南京大学
自然语言处理研究组
Natural Language Processing Group

南京大学
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Python和科学计算基础

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SciPy生态系统

- **SciPy (pronounced “Sigh Pie”) is a Python-based ecosystem of open-source software for mathematics, science, and engineering.**

NumPy
Base N-dimensional array package

SciPy library
Fundamental library for scientific computing

Matplotlib
Comprehensive 2-D plotting

IPy[y]: IPython

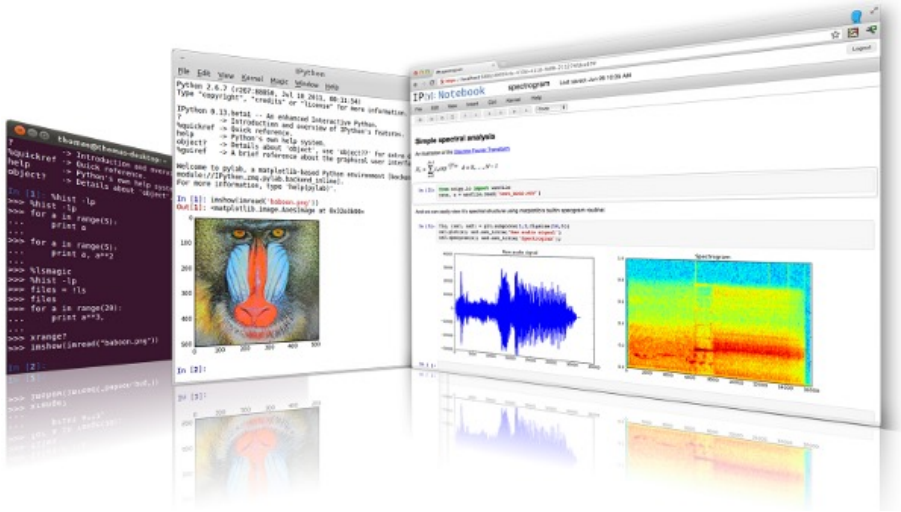
IPython
Enhanced interactive console

SymPy
Symbolic mathematics

pandas
Data structures & analysis

IPython

- **IPython provides a rich architecture for interactive computing with:**
  - A powerful interactive shell.
  - A kernel for Jupyter.
  - Support for interactive data visualization and use of GUI toolkits.
  - Flexible, embeddable interpreters to load into your own projects.
  - Easy to use, high performance tools for parallel computing.



IP[y]:
IPython

NumPy

- **NumPy is the fundamental package for scientific computing in Python.**
  - **a multidimensional array object**
  - various derived objects (such as masked arrays and matrices)
  - an assortment of routines for fast operations on arrays, including mathematical, logical, shape manipulation, sorting, selecting, I/O, discrete Fourier transforms, basic linear algebra, basic statistical operations, random simulation and much more.

SciPy

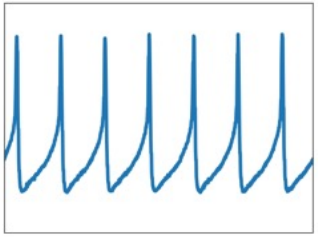
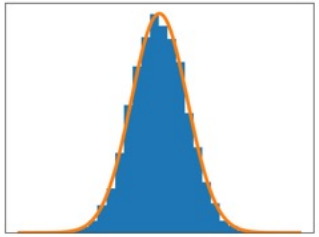
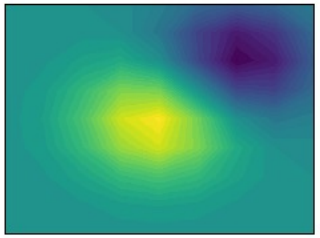
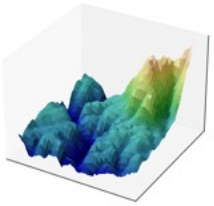
- **The SciPy library is one of the core packages that make up the SciPy stack. It provides many user-friendly and efficient numerical routines:**
  - numerical integration
  - interpolation
  - optimization
  - linear algebra
  - statistics.

Subpackage	Description
cluster	Clustering algorithms
constants	Physical and mathematical constants
fftpack	Fast Fourier Transform routines
integrate	Integration and ordinary differential equation solvers
interpolate	Interpolation and smoothing splines
io	Input and Output
linalg	Linear algebra
ndimage	N-dimensional image processing
odr	Orthogonal distance regression
optimize	Optimization and root-finding routines
signal	Signal processing
sparse	Sparse matrices and associated routines
spatial	Spatial data structures and algorithms
special	Special functions
stats	Statistical distributions and functions

Matplotlib

Matplotlib: Visualization with Python

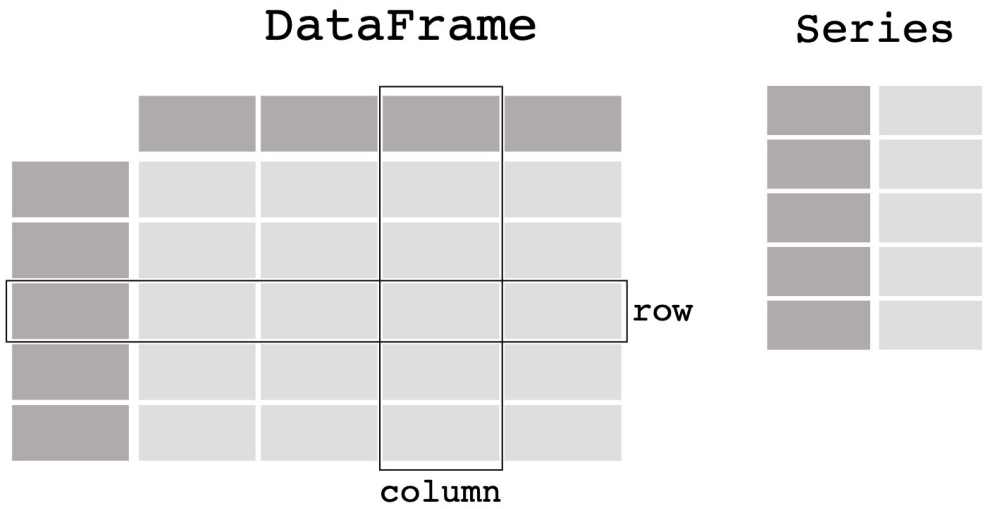
Matplotlib is a comprehensive library for creating static, animated, and interactive visualizations in Python.

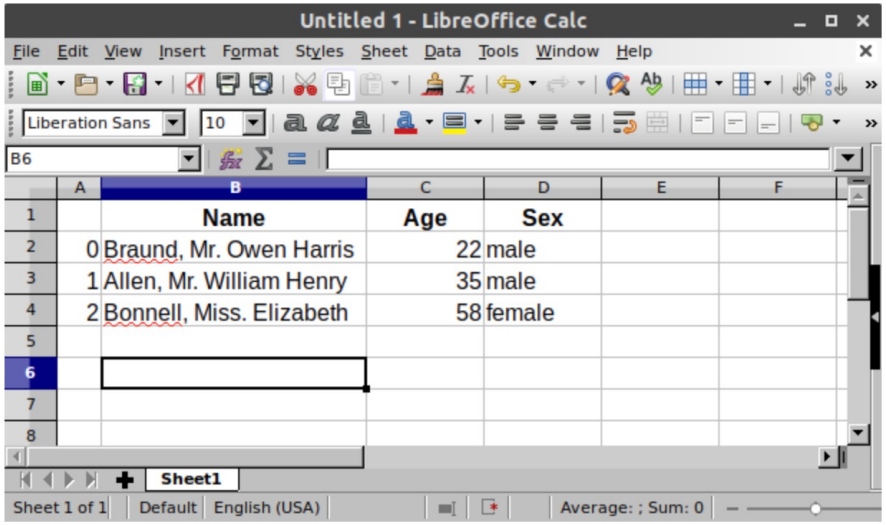





Matplotlib makes easy things easy and hard things possible.

Pandas

- **pandas is a Python package providing fast, flexible, and expressive data structures designed to make working with “relational” or “labeled” data both easy and intuitive.**





SymPy

- **SymPy is a Python library for symbolic mathematics.**
- **It aims to become a full-featured computer algebra system (CAS) while keeping the code as simple as possible in order to be comprehensible and easily extensible.**

SymPy:

```
exp (x)/(1+exp (2*x))
```

$$\frac{e^x}{e^{2x}+1}$$

SymPy:

```
23*pi +factorial (20)/(3**5)-2
```

$$23\pi + 100119424204799 98 \approx 1.00119424204801 \cdot 10^{16}$$

IPYTHON环境

IPython环境

- **启动IPython控制台**

```
(base) iMacS2:~ huangshujian$ ipython
Python 3.7.4 (default, Aug 13 2019, 15:17:50)
Type 'copyright', 'credits' or 'license' for more information
IPython 7.8.0 -- An enhanced Interactive Python. Type '?' for
help.

In [1]:
```

主要特点

- **输入输出缓存 In Out**
- **增强交互辅助功能**
  - 语法高亮、自动补全
- **系统命令交互！**
- **Magic functions %**
- **调试器、并行计算扩展等**

带编号的输入输出

- **用于记录和输出**

```
In [1]: 3 * 3
Out[1]: 9

In [2]: In[1]
Out[2]: '3 * 3'

In [3]: print('Hello World')
Hello World

In [4]: x = 5
```

带编号的输入输出

- **所有历史输入被组织为一个列表 In**
- **所有历史输出被组织为一个字典 Out**

```
In [5]: In
Out[5]: ['', '3 * 3', 'In[1]', "print('Hello World')", 'x = 5', 'In']


In [6]: Out
Out[6]:
{1: 9,
 2: '3 * 3',
 5: ['', '3 * 3', 'In[1]', "print('Hello World')", 'x = 5', 'In',
'Out']}
```

增强交互辅助功能

- **定义复合语句时，自动提示输入后续内容**
- **语法高亮，自动补全等**

```
In [8]: def print_func(x):
   ...:     x = x + 5
   ...:     print(x)
   ...:

In [9]: print_func(100)
105
```

获取帮助

- **快速了解主要功能和查阅文档**

command	description
?	Introduction and overview of IPython's features.
%quickref	Quick reference.
help	Python's own help system.
object?	Details about 'object', use 'object??' for extra details.

- **查看对象的文档注释**

```
In [13]: list?
Init signature: list(iterable=(), /)
Docstring:
Built-in mutable sequence.


If no argument is given, the constructor creates a new empty list.
The argument must be an iterable if specified.
Type:           type
Subclasses:     _HashedSeq, StackSummary, SList, _ImmutableLineList,
FormattedText, NodeList, _ExplodedList, Stack, _Accumulator
```

与系统shell交互

- **！开头的命令将被解析为调用系统shell**

```
In [24]: !pwd
/Users/huangshujian

In [26]: !ls
Applications   My Cloud              gensim-data
Desktop        Overall               nltk_data
Documents      PaperWithCitations    opt
```

与系统shell交互

- **将系统命令结果赋值给python变量**

```
In [28]: file = !ls

In [29]: file
Out[29]:
['Applications',
 'Desktop',
 'Documents',
 'Downloads',
 'Library',
……
```

- **使用python变量执行系统命令**

```
In [30]: filename = "Working"

In [36]: !ls
$filename

Icon? mactex-20200407.pkg screen
erhan10a.pdf python 名单.txt
```

Magic functions

- **一系列%开头的辅助命令，用于控制IPython环境和系统行为等**
  - %开头为单行命令（line magic）
  - %%开头为多行命令（cell magic）

- **The magic function system provides a series of functions which allow you to control the behavior of IPython itself, plus a lot of system-type features.**

使用%magic 查看magic function的相关说明

Magic functions

- **一系列%开头的辅助命令，用于控制IPython环境和系统行为等**
  - %开头为单行命令（line magic）
  - %%开头为多行命令（cell magic）
- **关于代码控制:**
  - %run, %edit, %save, %macro, %recall, etc.
- **关于文件系统：**
  - %ls, %pwd, %cd, %cp, %less, %writefile
- **关于缓存：**
  - %load, %paste
- **……**

- **通过？和？？查看不同详细程度的文档资料**

```
In [17]: %lsmagic?
Docstring: List currently available magic functions.
File:      ~/opt/anaconda3/lib/python3.7/site-
packages/IPython/core/magics/basic.py

In [18]: %lsmagic??
Source:
    @line_magic
    def lsmagic(self, parameter_s=''):
        """List currently available magic functions."""
        return MagicsDisplay(self.shell.magics_manager, ignore=[])
File:   ~/opt/anaconda3/lib/python3.7/site-
packages/IPython/core/magics/basic.py
```

```
In [16]: %lsmagic
Out[16]:
Available line magics:
%alias  %alias_magic  %autoawait  %autocall  %autoindent  %automagic  %boo
kmark  %cat  %cd  %clear  %colors  %conda  %config  %cp  %cpaste  %debug
%dhist  %dirs  %doctest_mode  %ed  %edit  %env  %gui  %hist  %history  %ki
llbgscripts  %ldir  %less  %lf  %lk  %ll  %load  %load_ext  %loadpy  %logo
ff  %logon  %logstart  %logstate  %logstop  %ls  %lsmagic  %lx  %macro  %m
agic  %man  %matplotlib  %mkdir  %more  %mv  %notebook  %page  %paste  %pa
stebin  %pdb  %pdef  %pdoc  %pfile  %pinfo  %pinfo2  %pip  %popd  %pprint
%precision  %prun  %psearch  %psource  %pushd  %pwd  %pycat  %pylab  %quic
kref  %recall  %rehashx  %reload_ext  %rep  %rerun  %reset  %reset_selecti
ve  %rm  %rmdir  %run  %save  %sc  %set_env  %store  %sx  %system  %tb  %t
ime  %timeit  %unalias  %unload_ext  %who  %who_ls  %whos  %xdel  %xmode

Available cell magics:
%%!  %%HTML  %%SVG  %%bash  %%capture  %%debug  %%file  %%html  %%javascri
pt  %%js  %%latex  %%markdown  %%perl  %%prun  %%pypy  %%python  %%python2
  %%python3  %%ruby  %%script  %%sh  %%svg  %%sx  %%system  %%time  %%time
it  %%writefile
```

```
In [39]: %automagic
Automagic is ON, % prefix IS NOT needed for line magics.

In [40]: pwd
Out[40]: '/Users/huangshujian'

In [41]: cd
/Users/huangshujian

In [42]: cd Working/python
/Users/huangshujian/Working/python
```

使用%automagic可以省略开头的%

```
In [43]: %%writefile fib.py
    ...: def fib(N):
    ...:     """
    ...:     Return a list of the first N Fibonacci numbers.
    ...:     """
    ...:     f0, f1 = 0, 1
    ...:     f = [1] * N
    ...:     for n in range(1, N):
    ...:         f[n] = f0 + f1
    ...:         f0, f1 = f1, f[n]
    ...:
    ...:     return f
    ...:
    ...: print(fib(10))
    ...:
    ...:

Writing fib.py
```

```
In [44]: !python fib.py
[1, 1, 2, 3, 5, 8, 13, 21, 34, 55]

In [45]: run fib.py
[1, 1, 2, 3, 5, 8, 13, 21, 34, 55]

In [46]: fib(6)
Out[46]: [1, 1, 2, 3, 5, 8]
```

可以通过系统命令执行

可以通过magic执行

magic执行过后，相当于导入了该脚本，脚本中的变量名可以在后续代码中使用

代码性能分析

- **%timeit**
  - 多次运行给定语句，并给出平均运行时间
- **%time和%%time**
  - 对给定的line或cell进行运行计时
- **%prun**
  - 分析运行过程中不同部分的执行频率和时间
  - 利用profiler进行性能分析

更多性能分析内容参见：https://docs.python.org/3/library/profile.html

```
In [47]: %timeit fib(100)
9.71 µs ± 15.4 ns per loop (mean ± std. dev. of 7 runs, 100000
loops each)

In [48]: %time fib(100)
CPU times: user 14 µs, sys: 0 ns, total: 14 µs
Wall time: 14.8 µs
Out[48]:
[1,
 1,
 2,
 3,
 5,
 8,
```

```
def improve(update, close, guess = 1):
    while not close(guess):
        guess = update(guess)
        print(guess)
    return guess
def appr_equal(x, y, epsilon = 1e-10):
    return abs(x - y) < epsilon
```

```
def improve(update, close, guess = 1):
    while not close(guess):
        guess = update(guess)
        print(guess)
    return guess
```

```
def my_sqrt(x):
    def sqrt_update(guess):
        mid = average(guess)
        if mid * mid > x :
            return guess[0], mid
        else :
            return mid, guess[1]
    def average(tup):
        return (tup[0] + tup[1]) / 2
    def sqrt_accurate(guess):
        mid = average(guess)
        return appr_equal(mid * mid, x)
    return average(improve(sqrt_update, sqrt_accurate, (0, x)))
```

%prun print(my_sqrt(2))

```
     214 function calls in 0.000 seconds

Ordered by: internal time

ncalls  tottime  percall  cumtime  percall filename:lineno(function)
    30    0.000    0.000    0.000    0.000 {built-in method builtins.print}
    30    0.000    0.000    0.000    0.000 <ipython-input-54-9121da0881e4>:10(sqrt_accurate)
     1    0.000    0.000    0.000    0.000 {built-in method builtins.exec}
     1    0.000    0.000    0.000    0.000 <ipython-input-53-56a84c2e6d1e>:1(improve)
    29    0.000    0.000    0.000    0.000 <ipython-input-54-9121da0881e4>:2(sqrt_update)
    30    0.000    0.000    0.000    0.000 <ipython-input-53-56a84c2e6d1e>:6(appr_equal)
    60    0.000    0.000    0.000    0.000 <ipython-input-54-9121da0881e4>:8(average)
    30    0.000    0.000    0.000    0.000 {built-in method builtins.abs}
     1    0.000    0.000    0.000    0.000 <ipython-input-54-9121da0881e4>:1(my_sqrt)
     1    0.000    0.000    0.000    0.000 {method 'disable' of '_lsprof.Profiler' objects}
     1    0.000    0.000    0.000    0.000 <string>:1(<module>)
```

%debug my_sqrt(2)

Jupyter Notebook

- **基于Client-Server模式的交互式运行环境**
  - 以cell的形式组织和运行代码
  - 将控制台运行结果通过网页进行更好的呈现

  - 方便编辑修改代码并查看运行结果
  - 支持markdown、latex等编辑功能
  - 可以显示图片等多媒体资源

  - 支持代码和运行结果保存和导出
    - html、pdf等

https://jupyter-notebook.readthedocs.io/en/latest/notebook.html#introduction

jupyter testNotebook Last Checkpoint: 3 hours ago (autosaved)

注销

文件 编辑 查看 插入 单元格 服务 Widgets 帮助 Trusted Python 3

Run Code

```
In [1]: print('Hello World')

        Hello World

In [2]: 2 * 3.14

Out[2]: 6.28

In [3]: x = 5

In [4]: x

Out[4]: 5

In [5]: In

Out[5]: ['', "print('Hello World')", '2 * 3.14', 'x = 5', 'x', 'In']

In [6]: Out

Out[6]: {2: 6.28,
         4: 5,
         5: ['', "print('Hello World')", '2 * 3.14', 'x = 5', 'x', 'In', 'Out']}
```

基础运行环境配置

利用conda系统管理运行环境

- **本部分内容需要安装的包: ipython, notebook**
- **后续部分根据进程依次需要安装: numpy, scipy, matplotlib等**

- **如果完全安装anaconda，上述基础包应该已经安装在环境中**
- **如果安装的是miniconda等原因，无上述包，可以利用conda方便的进行环境配置**
  - conda upate conda
  - conda create --name scipy-basic
  - conda activate scipy-basic
  - conda install PACKAGENAME

https://docs.conda.io/projects/conda/en/latest/user-guide/cheatsheet.html

```
(base) MBP2SJ:~ huangshujian$ conda update conda
```

更新conda环境

```
## Package Plan ##

  environment location: /Users/huangshujian/miniforge3

  added / updated specs:
    - conda

The following packages will be downloaded:
    package                    |            build
    ---------------------------|-----------------
    conda-package-handling-1.7.3|   py39h5161555_0         1.5 MB  conda-forge
    cryptography-3.4.7         |   py39h73257c9_0         792 KB  conda-forge
...
```

提示下载的package

```
The following packages will be UPDATED:
  conda-package-han~                 1.7.2-py39h51e6412_0 --> 1.7.3-py39h5161555_0
  cryptography                       3.4.4-py39h6e07874_0 --> 3.4.7-py39h73257c9_0
...
```

提示更新的package

```
Proceed ([y]/n)?
```

提示进行

此处显示当前正在使用的环境，默认为base

```
(base) MBP2SJ:~ huangshujian$ conda env list

# conda environments:
#
base                  *  /Users/huangshujian/miniforge3
```

查看系统中所有环境

```
(base) MBP2SJ:~ huangshujian$ conda create --name scipy-basic
Collecting package metadata (current_repodata.json): done
Solving environment: done

## Package Plan ##

  environment location: /Users/huangshujian/miniforge3/envs/scipy-basic

Proceed ([y]/n)?

Preparing transaction: done
Verifying transaction: done
Executing transaction: done
#
# To activate this environment, use
#
#     $ conda activate scipy-basic
#
# To deactivate an active environment, use
#
#     $ conda deactivate
```

创建一个新环境 scipy-basic

```
(base) MBP2SJ:~ huangshujian$ conda activate scipy-basic
```

切换至环境scipy-basic

```
(scipy-basic) MBP2SJ:~ huangshujian$ conda list
# packages in environment at /Users/huangshujian/miniforge3/envs/scipy-basic:
#
# Name                    Version                   Build  Channel
```

查看当前环境中的包列表

此处显示当前正在使用的环境，已切换至scipy-basic

```
(scipy-basic) MBP2SJ:~ huangshujian$ conda install ipython
...

(scipy-basic) MBP2SJ:~ huangshujian$ ipython
...
```

安装ipython包

启动ipython交互环境

```
(scipy-basic) MBP2SJ:~ huangshujian$ conda install notebook
...

(scipy-basic) MBP2SJ:~ huangshujian$ jupyter notebook
...
```

安装notebook包

启动jupyter notebook

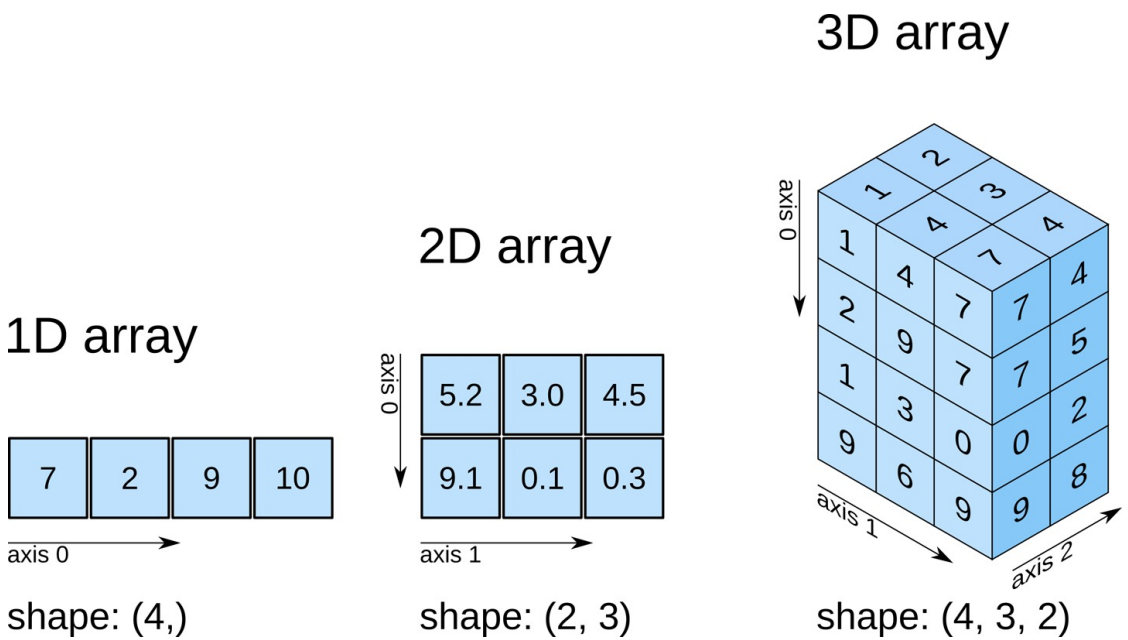
回顾

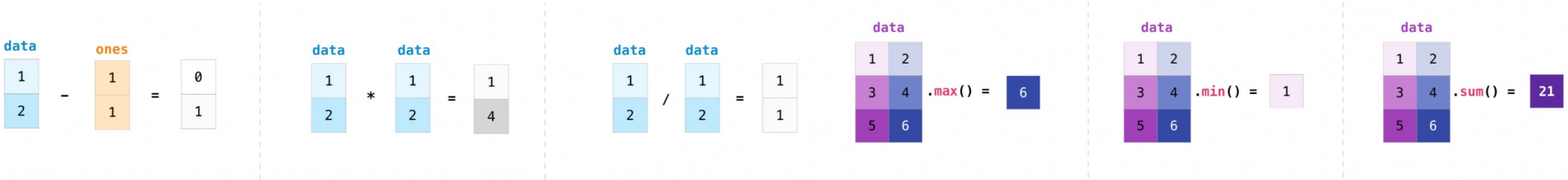
- **Python科学计算环境**
  - IPython环境、NumPy、SciPy、matplotlib、SymPy、Pandas
- **IPython环境使用**
  - magic functions
  - 代码性能分析
  - jupyter notebook

- **部分内容参考：《Python科学计算和数据科学应用》**

NUMPY

multi-dimensional array





https://numpy.org/doc/stable/user/absolute_beginners.html