

M. Hohle:

Physics 77: Introduction to Computational Techniques in Physics





Introduction to Computational Techniques in Physics Scientific Computing

Programmer's Problem



<u>Outline</u>

- introduction to numpy
- linear algebra with numpy
- avoiding loops



Introduction to Computational Techniques in Physics Scientific Computing

Programmer's Problem

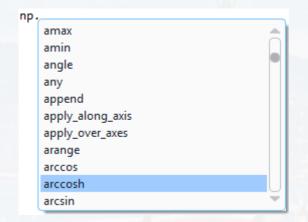


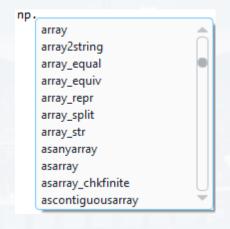
Outline

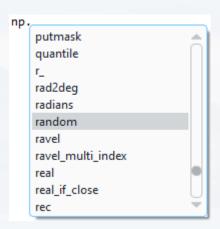
- introduction to numpy
- linear algebra with numpy
- avoiding loops

so far, we have used math faster and more functions: numpy

import numpy as np







basic math function (like math)

manipulating/creating arrays

random number generator

...and much, much more...

type: numpy array

```
M = np.array([[1,2,5,6], [0,8,5,-4], [-4,4,6,1], [2,3,-1,0]])
print(M)
```

type(M)

type(M)
numpy.ndarray



useful numpy commands:

$$V = np.arange(start = -1, stop = 3, step = 0.01)$$

V - NumPy object array

	0
0	-1
1	-0.99
2	-0.98
3	-0.97
4	-0.96
5	-0.95

creating an array, that contain floats which start at start, continue in steps of step until the stop value stop

useful numpy commands:

$$Z = np.zeros((5,6,7))$$

Z - NumPy object array

	0	1	2
0	0	0	0
1	0	0	0
2	0	0	0
3	0	0	0
4	0	0	0
5	0	0	0

creating an **array** of any shape that only contains zeros.
Ideal for pre-allocating matrices

see also

$$Z = np.ones((5,6,7))$$

useful numpy commands:

$$I = np.eye(5)$$

creating the N x N identity matrix

I - NumPy object array

	0	1	2	3	4
0	1	0	0	0	0
1	0	1	0	0	0
2	0	0	1	0	0
3	0	0	0	1	0
4	0	0	0	0	1

useful numpy commands:

$$T = np.tile([1, 2, 4, 5], reps = (5, 1))$$

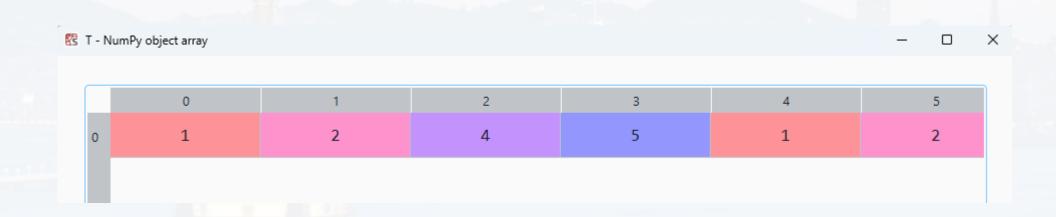
creating multiple replicates of an array

S S	T - NumPy object array					
		0	1	2	3	
	0	1	2	4	5	
	1	1	2	4	5	
	2	1	2	4	5	
	3	1	2	4	5	
	4	1	2	4	5	

useful numpy commands:

$$T = np.tile([1, 2, 4, 5], reps = (1, 5))$$

creating multiple replicates of an array



math vs numpy

Task: Calculating cosine from an array!

A = np.arange(-1, 3, 1/1000000)

```
from math import cos as math_cos as math_cos cos as np_cos

import time

assigning different names in order to be able to distinguish between the different methods
```

```
t1 = time.monotonic()
```

```
for a in A:
    math_cos(a)
```

0.36 sec

```
t2 = time.monotonic()

dt = t2 - t1
print('Total runtime: ' + str(dt) + ' seconds')
```

```
math vs numpy
```

Task: Calculating cosine from an array!

```
A = np.arange(-1, 3, 1/1000000)
```

```
from math import cos as math_cos
from numpy import cos as np_cos
import time
```

```
t1 = time.monotonic()
```

2.26 sec

```
for a in A:
    np_cos(a)
```

That is 6 times slower!

```
t2 = time.monotonic()

dt = t2 - t1
print('Total runtime: ' + str(dt) + ' seconds')
```

```
math vs numpy
```

Task: Calculating cosine from an array!

```
A = np.arange(-1, 3, 1/1000000)
```

```
from math import cos as math_cos
from numpy import cos as np_cos
import time
```

We actually don't need the loop at all!

```
t1 = time.monotonic()
```

```
np_cos(A)
```

0.016 sec

```
t2 = time.monotonic()

dt = t2 - t1
print('Total runtime: ' + str(dt) + ' seconds')
```

```
math vs numpy
```

dt = t2 - t1

Task: Calculating cosine from an array!

```
A = np.arange(-1, 3, 1/1000000)
```

```
from math import cos as math_cos
from numpy import cos as np_cos
import time
```

print('Total runtime: ' + str(dt) + ' seconds')

```
t1 = time.monotonic()

math_cos(A)

Traceback (most recent call last):

Cell In[40], line 2
    math_cos(A)

TypeError: only length-1 arrays can be converted to Python scalars
t2 = time.monotonic()
```

math vs numpy

	math	numpy	
loop	0.36 sec	2.26 sec	math is optimized for scalars. It doesn't need arrays
vector	n. a.	0.016 sec	arrays are actually slow but faster than a for loop → use numpy



Introduction to Computational Techniques in Physics Scientific Computing

Programmer's Problem



<u>Outline</u>

- introduction to numpy
- linear algebra with numpy
- avoiding loops

Why do we need matrices:

- "vectorized" code is : faster

shorter

maintainable

readable

scalable

- AI/ANN: essentially matrix operations

- regression, linear models etc

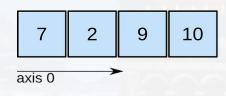
- easy to parallelize

in python:

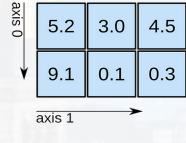
see <u>here</u>

2D array

1D array



shape: (4,)



shape: (2, 3)

3D array

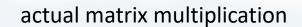
shape: (4, 3, 2)

... and higher

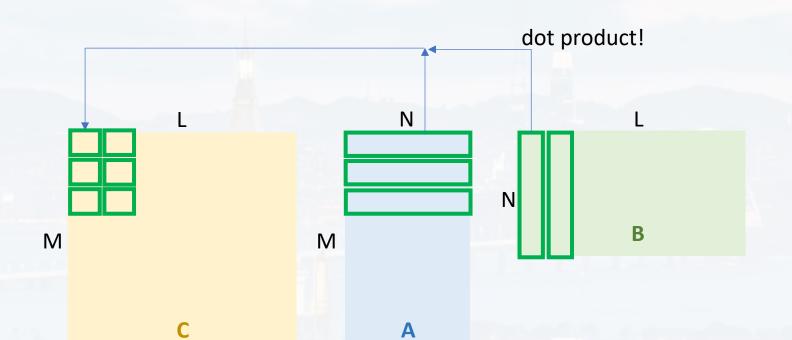
note:

higher dimensional arrays are called **tensor** in the CS community, but they are not the same tensors as in math & physics

the math:



$$C = A*B$$



$$c_{m,l} = \sum_{n=0}^{N} a_{m,n} b_{n,l}$$

- only works if $n_{column}(A) = n_{row}(B)$
- result: $C(n_{row}(A), n_{column}(B))$

```
v1 = np.array([1,5,0,-3])
v2 = np.array([3,-1,2,2])

1) np.dot(v1,v2)
2) np.outer(v1,v2)
```

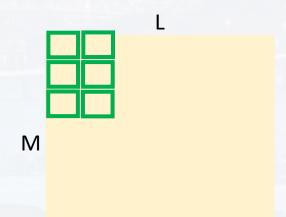
$$(a \quad b \quad c) \quad \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = a\alpha + b\beta + c\gamma$$

$$\begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} \quad (a \quad b \quad c) = \begin{pmatrix} a\alpha & \alpha b & \alpha c \\ \alpha \beta & \beta b & \beta c \\ \alpha \gamma & \gamma b & \gamma c \end{pmatrix}$$

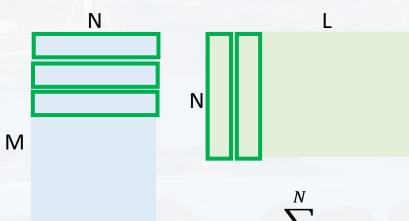
```
M = np.array([[1,2,5,6], [0,8,5,-4], [-4,4,6,1], \\ [2,3,-1,0]])
```

np.dot(M,M)

actual matrix multiplication



C = A*B



$$c_{m,l} = \sum_{n=0}^{N} a_{m,n} \ b_{n,l}$$

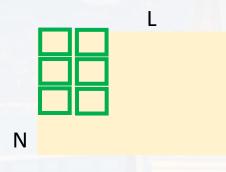
identity matrix

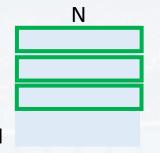
$$I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

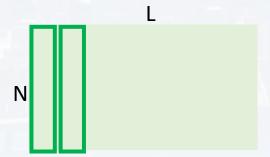
$$I = \begin{pmatrix} 1 & \cdots & 0 \\ \vdots & 1 & \vdots \\ 0 & \cdots & 1 \end{pmatrix}$$

actual matrix multiplication

$$B = I*B$$







$$c_{m,l} = \sum_{n=0}^{N} a_{m,n} b_{n,l}$$



Introduction to Computational Techniques in Physics Scientific Computing

Programmer's Problem



Outline

- introduction to numpy
- linear algebra with numpy
- avoiding loops

We saw earlier: loops are slow \rightarrow use linear algebra or numpy commands

broadcasting

"Broadcasting describes how NumPy treats arrays with different shapes during arithmetic operations."

last section: numpy operations following linear algebra

now: additional useful operations

```
import numpy as np
```

A1 =
$$np.array([1, 3, 4, 6])$$

A2 =
$$np.array([2, 4, -1, 0])$$

$$A3 = A1*A2$$

automatically performs element wise multiplication

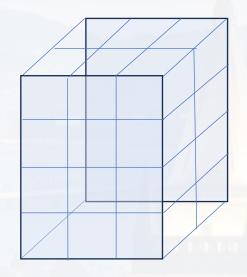
```
import numpy as np
                                                                               broadcasting
A1 = np.array([1, 3, 4, 6])
A2 = np.array([2, 4, -1, 0])
                                                         automatically performs element wise
                                                         multiplication
A3 = A1*A2
А3
array([ 2, 12, -4, 0])
A1.shape
(4,)
A2.shape
(4,)
A2 = A2.reshape((1, len(A2)))
A2.shape
                                                         Works too!
(1, 4)
A1*A2
array([[ 2, 12, -4, 0]])
```

```
import numpy as np
                                                                                  broadcasting
 A1 = np.array([1, 3, 4, 6])
 A2 = np.array([2, 4, -1, 0])
                                                           Multiplying with a number (no shape!)
                                                            → still element wise multiplication
 A3 = A1*A2
A1*3
array([ 3, 9, 12, 18])
A4 = np.array([3, -5, 6])
A4*A1
Traceback (most recent call last):
                                                                                  What are the
                                                                                  broadcasting
  Cell In[23], line 1
                                                                                  rules?
    A4*A1
                                                               broadcasting error!
ValueError: operands could not be broadcast together with shapes (3,) (4,)
```

broadcasting

What are the broadcasting rules?

Think about matrices like boxes! As long as you can turn them such a way that the edges match, broadcasting is applicable!



```
A1 = np.array(

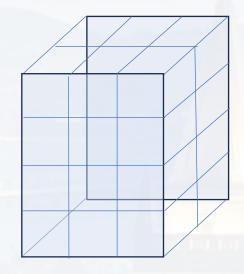
[ [[1, -1], [2, -2], [3, -3]],
      [[4, -4], [5, -5], [6, -6]],
      [[7, -7], [8, -8], [9, -9]],
      [[10, -10], [11, -11], [12, -12]] ]
```

A1.shape (4, 3, 2)

What are the broadcasting rules?

broadcasting

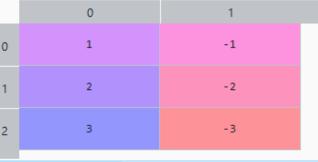
Think about matrices like boxes! As long as you can turn them such a way that the edges match, broadcasting is applicable!



$$A1 = np.array($$

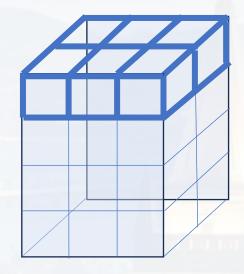
```
[ [[1, -1], [2, -2], [3, -3]], [4, -4], [5, -5], [6, -6]], [7, -7], [8, -8], [9, -9]], [10, -10], [11, -11], [12, -12]]
```

A1.shape (4, 3, 2)



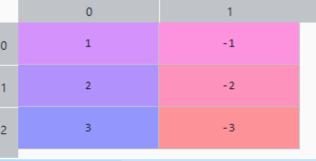
broadcasting

Think about matrices like boxes! As long as you can turn them such a way that the edges match, broadcasting is applicable!



$$A1 = np.array($$

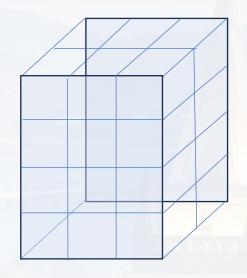
A1.shape (4, 3, 2)



What are the broadcasting rules?

broadcasting

Think about matrices like boxes! As long as you can turn them such a way that the edges match, broadcasting is applicable!



```
A1 = np.array([ [[1, -1], [2, -2], [3, -3]], [4, -4], [5, -5], [6, -6]], [7, -7], [8, -8], [9, -9]], [[10, -10], [11, -11], [12, -12]]])
```



adding/multiplying an object of shape 0, (1,) or (1,1)

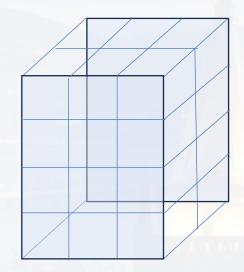
A1.shape (4, 3, 2)

Always fits any part of the box \rightarrow works!



broadcasting

Think about matrices like boxes! As long as you can turn them such a way that the edges match, broadcasting is applicable!





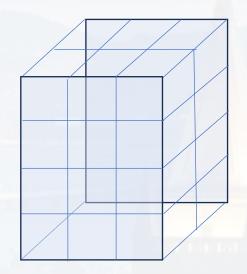
a = 3

A1.shape (4, 3, 2)

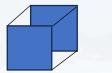
adding/multiplying an object of shape 0, (1,) or (1,1)

broadcasting

Think about matrices like boxes! As long as you can turn them such a way that the edges match, broadcasting is applicable!



```
A1 = np.array([
                     [[1, -1], [2, -2], [3, -3]],
                     [[4, -4], [5, -5], [6, -6]],
[[7, -7], [8, -8], [9, -9]],
                     [[10, -10], [11, -11], [12, -12]])
```



```
a.shape
a = np.array([3])
                    (1,)
```

A1.shape (4, 3, 2)

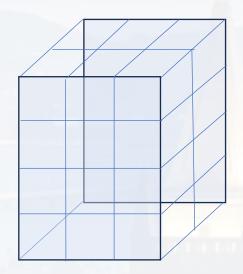
adding/multiplying an object of shape 0, (1,) or (1,1)

```
In [4]: A1 * a
Out[4]:
array([[[ 3, -3],
          6, -6],
          9, -9]],
       [[ 12, -12],
       [ 15, -15],
        [ 18, -18]],
       [[ 21, -21],
        [ 24, -24],
       [ 27, -27]],
       [[ 30, -30],
        [ 33, -33],
        [ 36, -36]]])
```



broadcasting

Think about matrices like boxes! As long as you can turn them such a way that the edges match, broadcasting is applicable!



```
A1 = np.array([ [[1, -1], [2, -2], [3, -3]], [4, -4], [5, -5], [6, -6]], [7, -7], [8, -8], [9, -9]], [[10, -10], [11, -11], [12, -12]]])
```

```
a = np.array([[3]])
```

a.shape (1, 1)

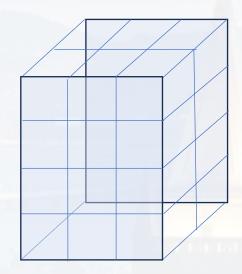
```
A1.shape (4, 3, 2)
```

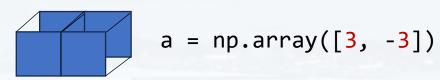
adding/multiplying an object of shape 0, (1,) or (1,1)



broadcasting

Think about matrices like boxes! As long as you can turn them such a way that the edges match, broadcasting is applicable!





A1.shape (4, 3, 2)

adding/multiplying an object of shape (2,)

[[12, 12], [15, 15], [18, 18]], [[21, 21], [24, 24], [27, 27]], [[30, 30], [33, 33], [36, 36]]])

6],

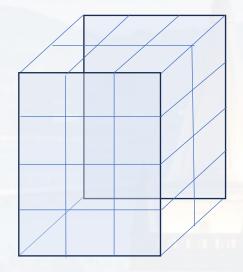
9]],

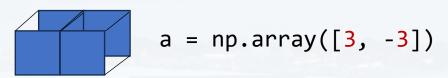
6,



broadcasting

Think about matrices like boxes! As long as you can turn them such a way that the edges match, broadcasting is applicable!





A1.shape (4, 3, 2)

adding/multiplying an object of shape (2,)

Works, because **a** was just oriented the right way!

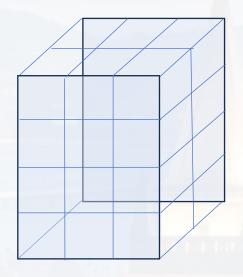
6], 9]], [[12, 12], [15, 15], 18]], [18, [[21, 21], [24, 24], 27]], [27, [[30, 30], [33, 33],

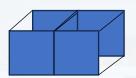
[36, 36]]])

What are the broadcasting rules?

broadcasting

Think about matrices like boxes! As long as you can turn them such a way that the edges match, broadcasting is applicable!





$$a = np.array([[3], [-3]])$$

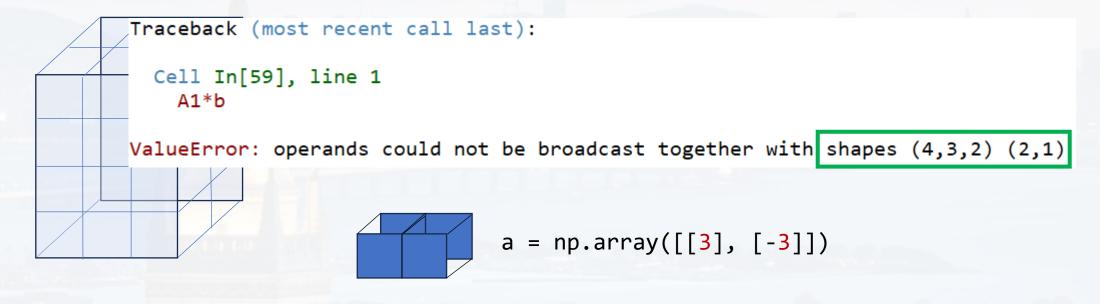
A1.shape (4, 3, 2)

adding/multiplying an object of shape (2,1)

What are the broadcasting rules?

broadcasting

Think about matrices like boxes! As long as you can turn them such a way that the edges match, broadcasting is applicable!



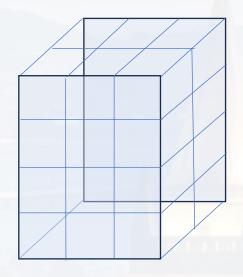
A1.shape (4, 3, 2)

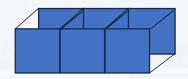
adding/multiplying an object of shape (2,1)

What are the broadcasting rules?

broadcasting

Think about matrices like boxes! As long as you can turn them such a way that the edges match, broadcasting is applicable!





$$a = np.array([3, 0, -3])$$

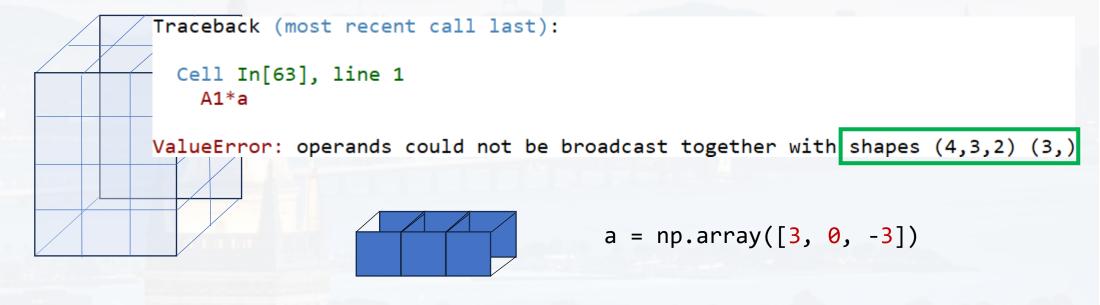
A1.shape (4, 3, 2)

adding/multiplying an object of shape (3,)

What are the broadcasting rules?

broadcasting

Think about matrices like boxes! As long as you can turn them such a way that the edges match, broadcasting is applicable!



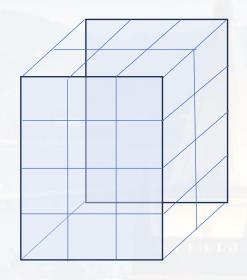
A1.shape (4, 3, 2)

adding/multiplying an object of shape (3,)

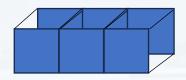
broadcasting

What are the broadcasting rules?

Think about matrices like boxes! As long as you can turn them such a way that the edges match, broadcasting is applicable!



$$a = np.array([[3], [0], [-3]])$$



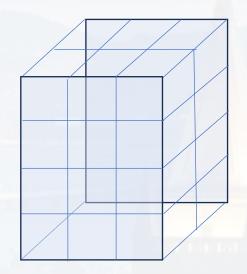
A1.shape (4, 3, 2)

adding/multiplying an object of shape (3,1)

What are the broadcasting rules?

broadcasting

Think about matrices like boxes! As long as you can turn them such a way that the edges match, broadcasting is applicable!



```
A1 = np.array([
```

[[12, -12], a = np.array([[3], [0],[-

[[21, -21], [0, 0],

[0, 0], [-18, 18]],

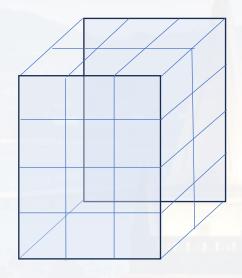
adding/multiplying an object of shape (3,1)

[-36, 36]]])

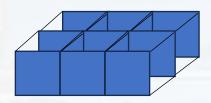
A1.shape (4, 3, 2) What are the broadcasting rules?

broadcasting

Think about matrices like boxes! As long as you can turn them such a way that the edges match, broadcasting is applicable!



$$a = np.array([[3, 0, -3], [2, 0, -2]])$$



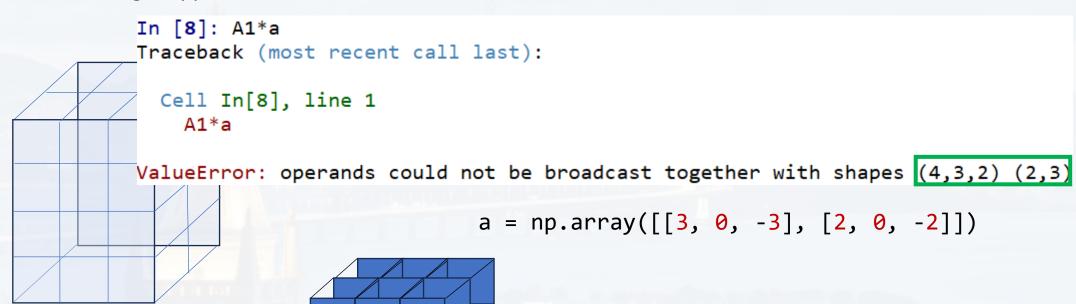
A1.shape (4, 3, 2)

adding/multiplying an object of shape (2,3)

What are the broadcasting rules?

broadcasting

Think about matrices like boxes! As long as you can turn them such a way that the edges match, broadcasting is applicable!



A1.shape (4, 3, 2)

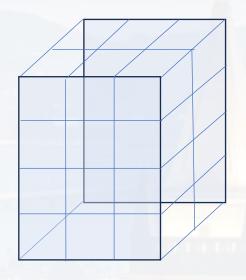
adding/multiplying an object of shape (2,3)

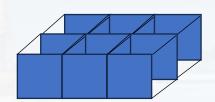


What are the broadcasting rules?

broadcasting

Think about matrices like boxes! As long as you can turn them such a way that the edges match, broadcasting is applicable!





$$a = np.array([[3, 0, -3], [2, 0, -2]])$$

a = a.reshape((3,2))

A1.shape (4, 3, 2)

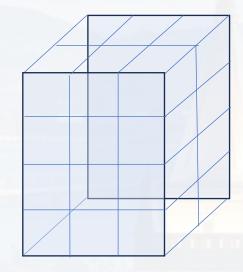
adding/multiplying an object of shape (3,2)

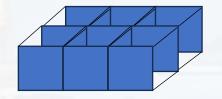


What are the broadcasting rules?

broadcasting

Think about matrices like boxes! As long as you can turn them such a way that the edges match, broadcasting is applicable!





a = a.reshape((3,2))

A1.shape (4, 3, 2)

adding/multiplying an object of shape (3,2)

```
[ 0, 6]],

[[ 12, 0],
 [-15, -10],
 [ 0, 12]],

[[ 21, 0],
 [-24, -16],
 [ 0, 18]],

[[ 30, 0],
 [-33, -22],
 [ 0, 24]]])
```



What are the broadcasting rules?

broadcasting

note: these broadcasting rules work for addition/subtraction too

```
ValueError: operands could not be broadcast together with shapes (4,3,2) (2,1)
didn't work because (2, 1) doesn't match (4, 3, 2)
solution: (2,), it matches (4, 3, 2)
```

```
ValueError: operands could not be broadcast together with shapes (4,3,2) (3,) didn't work because (3,) doesn't match (4, 3, 2) solution: (3, 1), it matches (4, 3, 2) two times
```

```
ValueError: operands could not be broadcast together with shapes (4,3,2) (2,3) didn't work because (2, 3) doesn't match (4, 3, 2) solution: reshape to (3, 2), it matches (4, 3, 2)
```

more useful numpy commands to avoid loops:

np.max() np.min() np.mean() np.median() np.std() np.argwhere() np.historgram() ...

rearranging arrays

```
np.reshape()
np.sort()
np.transpose()
np.hstack()
np.vstack()
np.tile()
np.arange()
...
```

resetting values

```
np.clip()
np.abs()
np.round()
np.eye()
...
```

math functions

```
np.exp()
np.sin()
np.cos()
np.tan()
np.arcsin()
np.arccos()
np.arctan()
np.arctanh()
```



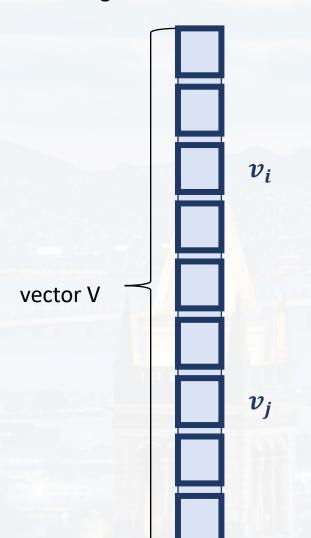
Let's combine some of those commands

```
np.zeros()
np.arange()
np.tile()
np.transpose()
```

for a particular example about avoiding loops!

We saw earlier: loops are slow \rightarrow use lin algebra or numpy commands

calculating distances d

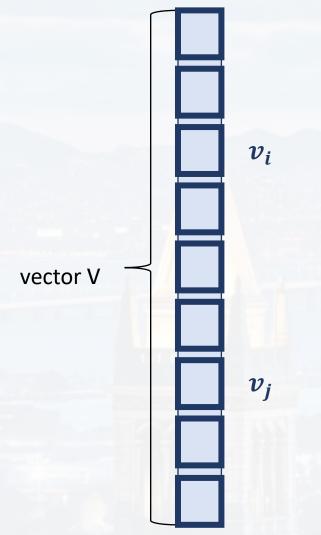


calculating the distance between each element

$$d(v_i, v_j) = (v_i - v_j)^2$$

We saw earlier: loops are slow \rightarrow use lin algebra or numpy commands

calculating distances d



calculating the distance between each element

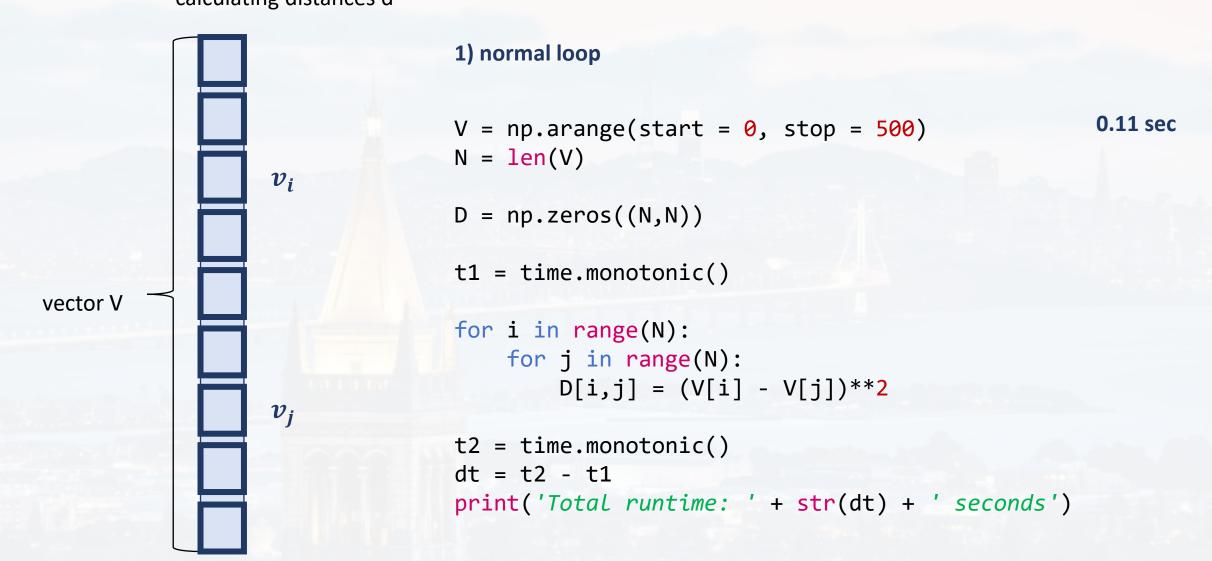
$$d(v_i, v_j) = (v_i - v_j)^2$$

efficiency:

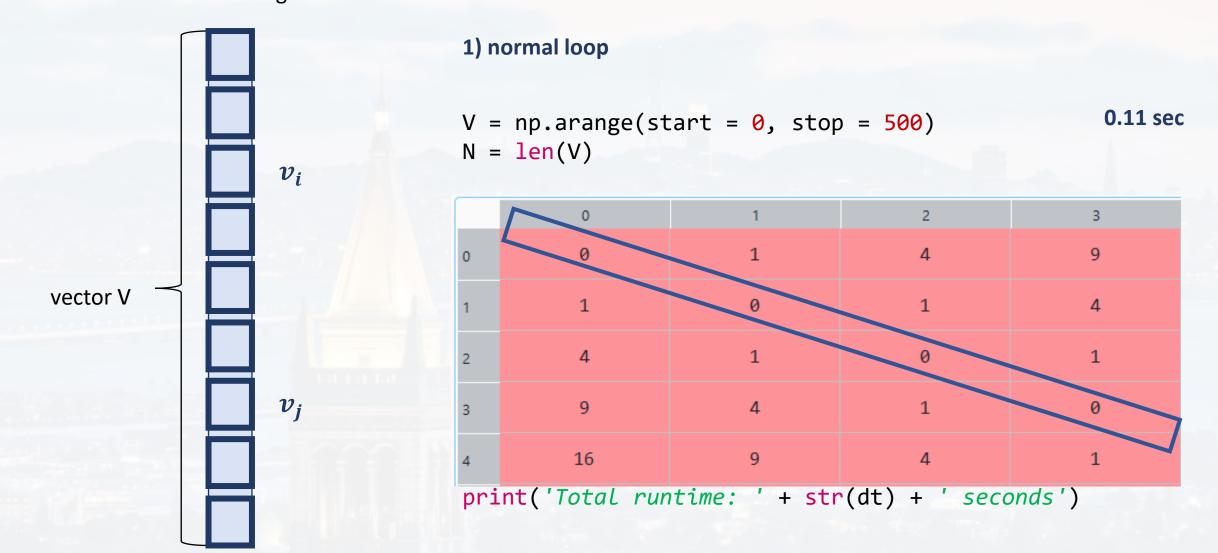
vector of length N \rightarrow N*N operations we know that the diagonal $d(v_i, v_i) = 0 \rightarrow$ N fewer operations only half the operations are necessary: $d(v_i, v_j) = d(v_j, v_i)$

 \rightarrow instead of N*N operations: only (N-1)*(N-1)/2 needed

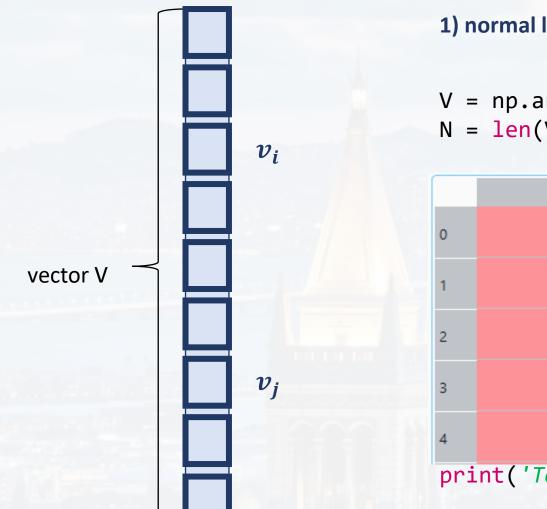
We saw earlier: loops are slow → use lin algebra or numpy commands calculating distances d



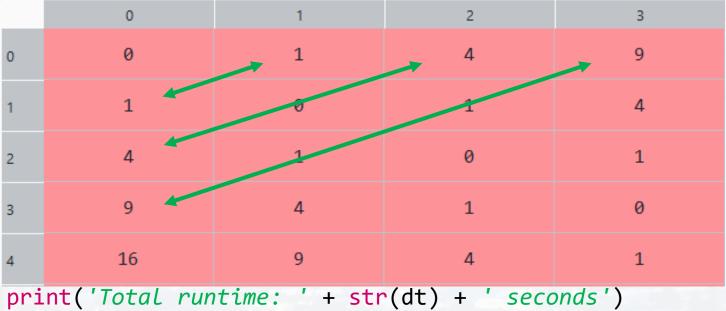
We saw earlier: loops are slow → use lin algebra or numpy commands calculating distances d



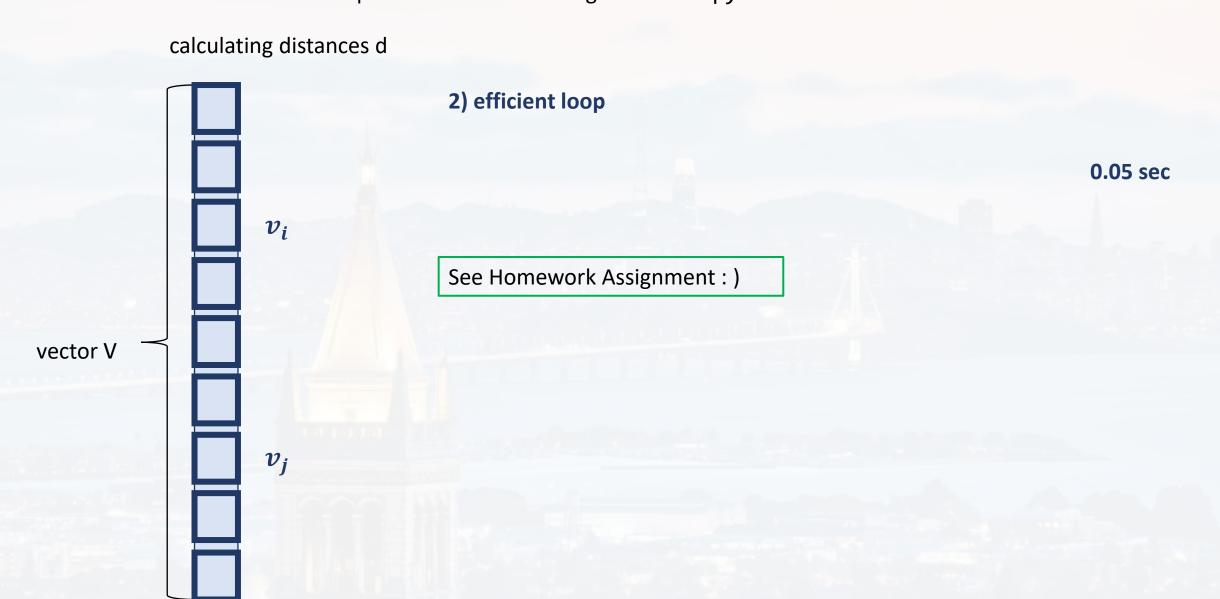
We saw earlier: loops are slow \rightarrow use lin algebra or numpy commands calculating distances d



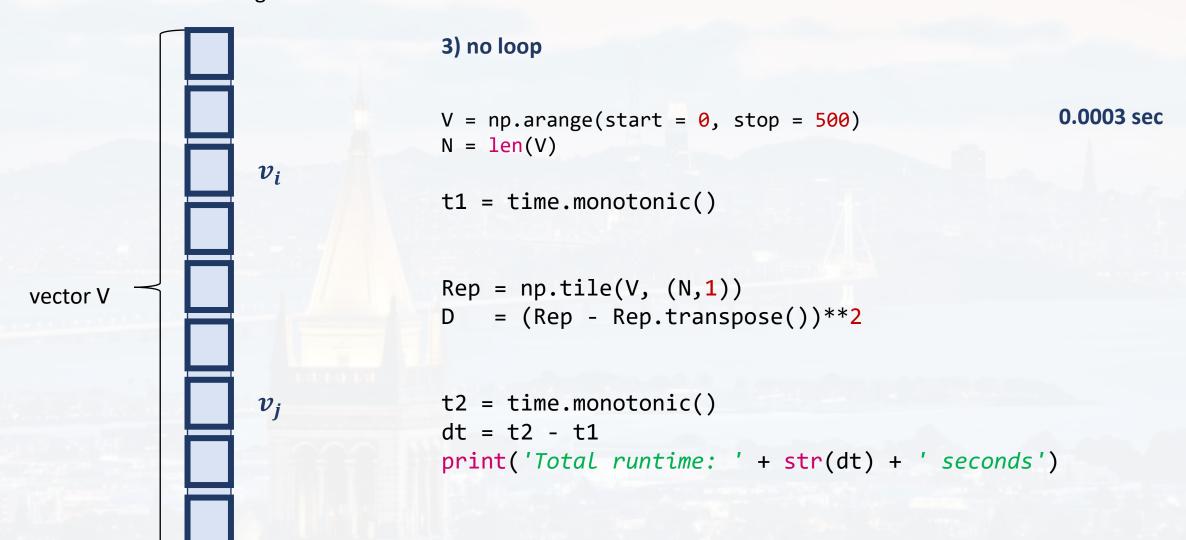
1) normal loop



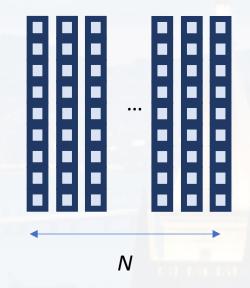
We saw earlier: loops are slow → use lin algebra or numpy commands

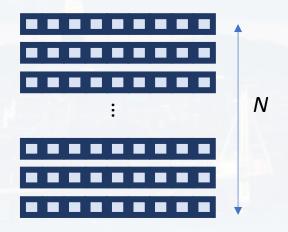


We saw earlier: loops are slow → use lin algebra or numpy commands calculating distances d



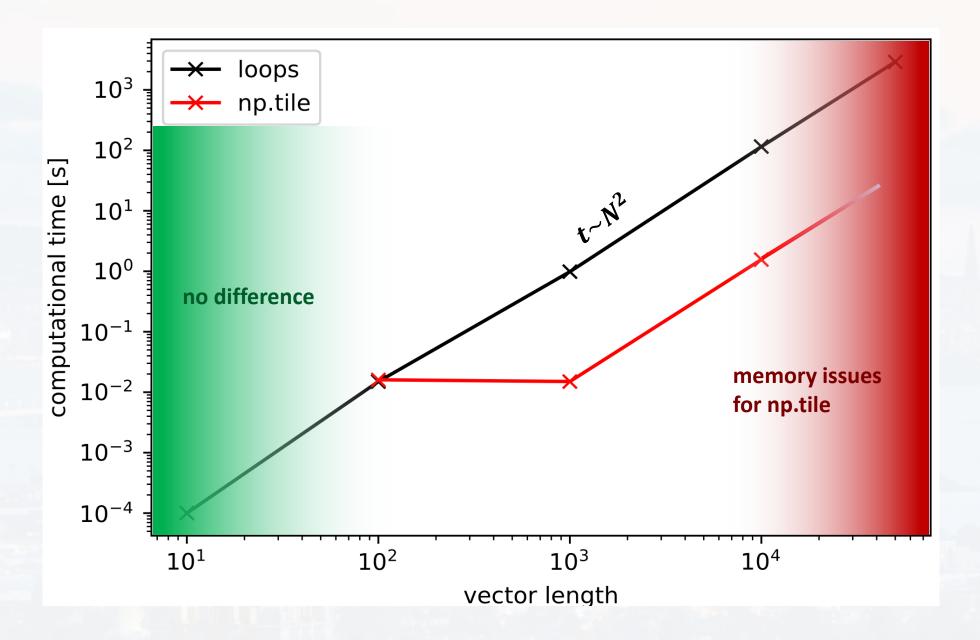
We saw earlier: loops are slow → use lin algebra or numpy commands calculating distances d





	loop	efficient loop	np.tile
N = 500	0.11 sec	0.05 sec	0.0003 sec
N = 10,000	35.0 sec	17.8 sec	1.25 sec
N = 50,000			180 sec







Introduction to Computational Techniques in Physics Scientific Computing

Thank you very much for your attention!

