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Python与机器学习

——Python库的使用

华算科技 黄老师 2022年2月22日



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- 1. Python库介绍
- 2. NumPy库
- 3. pandas库
- 4. 案例: 谱数据平滑
- 5. matplotlib库与数据可视化

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库是完成一定功能的代码的集合















pymatgen



库的优势

提高开发效率

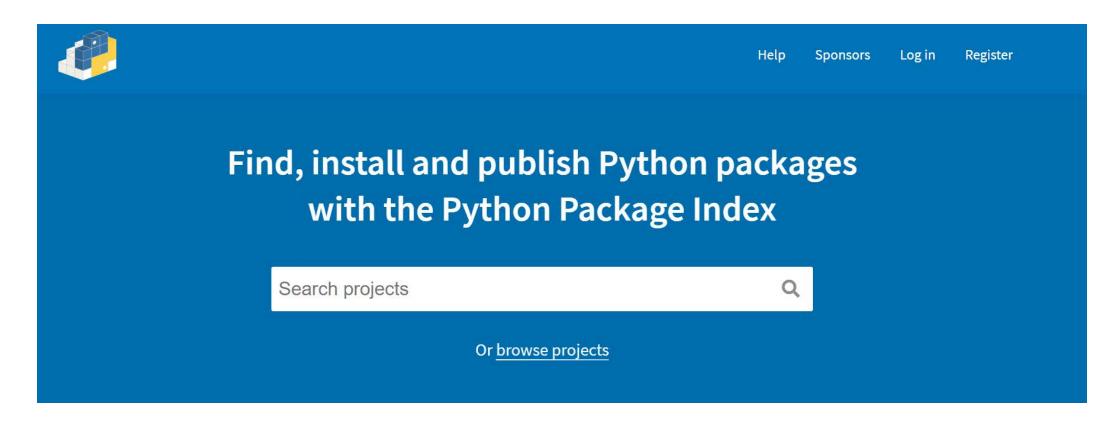
例如: 前面的求list平均

[2. 27e-12, 2. 24e-12, 2. 3e-12, 2. 25e-12, 2. 22e-12, 2. 25e-12, 2. 24e-12] 2. 252857142857143e-12 2. 547142857142857e-12

库的安装

pip install xxx命令

Python库官方索引网站: PyPI(Python Package Index) https://pypi.org



镜像源

清华: https://pypi.tuna.tsinghua.edu.cn/simple

阿里云: http://mirrors.aliyun.com/pypi/simple

中国科技大学 https://pypi.mirrors.ustc.edu.cn/simple

豆瓣: http://pypi.douban.com/simple

0-0 0-0-1 0-0-5 0-core-client 0-orchestrator 00000a 007 007-no-time-to-die-2021-watch-full-online-free 00print-lol 00smalinux 01-distributions 0121 01changer 01d61084-d29e-11e9-96d1-7c5cf84ffe8e 021 024travis-test024 02exercicio 0805nexter 090807040506030201testpip 0c429e768e524e4f61297d472c0ab06c 0fela 0html 0imap Olever-so Olever-utils **Oproto** <u>Orest</u> Orss

<u>0wdg9nbmpm</u>

<u>0x-contract-artifacts</u>

库的导入

1. import 语句

使用方法: import A (导入A模块,例如导入numpy模块,import numpy)

可添加别名,例如 import numpy as np,程序中则可使用np代表numpy

2. from ... import ... 语句

使用方法: from A import a1 (在内存中创建并加载A模块中a1工具的副本,例如导入 numpy模块中的zeros函数, from numpy import zeros)

与import A.a1的区别,前者可直接调用,后者只能使用全名

查看帮助文件

help 语句

使用方法: help(A) (查看A模块下的所有函数, help(numpy))

help(A.a1) (查看A模块中的a函数, help(numpy.zero))

```
In [5]: help(numpy.zeros)
In [4]: help(numpy)
                                                                                                   Help on built-in function zeros in module numpy:
         Help on package numpy:
                                                                                                    zeros(...)
         NAME
                                                                                                        zeros(shape, dtype=float, order='C', *, like=None)
             numpy
         DESCRIPTION
                                                                                                        Return a new array of given shape and type, filled with zeros.
             NumPv
             =====
                                                                                                        Parameters
             Provides
                                                                                                        shape : int or tuple of ints
                                                                                                            Shape of the new array, e.g., ``(2, 3)`` or ``2``.
               1. An array object of arbitrary homogeneous items
               2. Fast mathematical operations over arrays
                                                                                                        dtype : data-type, optional
               3. Linear Algebra, Fourier Transforms, Random Number Generation
                                                                                                            The desired data-type for the array, e.g., `numpy.int8`. Default is
                                                                                                             numpy.float64.
             How to use the documentation
                                                                                                        order: {'C', 'F'}, optional, default: 'C'
                                                                                                            Whether to store multi-dimensional data in row-major
             Documentation is available in two forms: docstrings provided
                                                                                                            (C-style) or column-major (Fortran-style) order in
             with the code, and a loose standing reference guide, available from
              `the NumPy homepage <a href="https://www.scipy.org">https://www.scipy.org</a>.
                                                                                                        like : array_like
                                                                                                            Reference object to allow the creation of arrays which are not
              We recommend exploring the docstrings using
                                                                                                            NumPy arrays. If an array-like passed in as `like` supports
              `IPython <a href="https://ipython.org">https://ipython.org</a>, an advanced Python shell with
                                                                                                            the ``__array_function__` protocol, the result will be defined
             TAB-completion and introspection capabilities. See below for further
                                                                                                            by it. In this case, it ensures the creation of an array object
             instructions.
                                                                                                            compatible with that passed in via this argument.
             The docstring examples assume that `numpy` has been imported as `np`::
                                                                                                            .. versionadded:: 1.20.0
               >>> import numpy as np
```

科学计算库

NumPy, SciPy, matplotlib的组合, 广泛用于替代MATLAB

最优化、线性代数等科学计算

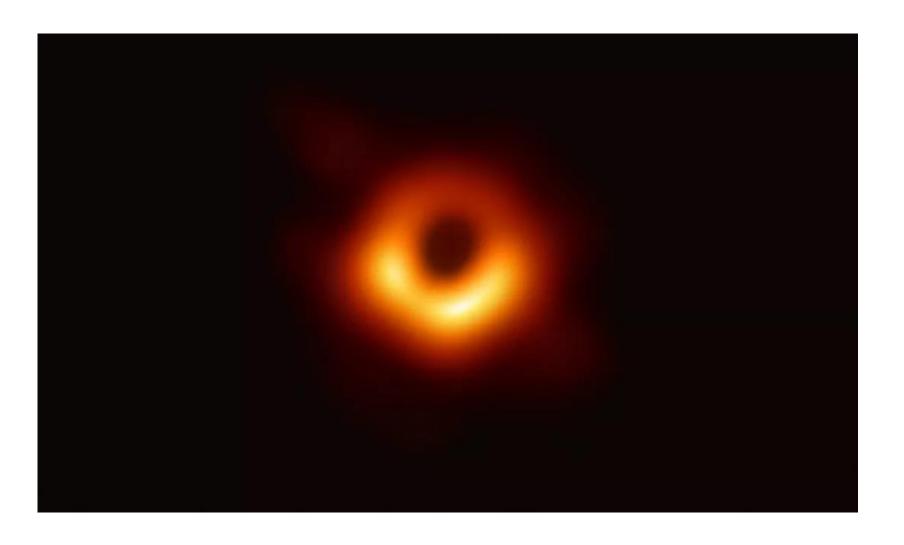






2019年,人类首次拍到了黑洞的照片

https://github.com/achael/eht-imaging



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NumPy库的使用

NumPy中封装有array(数组),其结构与Python中自带的list相似,但在科学计算中更为方便与强大。

```
list = [3.3, 2.2, 2.5, 3.1, 3.0, 'eV']
```

a = np.array([3.3, 2.2, 2.5, 3.1, 3.0]) array中存放的数据类型相同

```
In [1]: import numpy as np
In [2]: a = np.array([1, 2, 3, 4, 5, 6])
b = np.array([[1, 2, 3], [4, 5, 6]])
c = np.zeros(5)
```

```
[1 2 3 4 5 6]
[[1 2 3]
[4 5 6]]
[0. 0. 0. 0. 0.]
```

print(a)
print(b)
print(c)

NumPy库的使用

数组属性

```
print (a. ndim)
[3]:
      print (a. shape)
      print(b.ndim)
      print (b. shape)
      print (b. size)
      print(b.dtype)
       (6,)
       (2, 3)
       int32
```

ndim:数组维度

shape: n行m列

size: 总元素个数

dtype:数据类型

NumPy库的使用

维度与形状调整

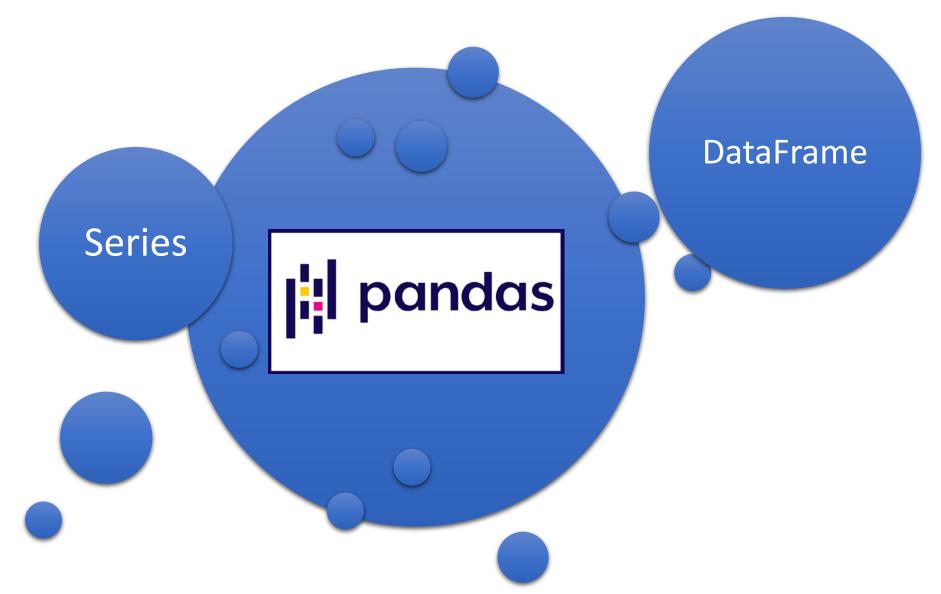
```
b. reshape (3, 2)
In [4]:
           print (b. shape)
           b = b. reshape (3, 2)
           print (b. shape)
           b = b. reshape (-1, 1)
           print(b)
           (2, 3)
            [2]
            [3]
             [4]
            [5]
             [6]]
```

```
In [5]: | c = np. zeros (24)
          print(c.ndim)
          c = c. reshape(2, 4, 3)
          print(c.ndim)
          print(c)
          [[[0. 0. 0.]
            [0. 0. 0.]
            [0. 0. 0.]
            [0. 0. 0.]]
           [[0. 0. 0.]
            [0. 0. 0.]
            [0. 0. 0.]
            [0. 0. 0.]]]
```

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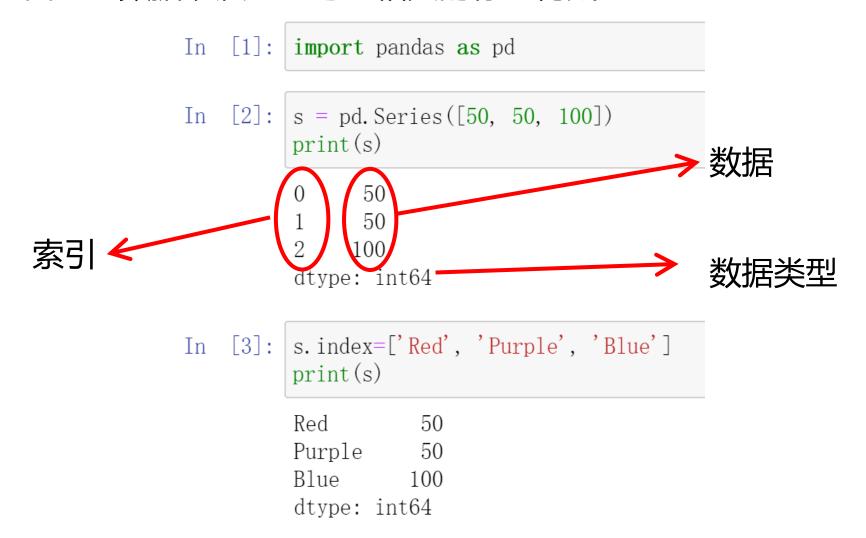
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pandas数据结构



Series

Series: 由一组数据以及一组与之相关的标签构成



DataFrame

DataFrame: 由若干个共用一个索引的Series组成

```
In [34]: data = [['Red', 50, 60], ['Purple', 60, 50], ['Blue', 100, 100]]
   df = pd. DataFrame(data, columns = ['name', 'score1', 'score2'])
   df
```

Out[34]:

	name	score1	score2
0	Red	50	60
1	Purple	60	50
2	Blue	100	100

pandas读取csv

read_csv()函数 把csv文件读入DataFrame中

```
[9]:
              df = pd. read_csv('didz.csv', header = None)
              df
Out [9]:
                                                               3
                       0
                         2.270000e-12 2.240000e-12 2.300000e-12 2.250000e-12 2.220000e-12 2.250000e-12 2.240000e-12
                          2.810000e-12
                                       1.840000e-12 2.990000e-12 2.580000e-12 2.310000e-12
                                                                                           2.800000e-12
                                                                                                         2.500000e-12
          2 3.000000e-10 2.270000e-12 2.240000e-12 2.300000e-12 2.250000e-12 2.220000e-12 2.250000e-12
                                                                                                         2.240000e-12
                          2.810000e-12 1.840000e-12 2.990000e-12 2.580000e-12 2.310000e-12
             2.900000e-10
                                                                                           2.800000e-12
                                                                                                         2.500000e-12
```

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实操: 谱图平滑

```
[1]:
In
           1 import pandas as pd
In [2]:
           1 | df = pd. read_csv('UV_noise.csv', header = None)
           2 df
Out[2]:
                   0
             0 200.0 0.128823
             1 200.2 0.117582
             2 200.4 0.125130
             3 200.6 0.121738
             4 200.8 0.104534
          1096 419.2 0.022818
          1097 419.4 0.025858
          1098 419.6 0.029388
          1099 419.8 0.021187
          1100 420.0 0.028926
```

1101 rows × 2 columns

实操: 谱图平滑

```
In [4]:
                import numpy as np
             3 \text{ wl} = \text{np.array}(\text{df}[0])
             4 Abs = np. array(df[1])
In [5]:
                import matplotlib.pyplot as plt
                plt.plot(wl, Abs)
                plt.show()
            0.6
            0.5
            0.4
            0.3
            0.2
            0.1
            0.0
                            250
                                        300
                 200
                                                    350
                                                               400
```

实操: 谱图平滑

Savitzky-Golay平滑法

```
[6]:
            1 from scipy.signal import savgol_filter
            2 Abs_smooth = savgol_filter(Abs, 9, 2)
In
    [9]:
           1 plt.plot(wl, Abs)
              plt.plot(wl, Abs_smooth)
              plt.show()
          0.6
          0.5
          0.4
          0.3
          0.2
          0.1
          0.0
                                   300
               200
                         250
                                             350
                                                       400
```

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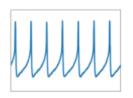


matplotlib库

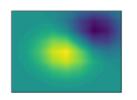
https://matplotlib.org

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.

Create

- Develop publication quality plots with just a few lines of code
- Use interactive figures that can zoom, pan, update...

Customize

- Take full control of line styles, font properties, axes properties...
- Export and embed to a number of file formats and interactive environments

Extend

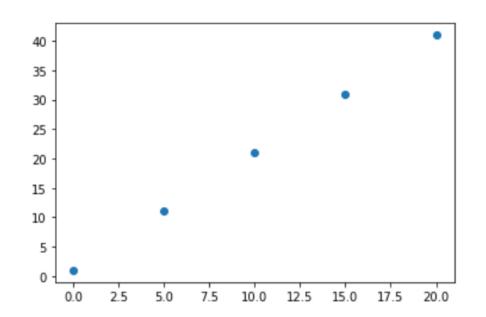
- Explore tailored functionality provided by third party packages
- Learn more about Matplotlib through the many external learning resources

实操: 散点图的绘制

```
In [1]: import numpy as np
import matplotlib.pyplot as plt

In [2]: x = np.linspace(0, 20, 5)
y = 2 * x + 1
In [3]: plt.scatter(x, y)
```

Out[3]: <matplotlib.collections.PathCollection at 0x248c8f8f550>



linspace() 在指定的间隔内返回均匀间隔的数字

$$x = [0, 5, 10, 15, 20]$$

$$y = [1, 11, 21, 31, 41]$$

图像点调整

20

15

10

2.5

5.0

7.5

调整点的大小

s = 200

调整点的形状

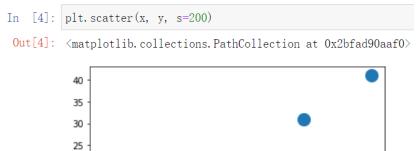
marker=','

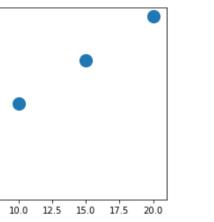
marker='v'

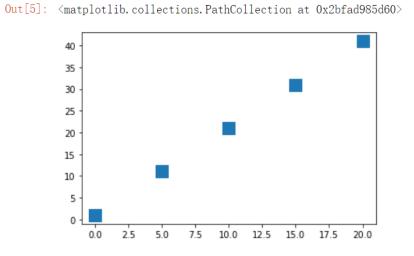
In [5]: plt.scatter(x, y, s=200, marker=',')

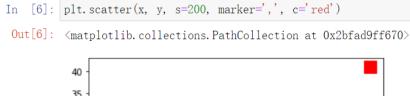
调整点的颜色

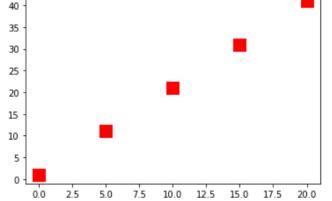
c='red'











常用颜色

color = 或c =	颜色	样例
None	靛青色	
'b'或'blue'	蓝色	
'g'或'green'	绿色	
'r'或'red'	红色	
'c'	青色(cyan)	
'm'	品红色(magenta)	
'y'	黄色(yellow)	
'k'或'black'	黑色	
'w'或'white'	白色	

坐标调整

调整坐标轴大小 plt.xlim((0, 30))

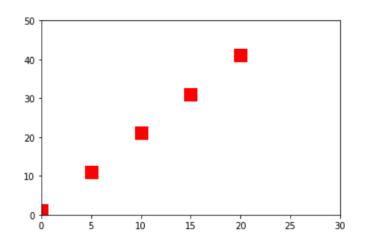
调整坐标轴刻度 plt.xticks()

调整坐标轴标签 plt.xlabel()

```
In [7]: plt.xlim((0, 30))
    plt.ylim((0, 50))

plt.scatter(x, y, s=200, marker=',', c='red')
```

Out[7]: <matplotlib.collections.PathCollection at 0x269cc785cd0>

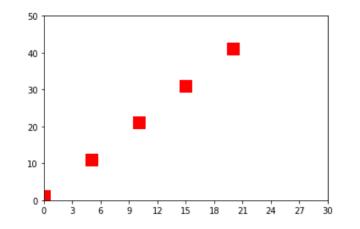


```
In [8]: plt.xlim((0, 30))
plt.ylim((0, 50))

x_ticks = np.linspace(0, 30, 11)
plt.xticks(x_ticks)

plt.scatter(x, y, s=200, marker=',', c='red')
```

Out[8]: \langle matplotlib.collections.PathCollection at 0x269cc7eb4f0>



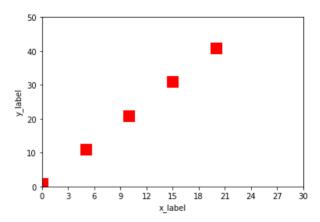
```
In [9]: plt.xlim((0, 30))
    plt.ylim((0, 50))

    x_ticks = np.linspace(0, 30, 11)
    plt.xticks(x_ticks)

    plt.xlabel('x_label')
    plt.ylabel('y_label')

plt.scatter(x, y, s=200, marker=',', c='red')
```

Out[9]: <matplotlib.collections.PathCollection at 0x269cc86ff40>



实操: 简单函数绘图

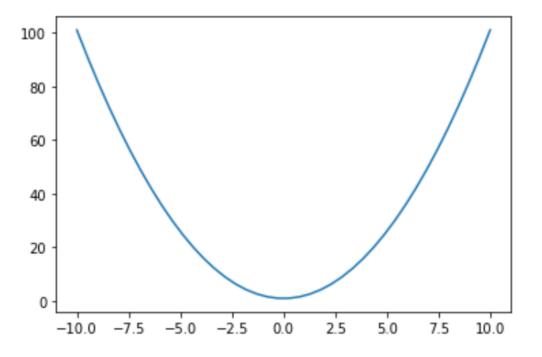
$$y = x^2 + 1$$

```
In [10]: x = \text{np.linspace}(-10, 10, 40)

y = x * x + 1

plt. plot(x, y)
```

Out[10]: [<matplotlib.lines.Line2D at 0x264d5962460>]



同一个图绘制多个函数

```
In [11]: x = np. linspace(-10, 10, 40)

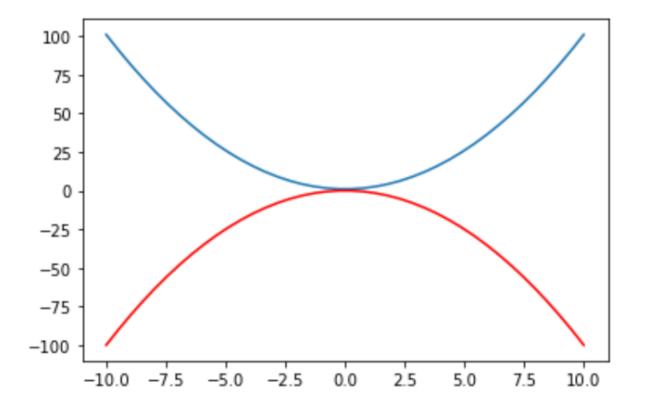
y = x * x + 1

y0 = -x * x

plt. plot(x, y)

plt. plot(x, y0, c='red')
```

Out[11]: [<matplotlib.lines.Line2D at 0x14b9dbf9130>]

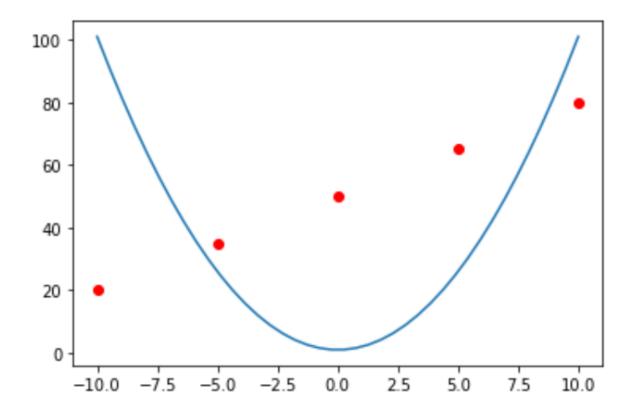


同时绘制散点与线

```
In [12]: x2 = np.linspace(-10, 10, 5)
y2 = 3 * x2 + 50

plt.scatter(x2, y2, c='red')
plt.plot(x, y)
```

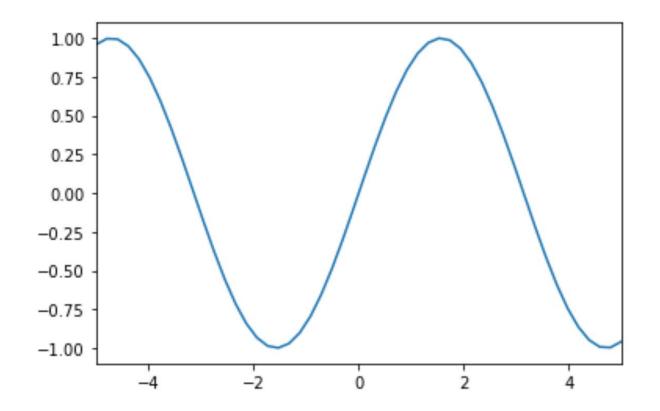
Out[12]: [<matplotlib.lines.Line2D at 0x14b9dc63d30>]



练习: 绘制正弦函数图像

绘制x在(-5,5)范围内正弦函数 y = sin(x) 的图像

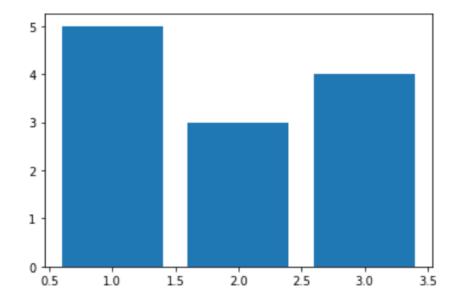
提示: sin函数调用方法为np.sin()



柱状图

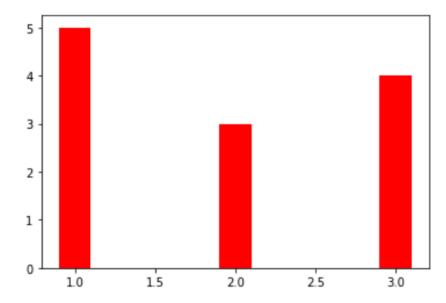
In [5]: x = [1, 2, 3] y = [5, 3, 4]plt. bar (x, y)

Out[5]: <BarContainer object of 3 artists>



In [6]: plt.bar(x, y, width = 0.2, color = 'r')

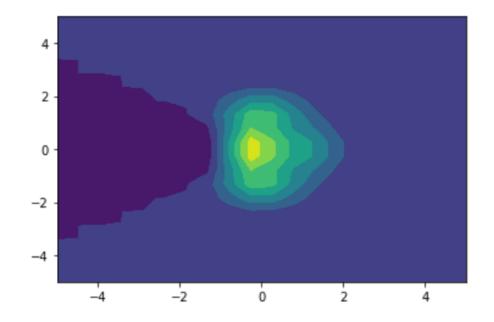
Out[6]: <BarContainer object of 3 artists>



阅读材料: 二维图

```
In [7]: x = np. linspace(-5, 5, 20)
y = np. linspace(-5, 5, 20)
X, Y = np. meshgrid(x, y)
Z = (1-X/2 + X**3 + Y**4)*np. exp(-X**2-Y**2)
plt. contourf(X, Y, Z)
```

Out[7]: <matplotlib.contour.QuadContourSet at 0x28fd484bd00>



```
In [8]: x = np. linspace (-5, 5, 20)
y = np. linspace (-5, 5, 20)
X, Y = np. meshgrid(x, y)
Z = (1-X/2 + X**3 + Y**4)*np. exp(-X**2-Y**2)
plt. pcolormesh(X, Y, Z)

C:\Users\26093\AppData\Local\Temp/ipykernel_30172/2048871572.py:5: Matimensions as C is deprecated since 3.3. Either specify the corners of 'gouraud', or set rcParams['pcolor.shading']. This will become an err plt. pcolormesh(X, Y, Z)
```

Out[8]: <matplotlib.collections.QuadMesh at 0x28fd47fbb20>

