Section 9: Introduction to `NumPy` and `SciPy`

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Motivation

We have learned all basic data structures...do we need more?

A question

You have an matrix like this:

$$\begin{bmatrix} 1 & 2 & 3 & 4 \\ 4 & 5 & 6 & 7 \\ 7 & 8 & 9 & 10 \end{bmatrix}$$

and you want to sum up numbers by each column. How do you write code for it?

In Python

a solution using native `list`

```
sums = []
for col_idx in range(len(matrix[0])):
    sum = 0
    for row_idx in range(len(matrix)):
        sum += matrix[row_idx][col_idx]
    sums.append(sum)
print sums
```

In Python

a solution if using numpy arrays

```
print matrix.sum(axis=1)
```

Another comparison

Sum benchmark: summing over a list

```
from numpy import arange
import time

N = 10000000
numpy_array = arange(N)
python_list = range(N)
print "### python list ###"
start = time.time()
sum = 0
for i in python_list:
    sum += i
print "average is: ", float(sum) / N
print "used time: ", time.time() - start
print "### numpy array ###"
start = time.time()
print "average is: ", numpy_array.mean()
print "used time: ", time.time() - start
```

First, `import`

```
import numpy
```

OR

```
import numpy as np
```
(assuming this from now on)

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- You can use the same indexing:
  - `a[:2]`
  - `a[1]`
  - `a[1:]`
- arrays can easily be multidimensional: `a = np.array([[1, 2, 3], [4, 5, 6]], float)`

Arrays shapes

```
a.shape == (3, 4)
```

$$\begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \\ 9 & 10 & 11 & 12 \end{bmatrix}$$

```
a.sum(axis=0)?
a.sum(axis=1)?
```

Arrays shapes

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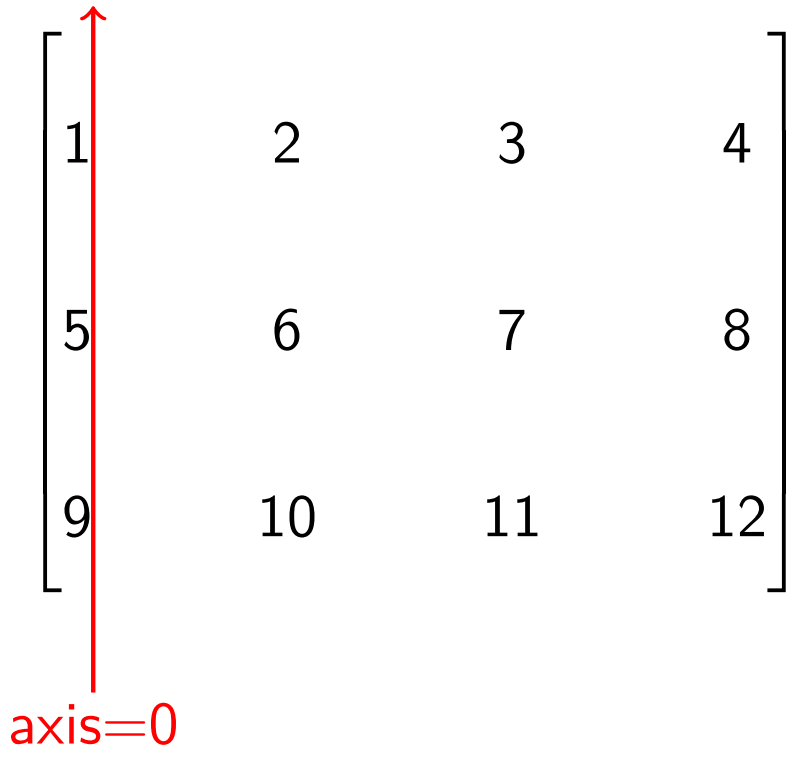


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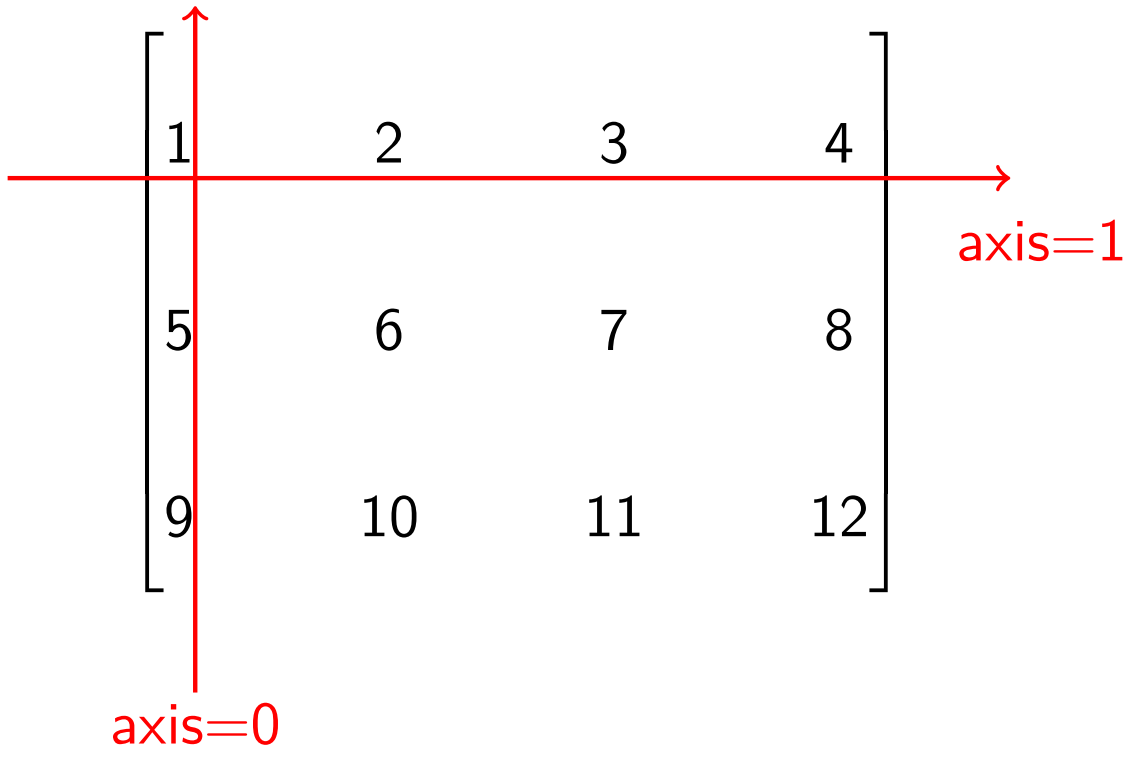


```
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Arrays, `reshape`

```
a = a.reshape((4, 3))
```

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \\ 10 & 11 & 12 \end{bmatrix}$$

Arrays, `reshape`

```
a = a.reshape((-1, 6))
```

$$\begin{bmatrix} 1 & 2 & 3 & 4 & 5 & 6 \\ 7 & 8 & 9 & 10 & 11 & 12 \end{bmatrix}$$

Other ways to create arrays

- `a = np.zeros(5)`

```
[0., 0., 0., 0., 0.]
```

Other ways to create arrays

- `a = np.zeros(5)`

  `[0., 0., 0., 0., 0.]`

- `a = np.arange(0, 10, 2)`

  `[0, 2, 4, 6, 8]`

Other ways to create arrays

- `a = np.zeros(5)`

`[0., 0., 0., 0., 0.]`

- `a = np.arange(0, 10, 2)`

`[0, 2, 4, 6, 8]`

- `a = np.full((2, 2), 2)`

$$\begin{bmatrix} 2 & 2 \\ 2 & 2 \end{bmatrix}$$

Array $\leftrightarrow$ list conversions

list to array

```
lst = [1, 2, 3]
a = np.asarray(lst)
```

array to list

```
a = np.array([1, 2, 3], int)
lst = a.tolist()
```

Useful operations

- `sum, mean`
- `np.var, np.std`
- `max, min, argmax, argmin`
- `zeros_like(), ones_like()`
- `concatenate`

Again, just like `matplotlib`, read the docs!!!

https://docs.scipy.org/doc/numpy/

Try it!

Practice

You are given a matrix with each row as a vector. Find the index of the row which has the smallest L_2 norm.
As a reference, for any vector $\vec{v}$, its L_2 norm is defined as:

$$||\vec{v}||_2 = \sqrt{\sum_{k=1}^{n} v_k^2}$$

example

```
matrix = [[1, 2, 3], [4, 5, 6], [7, 8, 9]]
return 0
```

A solution with just Python

```
import math

def l2_norm(lst):
    sum = 0
    for i in lst:
        sum += i ** 2
    return math.sqrt(sum)

smallest = None
idx = None
for i in range(len(matrix)):
    l2 = l2_norm(matrix[i])
    if smallest is None or l2 < smallest:
        idx = i
        smallest = l2
print "index: ", i
```

A solution with NumPy

```
import numpy as np
from numpy.linalg import norm

matrix = np.asarray(matrix)
all_norms = norm(matrix, axis=1)
print "index: ", all_norms.argmin()
```

Final word on NumPy: Vectorization

Do not waste NumPy's awesome performance by writing `for` loops on them!

`for` loop

```
a = np.arange(10000).reshape((-1, 2))
# square entries
for i in range(len(a)):
    for j in range(len(a[i])):
        a[i][j] = a[i][j] ** 2
```

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for loop

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vectorization code

```
a = np.arange(10000).reshape((-1, 2))
# square entries
a = a * a
```

Now let's switch to SciPy!

`scipy.cluster`	Vector quantization / Kmeans
`scipy.constants`	Physics/Math constants
`scipy.fftpack`	Fourier Transform
...	...
`scipy.signal`	Signal Processing
`scipy.stats`	Statistics

SciPy is built on NumPy

- You need to know how to deal with NumPy arrays to be comfortable with SciPy functions.
- Depending on your need, you can almost find anything in it!
- Commonly used by me: `stats`, `optimize`, `signal`

Optimization: Convex, Non-Convex, ...

`optimize` module deals with Lagrange multipliers for you!

A convex function

$$\min_x \frac{1}{2}x^2 \quad \texttt{s.t.} \quad x \geq -10$$

In SciPy: define objective function, and the constraints

```
def objective(x):
    return 0.5 * (x ** 2)
def constraint(x):
    # unlike definition (<=0), scipy constraints ar
    return x + 10
```

Optimization, cont'd

```
x0 = 0
cons = {'type': 'ineq', 'fun': constraint}
# minimize
minimize(objective, x0, method="SLSQP",
    constraints=cons)
```

Would still work on non-convex constraints such as $||\vec{v}||_2 = 0$

Statistics: Student T Test

Hypothesis testing: p values

```
from scipy.stats import ttest_ind
import numpy as np

# two independent random variables
X = np.random.rand(10, 1)
Y = np.random.rand(10, 1)
# T test (two tailed p value)
t, p = ttest_ind(X, Y)
```