Numpy

Numpy是Python中用于科学计算的核心库。它提供了高性能的多维数组对象，以及相关工具。

数组Arrays

一个numpy数组是一个由不同数值组成的网格。网格中的数据都是同一种数据类型，可以通过非负整型数的元组来访问。维度的数量被称为数组的阶，数组的大小是一个由整型数构成的元组，可以描述数组不同维度上的大小。

我们可以从列表创建数组，然后利用**方括号**访问其中的元素：

```
import numpy as np

a = np.array([1, 2, 3])   # Create a rank 1 array
print(type(a))            # Prints "<type 'numpy.ndarray'>"
print(a.shape)            # Prints "(3,)"
print(a[0], a[1], a[2])   # Prints "1 2 3"
a[0] = 5                  # Change an element of the array
print(a)                  # Prints "[5, 2, 3]"

b = np.array([[1,2,3],[4,5,6]])    # Create a rank 2 array
print(b)                           # 显示一下矩阵b
print(b.shape)                     # Prints "(2, 3)"
print(b[0, 0], b[0, 1], b[1, 0])   # Prints "1 2 4"
```

Numpy还提供了很多其他创建数组的方法：

```
import numpy as np

a = np.zeros((2,2))   # Create an array of all zeros
print(a)              # Prints "[[ 0.  0.]
                      #          [ 0.  0.]]"

b = np.ones((1,2))    # Create an array of all ones
print(b)              # Prints "[[ 1.  1.]]"

c = np.full((2,2), 7)  # Create a constant array
print(c)               # Prints "[[ 7.  7.]
                       #          [ 7.  7.]]"

d = np.eye(2)         # Create a 2x2 identity matrix
print(d)              # Prints "[[ 1.  0.]
                      #          [ 0.  1.]]"

e = np.random.random((2,2))  # Create an array filled with random values
print(e)                     # Might print "[[ 0.91940167  0.08143941]
                             #               [ 0.68744134  0.87236687]]"
```

访问数组

Numpy提供了多种访问数组的方法。

切片

和Python列表类似，numpy数组可以使用切片语法。因为数组可以是多维的，所以你必须为每个维度指定好切片。

```
import numpy as np

# Create the following rank 2 array with shape (3, 4)
# [[ 1  2  3  4]
#  [ 5  6  7  8]
#  [ 9 10 11 12]]
a = np.array([[1,2,3,4], [5,6,7,8], [9,10,11,12]])

# Use slicing to pull out the subarray consisting of the first 2 rows
# and columns 1 and 2; b is the following array of shape (2, 2):
# [[2 3]
#  [6 7]]
b = a[:2, 1:3]

# A slice of an array is a view into the same data, so modifying it
# will modify the original array.
print(a[0, 1])  # Prints "2"
b[0, 0] = 77    # b[0, 0] is the same piece of data as a[0, 1]
print(a[0, 1])  # Prints "77"
```

整型数组访问

当我们使用切片语法访问数组时，得到的总是原数组的一个子集。整型数组访问允许我们利用其它数组的数据构建一个新的数组。

```
import numpy as np

a = np.array([[1,2], [3, 4], [5, 6]])

# An example of integer array indexing.
# The returned array will have shape (3,) and
print(a[[0, 1, 2], [0, 1, 0]])  # Prints "[1 4 5]"

# The above example of integer array indexing is equivalent to this:
print(np.array([a[0, 0], a[1, 1], a[2, 0]]))  # Prints "[1 4 5]"

# When using integer array indexing, you can reuse the same
# element from the source array:
print(a[[0, 0], [1, 1]])  # Prints "[2 2]"

# Equivalent to the previous integer array indexing example
print(np.array([a[0, 1], a[0, 1]]))  # Prints "[2 2]"
```

整型数组访问语法还有个有用的技巧，可以用来选择或者更改矩阵中每行中的一个元素。

```
import numpy as np
```

```
# Create a new array from which we will select elements
a = np.array([[1,2,3], [4,5,6], [7,8,9], [10, 11, 12]])

print(a) # prints "array([[ 1,  2,  3],
         #                [ 4,  5,  6],
         #                [ 7,  8,  9],
         #                [10, 11, 12]])"

# Create an array of indices
b = np.array([0, 2, 0, 1])

# Select one element from each row of a using the indices in b
print(a[np.arange(4), b])  # Prints "[ 1  6  7 11]"

# Mutate one element from each row of a using the indices in b
a[np.arange(4), b] += 10

print(a) # prints "array([[11,  2,  3],
         #                [ 4,  5, 16],
         #                [17,  8,  9],
         #                [10, 21, 12]])
```

布尔型数组访问

布尔型数组访问可以让你选择数组中任意元素。通常，这种访问方式用于选取数组中满足某些条件的元素。

```
import numpy as np

a = np.array([[1,2], [3, 4], [5, 6]])


bool_idx = (a > 2)  # Find the elements of a that are bigger than 2;
                    # this returns a numpy array of Booleans of the same
                    # shape as a, where each slot of bool_idx tells
                    # whether that element of a is > 2.

print(bool_idx)     # Prints "[[False False]
                    #          [ True  True]
                    #          [ True  True]]"

# We use boolean array indexing to construct a rank 1 array
# consisting of the elements of a corresponding to the True values
# of bool_idx
print(a[bool_idx]) # Prints "[3 4 5 6]"

# We can do all of the above in a single concise statement:
print(a[a > 2])    # Prints "[3 4 5 6]"
```

数组类型

每个Numpy数组都是数据类型相同的元素组成的网格。Numpy提供了很多的数据类型用于创建数组。当你创建数组的时候，Numpy会尝试猜测数组的数据类型，你也可以通过参数直接指定数据类型。

```
import numpy as np

x = np.array([1, 2])  # Let numpy choose the datatype
print(x.dtype)        # Prints "int64"

x = np.array([1.0, 2.0])  # Let numpy choose the datatype
print(x.dtype)            # Prints "float64"

x = np.array([1, 2], dtype=np.int64)  # Force a particular datatype
print(x.dtype)                        # Prints "int64"
```

数组计算

基本数学计算函数会对数组中元素逐个进行计算，既可以利用操作符重载，也可以使用函数方式。

```
import numpy as np

x = np.array([[1,2],[3,4]], dtype=np.float64)
y = np.array([[5,6],[7,8]], dtype=np.float64)

# Elementwise sum; both produce the array
# [[ 6.0  8.0]
#  [10.0 12.0]]
print(x + y)
print(np.add(x, y))

# Elementwise difference; both produce the array
# [[-4.0 -4.0]
#  [-4.0 -4.0]]
print(x - y)
print(np.subtract(x, y))

# Elementwise product; both produce the array
# [[ 5.0 12.0]
#  [21.0 32.0]]
print(x * y)
print(np.multiply(x, y))

# Elementwise division; both produce the array
# [[ 0.2         0.33333333]
#  [ 0.42857143  0.5       ]]
print(x / y)
print(np.divide(x, y))

# Elementwise square root; produces the array
# [[ 1.          1.41421356]
#  [ 1.73205081  2.        ]]
print(np.sqrt(x))
```

> 注：这类的*是元素逐个相乘，而不是矩阵乘法。矩阵乘法通过**dot**来实现

```
import numpy as np

x = np.array([[1,2],[3,4]])
y = np.array([[5,6],[7,8]])
```

```
v = np.array([9,10])
w = np.array([11, 12])

# Inner product of vectors; both produce 219
print(v.dot(w))
print(np.dot(v, w))

# Matrix / vector product; both produce the rank 1 array [29 67]
print(x.dot(v))
print(np.dot(x, v))

# Matrix / matrix product; both produce the rank 2 array
# [[19 22]
#  [43 50]]
print(x.dot(y))
print(np.dot(x, y))
```

Numpy提供了很多计算数组的函数，其中最常用的一个是sum。

```
import numpy as np

x = np.array([[1,2],[3,4]])

print(np.sum(x))  # Compute sum of all elements; prints "10"
print(np.sum(x, axis=0))  # Compute sum of each column; prints "[4 6]"
print(np.sum(x, axis=1))  # Compute sum of each row; prints "[3 7]"
```

更多函数

除了计算，我们还常常改变数组或者操作其中的元素。其中将矩阵转置是常用的一个，在Numpy中，使用T来转置矩阵。

```
import numpy as np

x = np.array([[1,2], [3,4]])
print(x)   # Prints "[[1 2]
           #          [3 4]]"
print(x.T) # Prints "[[1 3]
           #          [2 4]]"

# Note that taking the transpose of a rank 1 array does nothing:
v = np.array([1,2,3])
print(v)   # Prints "[1 2 3]"
print(v.T) # Prints "[1 2 3]"
```

其他操作数组的方法

广播Broadcasting

广播是一种强有力的机制，它让Numpy可以让不同大小的矩阵在一起进行数学计算。我们常常会有一个小的矩阵和一个大的矩阵，然后我们会需要用小的矩阵对大的矩阵做一些计算。

举个例子，如果我们想要把一个向量加到矩阵的每一行，我们可以这样做：

```
import numpy as np

# We will add the vector v to each row of the matrix x,
# storing the result in the matrix y
x = np.array([[1,2,3], [4,5,6], [7,8,9], [10, 11, 12]])
v = np.array([1, 0, 1])
y = np.empty_like(x)   # Create an empty matrix with the same shape as x

# Add the vector v to each row of the matrix x with an explicit loop
for i in range(4):
    y[i, :] = x[i, :] + v

# Now y is the following
# [[ 2  2  4]
#  [ 5  5  7]
#  [ 8  8 10]
#  [11 11 13]]
print(y)
```

Numpy广播机制可以让我们不用创建vv，就能直接运算。

```
import numpy as np

# We will add the vector v to each row of the matrix x,
# storing the result in the matrix y
x = np.array([[1,2,3], [4,5,6], [7,8,9], [10, 11, 12]])
v = np.array([1, 0, 1])
y = x + v  # Add v to each row of x using broadcasting
print(y) # Prints "[[ 2  2  4]
         #          [ 5  5  7]
         #          [ 8  8 10]
         #          [11 11 13]]"
```

对两个数组使用广播机制要遵守下列规则：

1. 如果数组的秩不同，使用1来将秩较小的数组进行扩展，直到两个数组的尺寸的长度都一样。
2. 如果两个数组在某个维度上的长度是一样的，或者其中一个数组在该维度上长度为1，那么我们就说这两个数组在该维度上是相容的。
3. 如果两个数组在所有维度上都是相容的，他们就能使用广播。
4. 如果两个输入数组的尺寸不同，那么注意其中较大的那个尺寸。因为广播之后，两个数组的尺寸将和那个较大的尺寸一样。
5. 在任何一个维度上，如果一个数组的长度为1，另一个数组长度大于1，那么在该维度上，就好像是对第一个数组进行了复制。

支持广播机制的函数是全局函数。哪些是全局函数可以在文档中查找。 一些广播机制的使用:

```
import numpy as np

# Compute outer product of vectors
v = np.array([1,2,3])  # v has shape (3,)
w = np.array([4,5])    # w has shape (2,)
# To compute an outer product, we first reshape v to be a column
# vector of shape (3, 1); we can then broadcast it against w to yield
# an output of shape (3, 2), which is the outer product of v and w:
# [[ 4  5]
#  [ 8 10]
#  [12 15]]
print(np.reshape(v, (3, 1)) * w)

# Add a vector to each row of a matrix
x = np.array([[1,2,3], [4,5,6]])
# x has shape (2, 3) and v has shape (3,) so they broadcast to (2, 3),
# giving the following matrix:
# [[2 4 6]

#  [5 7 9]]
print(x + v)

# Add a vector to each column of a matrix
# x has shape (2, 3) and w has shape (2,).
# If we transpose x then it has shape (3, 2) and can be broadcast
# against w to yield a result of shape (3, 2); transposing this result
# yields the final result of shape (2, 3) which is the matrix x with
# the vector w added to each column. Gives the following matrix:
# [[ 5  6  7]
#  [ 9 10 11]]
print((x.T + w).T)

# Another solution is to reshape w to be a row vector of shape (2, 1);
# we can then broadcast it directly against x to produce the same
# output.
print(x + np.reshape(w, (2, 1)))

# Multiply a matrix by a constant:
# x has shape (2, 3). Numpy treats scalars as arrays of shape ();
# these can be broadcast together to shape (2, 3), producing the
# following array:
# [[ 2  4  6]
#  [ 8 10 12]]
print(x * 2)
```