Scientific Programming in Python

Inteligencia Artificial en los Sistemas de Control Autónomo
Máster Universitario en Ingeniería Industrial

Departamento de Automática

Objectives

1. Introduce some Python tools for scientific programming.
2. Motivate the need of efficient matrix manipulation.
3. Handle matrices and dataframes in Python.
4. Basic data visualization with Python.

Bibliography

Jake VanderPlas. *Python Data Science Handbook*. Chapters 1, 2, 3 and 4. O'Reilly. (Link).

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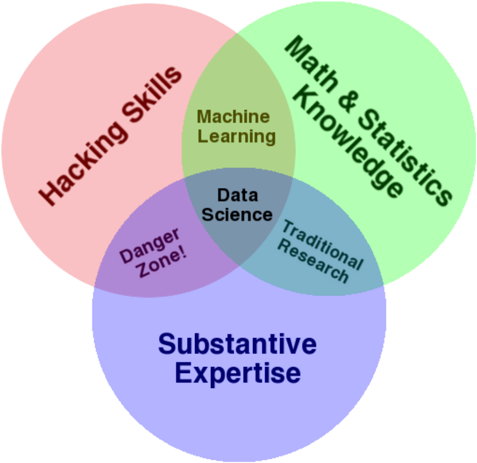
Overview

Data Science



Data Science

The data scientist tookit (I)

Data science is about manipulating data

- Need of specialized tools
- Two main languajes: R and Python

Python is a general purpose programming language

- Easy integration
- Huge ecosystem of packages and tools

Need of data-oriented tools

- Features provided by third-party tools

Data Science

The data scientist tookit (II)

Tool	Type	Description
`iPython`	Software	Advaced Python interpreter
`Jupiter`	Software	Python notebooks (Python interpreter)
`Numpy`	Package	Efficient array operations
`Pandas`	Package	Dataframe support
`Matplotlib`	Package	Data visualization
`Seaborn`	Package	Data visualization with dataframes
`Scikit-learn`	Package	AI/ML package for Python

Data Science
Anaconda

All those tools are packaged in `Anaconda`

- Python distribution for Data Science

Anaconda provides `Spyder`

- Python IDE designed for Data Science

Other tools provided by Anaconda

- Conda: Packages management tool
- TensorFlow: Deep Learning
- Many others

Data Science

Python IDEs for Data Science (I)

iPython

iPython = Interactive Python

- Extended funcionality
- Enhanced UI
- External editor

Running iPython:

```
$ ipython
```

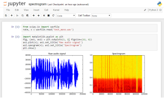
Jupyter

Python notebooks

- Web-based IDE
- Documentation
- Integration with GitHub
- Uses iPython

Running Jupyter:

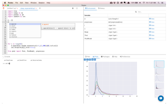
```
$ jupyter notebook
```



Rodeo

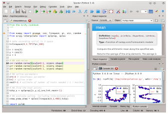
Python version of RStudio

- Good for R developers
- Not included in Anaconda
- Uses iPython



Spyder

Matlab-like IDE



Data Science

Python IDEs for Data Science (II)

Exercises

Write a Python script that shows the multiplication table of the number 5. Write the script using each one of the following environments:

1. iPython + text editor of your choice.
2. Jupiter.
   - Bonus track: Publish the notebook in GitHub.
3. Spyder.
4. Rodeo.

iPython

Basics (I)

In regular Python ...

- most objects come with a docstring attribute
- docstring accesible thorugh `help()`

iPython provides `` `?' ``, a shortcut to `help()`

- `len?`, `list?`, `list.append?`
- Try to type just `` `?' ``

Easy access to source code with `` `??' ``

- Does not work with most buildin functions!

iPython

Basics (II)

Press <tab> to complete almost everything

- Object contents

```
In [21]: a = [1,2,3]

In [22]: a.
          a.append   a.count    a.insert   a.reverse
          a.clear    a.extend   a.pop      a.sort
          a.copy     a.index    a.remove
```

- Packages

```
In [26]: import num
                   numba      numpy
                   numbers    numpydoc
                   numexpr
```

- Wildcards

```
In [29]: *Warning?
     %%!                        BaseException
     ArithmeticError            BlockingIOError
     AssertionError             BrokenPipeError
     AttributeError             BufferError
```

iPython

Basics (III): Keyboard shortcuts

Navigation

Keystroke	Action
`Ctrl-a`	Move cursor to the beginning of the line
`Ctrl-e`	Move cursor to the end of the line
`Ctrl-b`	Move cursor back one character
`Ctrl-f`	Move cursor forward one character

History

Keystroke	Action
`Ctrl-p` (↑)	Previous command
`Ctrl-n` (↓)	Next command
`Ctrl-r`	Reverse-search

Text entry

Keystroke	Action
`Ctrl-d`	Delete next character in line
`Ctrl-k`	Cut text from cursor to end of line
`Ctrl-u`	Cut text from beginning of line to cursor
`Ctrl-y`	Yank (paste) previously cut text

iPython

iPython magic commands

Magic commands: iPython extension of Python syntax

- Not valid in regular Python
- Provides handly features
- Widely used in DS and ML

Two flavours

- % prefix: Line magics - single line
- %% prefix: Cell magics - several lines

Help available

- `%magic`: Magic commands
- `%lsmagic`: List of magic commands

iPython

Pasting code blocks: %paste and %cpaste

Pasting code in Python is troublesome

- %paste: Paste one time
- %%cpaste: Paste several times

```python
def donothing(x):
    return x
```

%paste

```
In [20]: %paste
   def donothing(x):
    return x

## -- End pasted text --
```

%cpaste

```
In [25]: %cpaste
Pasting code; enter '--' alone on the line
to stop or use Ctrl-D.
:       def donothing(x):
            return x:
:--
```

iPython

Running external code: %run and %timeit

`%run`: Execute script

- Many optional arguments
- Checkout `%run?`

```
In [40]: %run donothing.py

In [41]: donothing(10)
Out[41]: 10
```

`%timeit`: Computes execution time

- Executes a single line
- Automatic adjustment of runs
- Shows basic statistics

```
In [33]: %timeit [n ** 2 for n in range(200)]
71.6 µs ± 1.84 µs per loop
(mean ± std. dev. of 7 runs, 10000 loops each)

In [34]: %timeit [n ** 2 for n in range(2000)]
753 µs ± 16.2 µs per loop
(mean ± std. dev. of 7 runs, 1000 loops each)
```

`%%timeit`: Several lines

iPython

Input and output history (I)

iPython stores its history as objects

- `In`: Input commands
  - List storing commands
- `Out`: Commands output
  - Dictionary storing outputs
  - Not all commands have outputs

```
In [1]: import math
In [2]: math.sin(2)
Out[2]: 0.9092974268256817
In [3]: math.cos(2)
Out[3]: -0.4161468365471424
In [4]: Out[2] ** 2 + Out[3] ** 2
Out[4]: 1.0
```

iPython

Input and output history (II)

Fast access to history: Underscore (_)

- Variable containing the last output
- Example: `print(_)`

Double and triple underscores

- Example: `print(__)`
- Example: `print(___)`

Trick: Shortcut to access (_*n*)

- Out[n] = _n, with n=number
- Example: `print(_2)`

Magic command to show history

- `%history`

Supressing command output (`;`)

- Example: `4 * 2;`

iPython

iPython shell commands

iPython provides easy interaction with the shell

- Execution of shell commands from iPython
- Use prefix `` `!' ``
- Example: `!ls`, `!pwd`

Save shell output in Python variables

- Example: `files = !ls`

Use Python variables in shell

- Example: `!echo {files}`

iPython

Automagic

Problems with some shell commands

```
In [23]: !pwd
/repositorios/pythonCourse
In [24]: !cd ..
In [25]: !pwd
/repositorios/pythonCourse
```

Some magic commands here to help

- `%cd`, `%ls`, `%mkdir`, `%pwd`, ...

Those magics are regularly used ...

- ... so common that % is no longer required (automagic)
- Working with iPython is almost like working with a Unix-like shell

Automagic commands

`cat`, `cp`, `env`, `ls`, `man`, `mkdir`, `more`, `mb`, `pwd`, `rm` and `rmdir`

NumPy

Understanding Data Types in Python (I)

Static typing

```
/* C code */
int result = 0;
for(int i=0; i<100; i++){
    result += i;
}
```

- Data types must be declared
- Data types cannot change
- Error detection in compilation
- Variables names are, basicly, labels

Dynamic typing

```
# Python code
result = 0
for i in range(100):
   result += i
```

- Data types are not declared
- Data types can change
- Error detection in run-time
- Variables are complex data structures (even for simple types)

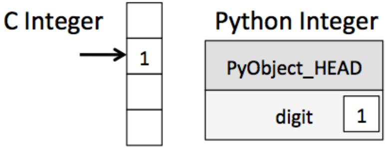
NumPy

Understanding Data Types in Python (II)

Dynamic typing must be implemented somewhere ...

Python 3.4 source code

```
struct _longobject {
    long ob_refcnt;
    PyTypeObject *ob_type;
    size_t ob_size;
    long ob_digit[1];
};
```

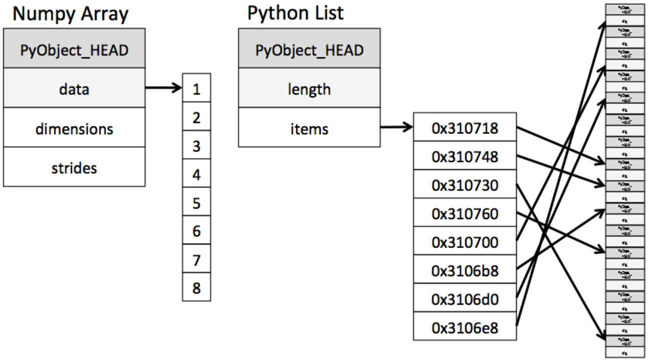


NumPy

Understanding Data Types in Python (III)

A Python list may contain different types

```
In [1]: L3 = [True, "2", 3.0, 4]
   ...: [type(item) for item in L3]
Out[1]: [bool, str, float, int]
```



NumPy

Understanding Data Types in Python (IV)

Standard Python data types are powerful and flexible

- Flexibility has a price: Reduced performance
- Not an big issue in generic programming
- A big issue in scientific programming
- We require efficient data manipulation mechanisms: NumPy

NumPy: Python package for numeric computation

- Efficient array implementation
- Fast mathematical functions
- Random numbers generation
- Static data types: Less flexibility

Most Python modules for AI/ML depend on NumPy, in particular

- Pandas (dataframes), Scikit-learn (ML), Seaborn (data visualization)

NumPy

Introduction

NumPy must be imported in order to be available

- Remember, you can use `np?` or `np.<TAB>`

The main component of NumPy is ndarray

- Python object
- Efficient matrix representation
- Homogeneus elements

Convention

```
import numpy as np
```

```
In [1]: array = np.array
    ([1,2,3])
In [2]: array
Out[1]: array([1, 2, 3])
In [3]: array = np.array
    ([[1,2],[3,4]])
```

NumPy

Matrix creation

NumPy functions for array creation from lists

- Lists must contain the same type, NumPy will upcast if needed
- `np.array([1, 4, 2, 5, 3])`
- `np.array([1, 2, 3, 4], dtype='float32')`: Explicit data type
- `np.array([3.14, 4, 2, 3])`: Upcast

NumPy functions for array creation from scratch

- `np.zeros(10, dtype=int)`: All zeros
- `np.ones((3, 5), dtype=float)`: All ones
- `np.full((3, 5), 3.14)`: Fill matrix
- `np.arange(0, 20, 2)`: Similar to Python's range()
- `np.linspace(0, 1, 5)`: Evenly spaced numbers
- `np.random.random((3, 3))`: Random numbers
- `np.random.normal(0, 1, (3, 3))`: Random normal numbers
- `np.random.randint(0, 10, (3, 3))`: Random integers
- `np.eye(3)`: Identity matrix
- `np.empty(3)`: Empty matrix

NumPy

NumPy data types

Python is implemented in C

- Data types in NumPy are based on those in C

Two styles to declare types

- String: `np.zeros(10, dtype='int16')`
- NumPy object: `np.zeros(10, dtype=np.int16)`

Data type	Description
`bool_`	Boolean (True or False) stored as a byte
`int_`	Default integer type
`intc`	Identical to C
`intp`	Integer used for indexing
`int8`	Byte
`int16`	Integer
`int32`	Integer
`int64`	Integer
`uint8`	Unsigned integer
`uint16`	Unsigned integer
`uint32`	Unsigned integer
`uint64`	Unsigned integer
`float_`	Shorthand for float64
`float16`	Half precision float
`float32`	Single precision float
`float64`	Double precision float
`complex_`	Shorthand for complex128
`complex64`	Complex number
`complex128`	Complex number

NumPy

NumPy array attributes

Ndarray objects expose several attributes

- `ndim`: Dimensions
- `shape`: Size of each dimension
- `size`: Number of elements
- `dtype`: Data type
- `itemsize`: Size of each element (in bytes)
- `nbytes`: Size of the array (in bytes)

```
x = np.random.randint(10, size
    =(3, 4))
print("x3 ndim: ", x3.ndim)
print("x3 shape:", x3.shape)
print("x3 size: ", x3.size)
print("dtype:", x3.dtype)
print("itemsize:", x3.itemsize,
    "bytes")
print("nbytes:", x3.nbytes, "
    bytes")
```

NumPy

Accessing single elements

Unidimensional array

- `array[index]`

Unidimensional array from the end

- `array[-index]`

Multidimensional array

- `array[row,column]`

```
x = np.array([5, 0, 3, 3, 7, 9])
x[0] # 5
x[4] # 7
x[-1] # 9
x[-2] # 7
x = np.array([[3, 5, 2, 4],
     [7, 6, 8, 8],
     [1, 6, 7, 7]])
x2[2, 0] # 1
x2[2, -1] # 7
```

Warning

Ndarray has fixed types, values can be truncaded without warning. Big source of problems!

NumPy

Accessing subarrays

Slice notation can be used with ndarray

- `x[start:stop:step]`

Default values

- Start = 0
- Stop = Size of dimension
- Step = 1

Step may take a negative value

- Reverse order

These operations return a view

- Use `copy()` to get a copy

Unidimensional array

```
x[:5]    # first five elements
x[5:]    # elements after index 5
x[4:7]   # middle sub-array
x[::2]   # every other element
x[1::2]  # every other element,
    starting at index 1
x[::-1]  # all elements, reversed
```

Multidimensional a rray

```
x[:2, :3]   # 2 rows, 3 columns
x[:3, ::2]  # all rows, every
    other column
x[::-1, ::-1]
```

NumPy

Reshaping of arrays

Reshaping arrays is a very common task

- Change data number of dimensions

Important ndarray method: `reshape()`

- Changes the dimensions of an array
- Sizes must match

Conversion of 1-D arrays into column or row matrices

- Using method `reshape()`
- Using the keyword np.newaxis

General reshaping

```
In [1]: x=np.array([1, 2, 3, 4])
In [2]: x.reshape((2,2))
Out[1]:
array([[1, 2],
       [3, 4]])
```

1-D to row

```
x = np.array([1, 2, 3])
x.reshape((1, 3))
x[np.newaxis, :]
```

1-D to column

```
x.reshape((3, 1))
x[:, np.newaxis]
```

NumPy

Concatenation of arrays

Three methods to join arrays

- `np.concatenate()`
- `np.vstack()`
- `np.hstack()`

np.concatenate()

```
In [1]: x = np.array([1, 2, 3])
In [2]: y = np.array([3, 2, 1])
In [3]: np.concatenate([x, y])
Out[1]: array([1, 2, 3, 3, 2, 1])
```

np.vstack()

```
In [1]: x = np.array([1, 2, 3])
In [2]: grid = np.array([[9, 8, 7],
   ...:                  [6, 5, 4]])
In [3]: np.vstack([x, grid])
Out[107]:
array([[1, 2, 3],
       [9, 8, 7],
       [6, 5, 4]])
```

NumPy

Splitting of arrays

Three methods to split arrays

- `np.split()`
- `np.vsplit()`
- `np.hsplit()`

np.split()

```
In [1]: x = [1, 2, 3, 99, 99, 3, 2, 1]
In [2]: x1, x2, x3 = np.split(x, [3, 5])
In [3]: print(x1, x2, x3)
[1 2 3] [99 99] [3 2 1]
```

np.vstack()

```
In [1]: grid = np.arange(16).reshape((4, 4))
In [2]: print(grid)
[[ 0  1  2  3]
 [ 4  5  6  7]
 [ 8  9 10 11]
 [12 13 14 15]]
In [3]: upper, lower = np.vsplit(grid, [2])
In [4]: print(upper)
    [[0 1 2 3]
     [4 5 6 7]]
```

NumPy

Universal functions (I)

Python may be ridiculously slow

- Run-time type checks and function dispatching
- Evident when an operation is repeated over a collection of data

Performance test

```
def compute_reciprocals(values):
    output = np.empty(len(values))
    for i in range(len(values)):
        output[i] = 1.0 / values[i]
    return output

big_array = np.random.randint(1, 100, size=1000000)
# Stardand CPython
%timeit compute_reciprocals(big_array)
# 3.59 s ± 139 ms per loop
# NumPy
%timeit (1.0 / big_array)
#5.41 ms ± 182 µs per loop
```

NumPy

Universal functions (II)

Vectorized operations: Functions that are aware of NumPy's static typing

- Avoid dynamic type-checking
- Loop related code pushed into the compiled layer
- Hugely improved performance
- Perform an operation with the first element and then it to the rest

In NumPy, vectoriced operations are named universal functions, of ufuncs

- Regular functions
- Arrays as arguments (one or multi-dimensional)
- Operates between arrays of different sizes (broadcasting)

In order to take advantange of NumPy's performance, ufuncs must be used

NumPy

Universal functions: Arithmetic functions

NumPy makes use of Python's native arithmetic operators

- Used like regular Python operators
- Operators are wrappers for NumPy's functions

Operator	Equivalent ufunc	Description
`+`	`np.add`	Addition (e.g., 1 + 1 = 2)
`-`	`np.subtract`	Subtraction (e.g., 3 - 2 = 1)
`-`	`np.negative`	Unary negation (e.g., -2)
`*`	`np.multiply`	Multiplication (e.g., 2 * 3 = 6)
`/`	`np.divide`	Division (e.g., 3 / 2 = 1.5)
`//`	`np.floor_divide`	Floor division (e.g., 3 // 2 = 1)
`**`	`np.power`	Exponentiation (e.g., 2 ** 3 = 8)
`%`	`np.mod`	Modulus/remainder (e.g., 9 % 4 = 1)

NumPy

Universal functions (III)

Binary ufuncs

```
x = np.arange(4)
print("x     =", x)
print("x + 5 =", x + 5)
print("x - 5 =", x - 5)
print("x * 2 =", x * 2)
print("x / 2 =", x / 2)
print("x // 2 =", x // 2)  # floor division
np.add(x, 2)               # array plus scalar
```

Unary ufuncs

```
print("-x     = ", -x)
print("x ** 2 = ", x ** 2)
print("x % 2  = ", x % 2)
```

NumPy

Universal functions: Basic functions

Absolute value

- `np.absolute(x)` and `np.absolute(x)`

Trigonometric functions

- `np.sin(theta)`, `np.cos(theta)`, `np.tan(theta)`
- `np.arcsin(theta)`, `np.arccos(theta)`, `np.arctan(theta)`

Exponents and logarithms

- `np.exp(x)`, `np.exp2(x)`, `np.power(base, x)`
- `np.log(x)`, `np.log2(x)`, `np.log10(x)`

Advanced mathematical functions

- Checkout module `scipy.special` for exotic mathematical functions

Output as argument

- Avoid temporal variables using `out` argument in ufuncs
- Example: `np.multiply(x, 10, out=y)`

NumPy

Universal functions: Special functions

Aggregation functions

- Applied to any ufunc
- `reduce(x)`: Repeatedly applies an ufunc to the elements of an array until only a single result remains
- `accumulate(x)`: Like `reduce()`, but it stores intermediate values
- `outer(x)`: Compute the output of all pairs of two different inputs

reduce() example

```
In  [1]: x = np.arange(1, 6)
In  [2]: np.add.reduce(x)
Out [1]: 15
```

accumulate() example

```
In  [1]: np.add.reduce(x)
Out [1]: 15
```

Outer() example

```
In  [132]:np.multiply.outer(x, x)
array([[ 1,  2,  3,  4,  5],
       [ 2,  4,  6,  8, 10],
       [ 3,  6,  9, 12, 15],
       [ 4,  8, 12, 16, 20],
       [ 5, 10, 15, 20, 25]])
```

NumPy

Universal functions: Aggregations (I)

Many ufuncs to summarize data

- Basic step in exploratory data analysis
- Argument `axis` determines to which dimension the summary is to be applied

Function	NaN-safe version	Description
`np.sum`	`np.nansum`	Compute sum of elements
`np.prod`	`np.nanprod`	Compute product of elements
`np.mean`	`np.nanmean`	Compute mean of elements
`np.std`	`np.nanstd`	Compute standard deviation
`np.var`	`np.nanvar`	Compute standard deviation
`np.min`	`np.nanmin`	Find minimum value
`np.max`	`np.nanmax`	Find maximum value
`np.argmin`	`np.nanargmin`	Find index of minimum value
`np.argmax`	`np.nanargmax`	Find index of maximum value
`np.median`	`np.nanmedian`	Compute median of elements
`np.percentile`	`np.nanpercentile`	Compute rank-based statistics of elements
`np.any`	`N/A`	Evaluate whether any elements are true
`np.all`	`N/A`	Evaluate whether all elements are true

NumPy

Universal functions: Aggregations (II)

(Download dataset)

- Use wget or curl to download the file within iPython

Basic data analysis example

```
import pandas as pd
data = pd.read_csv('president_heights.csv')
heights = np.array(data['height(cm)'])
print(heights)

print("Mean height:          ", heights.mean())
print("Standard deviation:", heights.std())
print("Minimum height:     ", heights.min())
print("Maximum height:     ", heights.max())

print("25th percentile:    ", np.percentile(heights, 25))
print("Median:             ", np.median(heights))
print("75th percentile:    ", np.percentile(heights, 75))
```

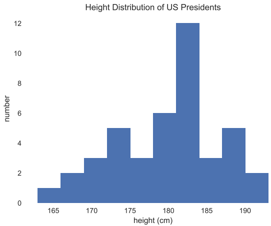
NumPy

Universal functions: Aggregations (III)

Basic data analysis example (Continuation)

```
%matplotlib inline
import matplotlib.pyplot as plt
import seaborn; seaborn.set()  # set plot style

plt.hist(heights)
plt.title('Height Distribution of US Presidents')
plt.xlabel('height (cm)')
plt.ylabel('number');
```



NumPy

Universal functions: Broadcasting (I)

Broadcasting is a mechanism to operate over arrays of different sizes

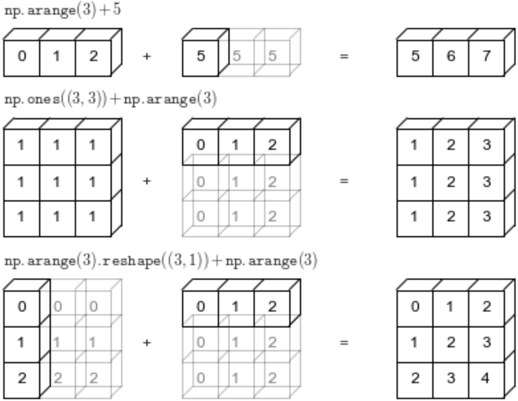
- Used in ufuncs
- Implicit array expansion through three rules

Broadcasting rules

1. Rule 1: If the two arrays differ in their number of dimensions, the shape of the one with fewer dimensions is padded with ones on its leading (left) side.
2. Rule 2: If the shape of the two arrays does not match in any dimension, the array with shape equal to 1 in that dimension is stretched to match the other shape.
3. Rule 3: If in any dimension the sizes disagree and neither is equal to 1, an error is raised.

NumPy

Universal functions: Broadcasting (II)



Array expansion does not consume memory!

NumPy

Universal functions: Broadcasting (III)

Normalization

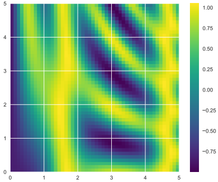
```
X = np.random.random((10, 3))
Xmean = X.mean(0)
X_centered = X - Xmean
```

3D plot

```
%matplotlib inline
import matplotlib.pyplot as plt

x = np.linspace(0, 5, 50)
y = np.linspace(0, 5, 50)[:, np.newaxis]
z = np.sin(x)**10+np.cos(10+y*x)*np.cos(x)

plt.imshow(z, origin='lower',
    extent=[0, 5, 0, 5], cmap='viridis')
plt.colorbar();
```



NumPy

Comparisons, masks, and Boolean logic (I)

(Download dataset)

Example

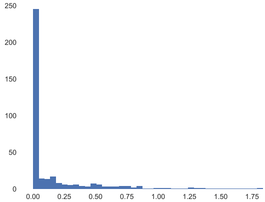
```
import numpy as np
import pandas as pd

# pandas to extract rainfall inches as a ndarray
rainfall = pd.read_csv('Seattle2014.csv')['PRCP'].values
inches = rainfall / 254.0  # 1/10mm -> inches
inches.shape
# Outputs (365,)

%matplotlib
import matplotlib.pyplot as plt
import seaborn; seaborn.set()
plt.hist(inches, 40);
```

NumPy

Comparisons, masks, and Boolean logic (II)



Data filtering is a recurrent task

- How many rainy days were there in the year?
- What is the average precipitation on those rainy days?
- How many days were there with more than half an inch of rain?

Two filtering methods in NumPy

- Boolean arrays masks
- Fancy indexing

NumPy

Comparisons, masks, and Boolean logic: Booleans arrays masks (I)

Syntax examples

```
x[x<5]
x[x==3]
x[(x>3)&(x<=5)]
```

We've seen arithmetic ufuncs ...

- ... but they also support comparison and boolean operations
- Return an array of booleans

Operator	Ufunc
==	`np.equal`
!=	`np.not_equal`
<	`np.less`
<=	`np.less_equal`
>	`np.greater`
>=	`np.greater_equal`

Operator	Ufunc
&	`np.bitwise_and`
|	`np.bitwise_or`
^	`np.bitwise_xor`
~	`np.bitwise_not`

NumPy

Comparisons, masks, and Boolean logic: Booleans arrays masks (II)

Example

```
print(x)
[[5,  0,  3,  3]
 [7,  9,  3,  5]
 [2,  4,  7,  6]]
np.count_nonzero(x < 6) # Returns 8
np.sum(x < 6) # Returns 8
np.sum(x < 6, axis=1) # By row, returns
    array([4,2,2])
np.any(x > 8) # Returns True
np.any(x < 0) # Returns False
np.all(x < 10)# Returns True

np.sum(~((inches <= 5) | (inches >= 1)))
```

NumPy

Comparisons, masks, and Boolean logic: Fancy indexing

So far we've seen three accessing methods

- Simple indices (`x[1]`)
- Slices (`x[:5]`)
- Boolean masks (`x[x>0]`)

Fancy indexing: Pass arrays on indices instead of scalars

Example

```
x = rand.randint(100, size=10)
[x[3], x[7], x[2]] # Simple indices
ind = [3, 7, 4] # Array of indices
x[ind] # Fancy indexing
x[[3,5,6]] # Also valid
```

The shape of the result reflects the shape of the index arrays rather than the shape of the array being indexed

NumPy

Structured arrays (I)

Some times, we need to group data

- Example: Store name, age and weight of several people
- Different data types for each attribute

Non-structured array

```
name = ['Alice', 'Bob', 'Cathy', 'Doug']
age = [25, 45, 37, 19]
weight = [55.0, 85.5, 68.0, 61.5]
```

Solution: Structured arrays

Structured arrays

```
# Use a compound data type for structured arrays
data = np.zeros(4, dtype={'names':('name', 'age', 'weight'),
                          'formats':('U10', 'i4', 'f8')})
```

NumPy

Structured arrays (II)

Structured array manipulation

```
data['name'] = name
data['age'] = age
data['weight'] = weight

# Get all names
data['name']
# Get first row of data
data[0]
# Get the name from the last row
data[-1]['name']
# Get names where age is under 30
data[data['age'] < 30]['name']
```

These kind of structures are day-to-day used

- Pandas is a much better choice

Pandas

Introduction

A data science workflow needs more features

- Label columns and rows
- Missing data
- Operations on groups
- Data input

Pandas implements all those features, and more

- Built on NumPy's ndarray

Pandas provides two main objects

- `Series`
- `DataFrame`

Convention

```
import numpy as np
import pandas as pd
```

Pandas

Introduction

A DS/ML workflow needs more features

- Missing data
- Data input
- Operations on groups
- Label columns and rows

Pandas provides all those features, and more

- Pandas = **PAN**el **DA**ta **S**ystem
- Built on NumPy's ndarray
- Provides dataframes

Pandas provides two main objects

- `Series` and `DataFrame`

Convention

```
import numpy as np
import pandas as pd
```

Pandas

The Pandas Series object (I)

A `Series` is a one-dimensional array of indexed data

- NumPy arrays indices are implicit (i.e. its position)
- Series indices are explicit, and can be any type

Two attributes

- `values`: ndarray
- `index`: pd.Index object

Accessing through regular Python syntax

```
data = pd.Series([0.25,
    0.5, 0.75, 1.0])
data.values
data.index
data[1:3]
```

Pandas

The Pandas Series object (II)

Custom indices

```
In[1] : data = pd.Series([0.25, 0.5, 0.75, 1.0],
                         index=['a', 'b', 'c', 'd'])
In [2]: data
Out[1]:
a       0.25
b       0.50
c       0.75
d       1.00
dtype: float64

In [3]: data['a']
Out[2]: 0.25
In [4]: data[0]
Out[3]: 0.25
```

Pandas

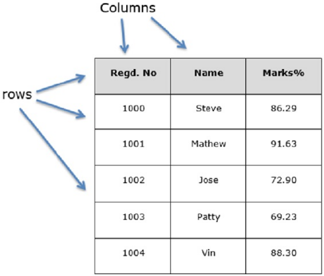
The Pandas `DataFrame` object (I)

A `DataFrame` is a 2-D tabular data structure

- Similar to a spreadsheet
- Homogeneous columns
- Heterogeneous rows

Two attributes, both `pd.Index`

- `index`: Rows
- `columns`: Columns



Regd. No	Name	Marks%
1000	Steve	86.29
1001	Mathew	91.63
1002	Jose	72.90
1003	Patty	69.23
1004	Vin	88.30

(Source)

Pandas

The Pandas DataFrame object (II)

DataFrame example

```
In [1]:  import seaborn as sns

In [2]:  iris = sns.load_dataset('iris')
In [3]:  iris.head()

Out[1]:
sepal_length  sepal_width  petal_length  petal_width  species
0          5.1          3.5           1.4          0.2   setosa
1          4.9          3.0           1.4          0.2   setosa
2          4.7          3.2           1.3          0.2   setosa
3          4.6          3.1           1.5          0.2   setosa
4          5.0          3.6           1.4          0.2   setosa
In [246]: iris.columns
Out[246]:
Index(['sepal_length', 'sepal_width', 'petal_length', '
    petal_width', 'species'],
    dtype='object')
```

Pandas

Constructing DataFrame objects

Manual initialization

- From a single `Series` object
  `pd.DataFrame(population, columns=['population'])`
- From several `Series` objects
  `pd.DataFrame('population': population, 'area': area)`
- From a dictionary
  `pd.DataFrame([{'a': 0, 'b': 0}, {'a': 1, 'b': 2}])`
- From a NumPy 2-D array
  ```
  pd.DataFrame(np.random.rand(3, 2),
  columns=['foo', 'bar'], index=['a', 'b', 'c'])
  ```

Read from a file

- CSV (very common!!!): `pd.read_csv('filename.csv')`
- Excel:
  `pd.read_excel('filename.xlsx', sheetname='mysheet')`