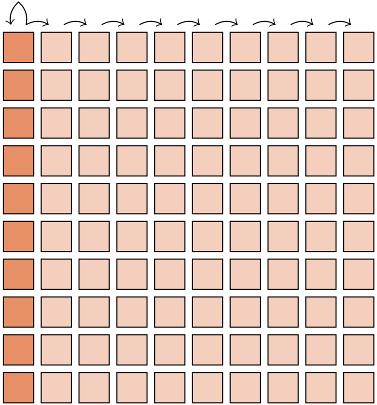
## Explicit Broadcasting

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

`dd` and `ee` are now $10 \times 10$-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 8×2×8 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)

# Pandas

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

https://pandas.pydata.org

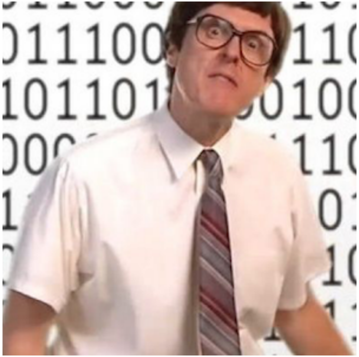
- Python data analysis library
- Offering data containers plus corresponding functionality
  - DataFrame object for data manipulation
  - time series `pd.Series` and their notorious functions (*i.e.* rolling-“whatever”-you-want function)
  - many SQL-like data operations (group, merge, join)
- Tools 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

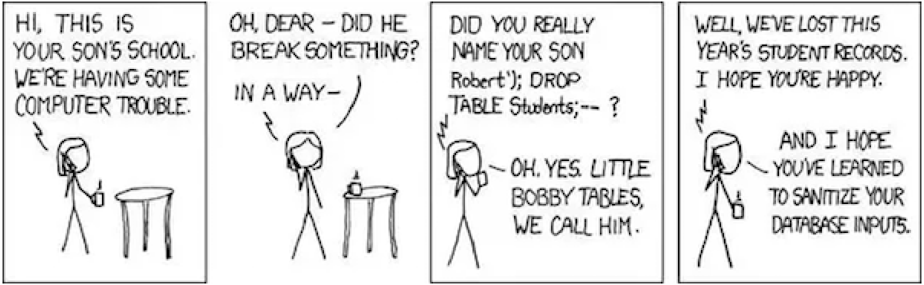
**Pandas**

```
>>> 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

**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

**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**

```
>>> 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 | Command |
|---|---|
| Retrieve all data from a table | `SELECT * FROM <table>` |
| Retrieve columns (`c1,c2`) from table `t` based on condition | `SELECT c1,c2 FROM t WHERE <cond>` |
| Group entries according to values | `SELECT SUM(c1),AVG(c2) FROM t GROUP BY c3,c4` |
| Add new entry | `INSERT INTO t (c1,c2) values (v1,v2)` |
| Delete one or more entries | `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

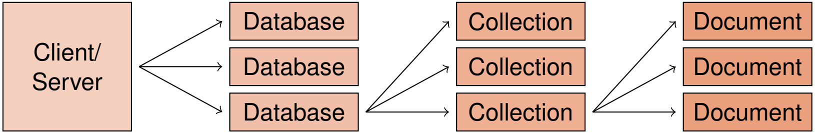
  $\Longrightarrow$ possibility to change the behaviour via the `row_factory` variable of the database
- Use `?` as placeholder instead of concatenating the SQL command by Python string operations
- Use `executemany()` to run same SQL command with several parameter sets
- All executed commands need to be commited 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” $\rightarrow$ 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 sued to insert, get, alter or delete entries

## 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 $\Longrightarrow$ {<variable> : <sub-query>} with sub-query as {<operator> : <value(s)>} or {"$and/$or" : <list of sub-queries>}

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

# 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`) $\Longrightarrow$ 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. Stéfan 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. Stéfan 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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Department of Physics

# Backup

# Data Structure (Advanced)

Further information via the `flags` variable accessible:

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

C-contiguous:
$a[0,0], a[0,1], \ldots, a[0,n], a[1,0], \ldots, a[m,n]$

F-contiguous:
$a[0,0], a[1,0], \ldots, a[m,0], a[0,1], \ldots, a[m,n]$

# Broadcasting (Dimensional)

This principle can be expanded to multi-dimensional arrays, *e.g.* a 3$\times$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)`