Introduction to NumPy arrays

Gert-Ludwig Ingold

https://github.com/gertingold/euroscipy-numpy-tutorial.git

Python comes with batteries included

➜ extensive Python standard library

What about batteries for scientists (and others as well)?

➜ scientific Python ecosystem

NumPy
Base N-dimensional array package

SciPy library
Fundamental library for scientific computing

Matplotlib
Comprehensive 2D Plotting

IP[y]:
IPython

IPython
Enhanced Interactive Console

Sympy
Symbolic mathematics

pandas
Data structures & analysis

from: www.scipy.org

+ SciKits and many other packages

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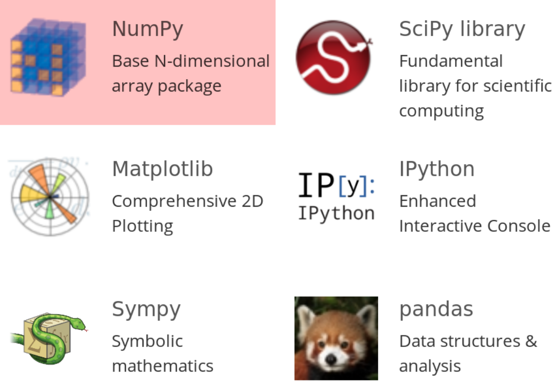

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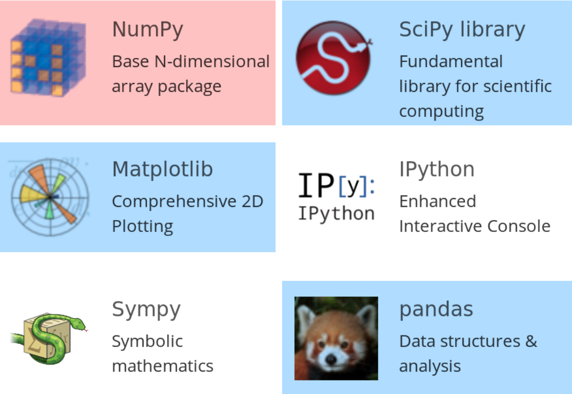
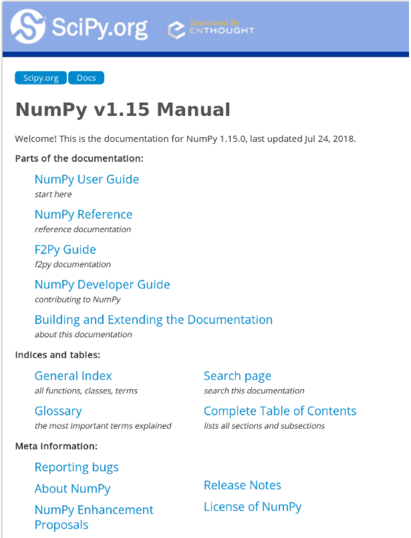


from: www.scipy.org

+ SciKits and many other packages

www.scipy-lectures.org

docs.scipy.org/doc/numpy/


SciPy.org Sponsored By ENTHOUGHT

Scipy.org Docs

NumPy v1.15 Manual

Welcome! This is the documentation for NumPy 1.15.0, last updated Jul 24, 2018.

Parts of the documentation:

- NumPy User Guide
  start here
- NumPy Reference
  reference documentation
- F2Py Guide
  f2py documentation
- NumPy Developer Guide
  contributing to NumPy
- Building and Extending the Documentation
  about this documentation

Indices and tables:

- General Index
  all functions, classes, terms
- Glossary
  the most important terms explained
- Search page
  search this documentation
- Complete Table of Contents
  lists all sections and subsections

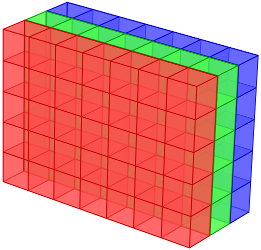
Meta information:

- Reporting bugs
- About NumPy
- NumPy Enhancement Proposals
- Release Notes
- License of NumPy

A wish list

- we want to work with vectors and matrices

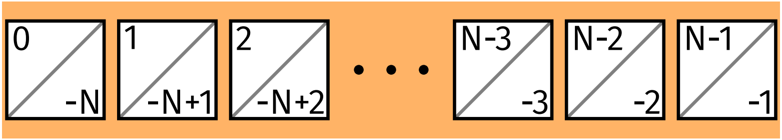
$$\begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}$$



colour image as $N \times M \times 3$-array

- we want our code to run fast
- we want support for linear algebra
- ...

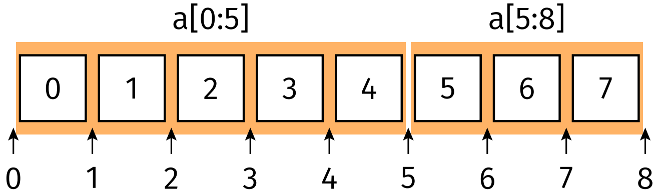
List indexing



- indexing starts at 0
- negative indices count from the end of the list to the beginning

List slicing

basic syntax: `[start:stop:step]`



- if `step=1`
  - slice contains the elements `start` to `stop-1`
  - slice contains `stop-start` elements
- `start`, `stop`, and also `step` can be negative
- default values:
  - `start` 0, i.e. starting from the first element
  - `stop` N, i.e up to and including the last element
  - `step` 1

Let’s do some slicing

Your turn

Matrices and lists of lists

Can we use lists of lists to work with matrices?

$$\begin{pmatrix} 0 & 1 & 2 \\ 3 & 4 & 5 \\ 6 & 7 & 8 \end{pmatrix}$$

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

- How can we extract a row?
- How can we extract a column?

Matrices and lists of lists

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

- How can we extract a row?
- How can we extract a column?

Let's do some experiments

Matrices and lists of lists

Can we use lists of lists to work with matrices?

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

- How can we extract a row? ☺
- How can we extract a column? ☹

Lists of lists do not work like matrices

Problems with lists as matrices

- different axes are not treated on equal footing
- lists can contain arbitrary objects
  matrices have a homogeneous structure
- list elements can be scattered in memory

Applied to matrices …

…lists are conceptually inappropriate

…lists have less performance than possible

We need a new object

ndarray

multidimensional, homogeneous array of fixed-size items

Getting started

Import the NumPy package:

```
from numpy import *
```

Getting started

Import the NumPy package:

```
from numpy import *
from numpy import array, sin, cos
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Getting started

Import the NumPy package:

~~`from numpy import *`~~

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`import numpy`

Getting started

Import the NumPy package:

```
from numpy import *
from numpy import array, sin, cos
import numpy
import numpy as np  ←
```

Getting started

Import the NumPy package:

~~`from numpy import *`~~

~~`from numpy import array, sin, cos`~~

~~`import numpy`~~

`import numpy as np`

Check the NumPy version:

`np.__version__`

Your turn

Data types

Some important data types:

integer	`int8`, `int16`, `int32`, `int64`, `uint8`, …
float	`float16`, `float32`, `float64`, …
complex	`complex64`, `complex128`, …
boolean	`bool8`
Unicode string	

default type: `float64`

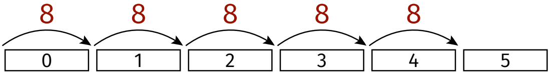
Beware of overflows!

Your turn

Strides

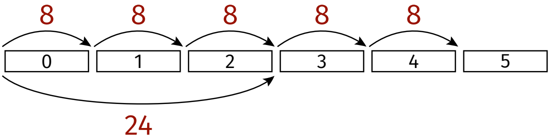
$$\begin{pmatrix} 0 & 1 & 2 & 3 & 4 & 5 \end{pmatrix}$$

(8,)



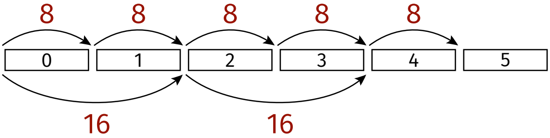
$$\begin{pmatrix} 0 & 1 & 2 \\ 3 & 4 & 5 \end{pmatrix}$$

(24, 8)



$$\begin{pmatrix} 0 & 1 \\ 2 & 3 \\ 4 & 5 \end{pmatrix}$$

(16, 8)



Views

For the sake of efficiency, NumPy uses views if possible.

- Changing one or more matrix elements will change it in all views.
- Example: transposition of a matrix `a.T`
  No need to copy the matrix and to create a new one

Some array creation routines

- numerical ranges: `arange`, `linspace`, `logspace`
- homogeneous data: `zeros`, `ones`
- diagonal elements: `diag`, `eye`
- random numbers: `rand`, `randint`

Numpy has an `append()`-method. Avoid it if possible.

Your turn

Indexing and slicing in one dimension

1d arrays: indexing and slicing as for lists

- first element has index 0
- negative indices count from the end
- slices: `[start:stop:step]`
  without the element indexed by `stop`
- if values are omitted:
  - `start`: starting from first element
  - `stop`: until (and including) the last element
  - `step`: all elements between `start` and `stop`-1

Indexing and slicing in higher dimensions

- usual slicing syntax
- difference to lists:
  slices for the various axes separated by comma

a[2, -3]

0	1	2	3	4	5	6	7
8	9	10	11	12	13	14	15
16	17	18	19	20	21	22	23
24	25	26	27	28	29	30	31
32	33	34	35	36	37	38	39

Indexing and slicing in higher dimensions

- usual slicing syntax
- difference to lists:
  slices for the various axes separated by comma

a[:3, :5]

0	1	2	3	4	5	6	7
8	9	10	11	12	13	14	15
16	17	18	19	20	21	22	23
24	25	26	27	28	29	30	31
32	33	34	35	36	37	38	39

Indexing and slicing in higher dimensions

Your turn

0	1	2	3	4	5	6	7
8	9	10	11	12	13	14	15
16	17	18	19	20	21	22	23
24	25	26	27	28	29	30	31
32	33	34	35	36	37	38	39

Indexing and slicing in higher dimensions

Your turn

a[-3:, -3:]

0	1	2	3	4	5	6	7
8	9	10	11	12	13	14	15
16	17	18	19	20	21	22	23
24	25	26	27	28	29	30	31
32	33	34	35	36	37	38	39

Indexing and slicing in higher dimensions

Your turn

0	1	2	3	4	5	6	7
8	9	10	11	12	13	14	15
16	17	18	19	20	21	22	23
24	25	26	27	28	29	30	31
32	33	34	35	36	37	38	39

Indexing and slicing in higher dimensions

Your turn

a[:, 3]

0	1	2	3	4	5	6	7
8	9	10	11	12	13	14	15
16	17	18	19	20	21	22	23
24	25	26	27	28	29	30	31
32	33	34	35	36	37	38	39

Indexing and slicing in higher dimensions

Your turn

0	1	2	3	4	5	6	7
8	9	10	11	12	13	14	15
16	17	18	19	20	21	22	23
24	25	26	27	28	29	30	31
32	33	34	35	36	37	38	39

Indexing and slicing in higher dimensions

Your turn

a[1, 3:6]

0	1	2	3	4	5	6	7
8	9	10	11	12	13	14	15
16	17	18	19	20	21	22	23
24	25	26	27	28	29	30	31
32	33	34	35	36	37	38	39

Indexing and slicing in higher dimensions

Your turn

0	1	2	3	4	5	6	7
8	9	10	11	12	13	14	15
16	17	18	19	20	21	22	23
24	25	26	27	28	29	30	31
32	33	34	35	36	37	38	39

Indexing and slicing in higher dimensions

Your turn

a[1::2, ::3]

0	1	2	3	4	5	6	7
8	9	10	11	12	13	14	15
16	17	18	19	20	21	22	23
24	25	26	27	28	29	30	31
32	33	34	35	36	37	38	39

Fancy indexing – Boolean mask

a[a % 3 == 0]

0	1	2	3	4	5	6	7
8	9	10	11	12	13	14	15
16	17	18	19	20	21	22	23
24	25	26	27	28	29	30	31
32	33	34	35	36	37	38	39

Fancy indexing – array of integers

a[(1, 1, 2, 2, 3, 3), (3, 4, 2, 5, 3, 4)]

0	1	2	3	4	5	6	7
8	9	10	11	12	13	14	15
16	17	18	19	20	21	22	23
24	25	26	27	28	29	30	31
32	33	34	35	36	37	38	39

Application: sieve of Eratosthenes

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49

0	1	**2**	3	~~4~~	5	~~6~~	7	~~8~~	9	~~10~~	11	~~12~~	13	~~14~~	15	~~16~~	17	~~18~~	19	~~20~~	21	~~22~~	23	~~24~~
25	~~26~~	27	~~28~~	29	~~30~~	31	~~32~~	33	~~34~~	35	~~36~~	37	~~38~~	39	~~40~~	41	~~42~~	43	~~44~~	45	~~46~~	47	~~48~~	49

0	1	**2**	**3**	~~4~~	5	~~6~~	7	~~8~~	~~9~~	~~10~~	11	~~12~~	13	~~14~~	~~15~~	~~16~~	17	~~18~~	19	~~20~~	~~21~~	~~22~~	23	~~24~~
25	~~26~~	~~27~~	~~28~~	29	~~30~~	31	~~32~~	~~33~~	~~34~~	35	~~36~~	37	~~38~~	~~39~~	~~40~~	41	~~42~~	43	~~44~~	~~45~~	~~46~~	47	~~48~~	49

0	1	**2**	**3**	~~4~~	**5**	~~6~~	7	~~8~~	~~9~~	~~10~~	11	~~12~~	13	~~14~~	~~15~~	~~16~~	17	~~18~~	19	~~20~~	~~21~~	~~22~~	23	~~24~~
~~25~~	~~26~~	~~27~~	~~28~~	29	~~30~~	31	~~32~~	~~33~~	~~34~~	~~35~~	~~36~~	37	~~38~~	~~39~~	~~40~~	41	~~42~~	43	~~44~~	~~45~~	~~46~~	47	~~48~~	49

0	1	**2**	**3**	~~4~~	**5**	~~6~~	**7**	~~8~~	~~9~~	~~10~~	11	~~12~~	13	~~14~~	~~15~~	~~16~~	17	~~18~~	19	~~20~~	~~21~~	~~22~~	23	~~24~~
~~25~~	~~26~~	~~27~~	~~28~~	29	~~30~~	31	~~32~~	~~33~~	~~34~~	~~35~~	~~36~~	37	~~38~~	~~39~~	~~40~~	41	~~42~~	43	~~44~~	~~45~~	~~46~~	47	~~48~~	~~49~~

0	1	**2**	**3**	~~4~~	**5**	~~6~~	**7**	~~8~~	~~9~~	~~10~~	**11**	~~12~~	**13**	~~14~~	~~15~~	~~16~~	**17**	~~18~~	**19**	~~20~~	~~21~~	~~22~~	**23**	~~24~~
~~25~~	~~26~~	~~27~~	~~28~~	**29**	~~30~~	**31**	~~32~~	~~33~~	~~34~~	~~35~~	~~36~~	**37**	~~38~~	~~39~~	~~40~~	**41**	~~42~~	**43**	~~44~~	~~45~~	~~46~~	**47**	~~48~~	~~49~~

Axes

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$

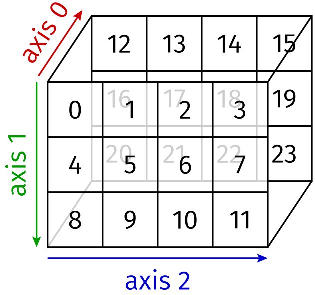
$$\begin{array}{cc} & \xrightarrow{\text{axis 1}} \\ \text{axis 0} \downarrow & \begin{pmatrix} \text{a[0, 0]} & \text{a[0, 1]} & \text{a[0, 2]} \\ \text{a[1, 0]} & \text{a[1, 1]} & \text{a[1, 2]} \\ \text{a[2, 0]} & \text{a[2, 1]} & \text{a[2, 2]} \end{pmatrix} \end{array}$$

Your turn

np.sum(a)

np.sum(a, axis=…)

Axes in more than two dimensions




```
array([[[ 0,  1,  2,  3],
        [ 4,  5,  6,  7],
        [ 8,  9, 10, 11]],

       [[12, 13, 14, 15],
        [16, 17, 18, 19],
        [20, 21, 22, 23]]])
```

create this array and produce 2d arrays by cutting perpendicular to the axes 0, 1, and 2

Matrix multiplication

$$\begin{pmatrix} 0 & 1 \\ 2 & 3 \end{pmatrix}\begin{pmatrix} 4 & 5 \\ 6 & 7 \end{pmatrix} = \begin{pmatrix} \boxed{6} & 7 \\ 26 & 31 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 \\ 2 & 3 \end{pmatrix}\begin{pmatrix} 4 & 5 \\ 6 & 7 \end{pmatrix} = \begin{pmatrix} 6 & \boxed{7} \\ 26 & 31 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 \\ 2 & 3 \end{pmatrix}\begin{pmatrix} 4 & 5 \\ 6 & 7 \end{pmatrix} = \begin{pmatrix} 6 & 7 \\ \boxed{26} & 31 \end{pmatrix}$$

$$\begin{pmatrix} 0 & 1 \\ 2 & 3 \end{pmatrix}\begin{pmatrix} 4 & 5 \\ 6 & 7 \end{pmatrix} = \begin{pmatrix} 6 & 7 \\ 26 & \boxed{31} \end{pmatrix}$$

Your turn

try `np.dot(•, •)`
`•.dot(•)`
`• @ •` *)

*) Python≥3.5, NumPy≥1.10

Mathematical functions in NumPy

Universal functions (ufuncs) take ndarrays as argument

Trigonometric functions

sin, cos, tan, arcsin, arccos, arctan, hypot, arctan2, degrees, radians, unwrap, deg2rad, rad2deg

Hyperbolic functions

sinh, cosh, tanh, arcsinh, arccosh, arctanh

Rounding

around, round_, rint, fix, floor, ceil, trunc

Sums, products, differences

prod, sum, nansum, cumprod, cumsum, diff, ediff1d, gradient, cross, trapz

Exponents and logarithms

exp, expm1, exp2, log, log10, log2, log1p, logaddexp, logaddexp2

Other special functions

i0, sinc

Floating point routines

signbit, copysign, frexp, ldexp

Arithmetic operations

add, reciprocal, negative, multiply, divide, power, subtract, true_divide, floor_divide, fmod, mod, modf, remainder

Handling complex numbers

angle, real, imag, conj

Miscellaneous

convolve, clip, sqrt, square, absolute, fabs, sign, maximum, minimum, fmax, fmin, nan_to_num, real_if_close, interp

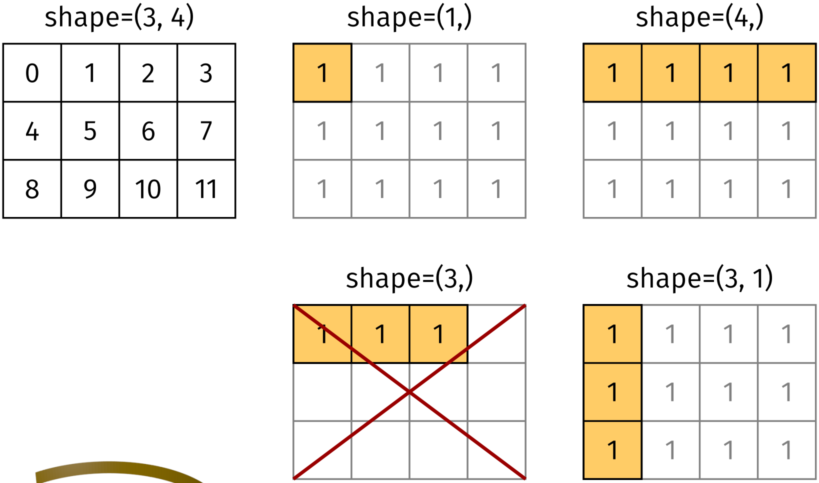
Many more special functions are provided as ufuncs by SciPy

Rules for broadcasting

Arrays can be broadcast to the same shape if one of the following points is fulfilled:

1. The arrays all have exactly the same shape.
2. The arrays all have the same number of dimensions and the length of each dimension is either a common length or 1.
3. The arrays that have too few dimensions can have their shapes prepended with a dimension of length 1 to satisfy property 2.

Broadcasting

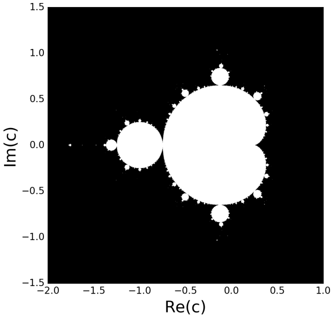


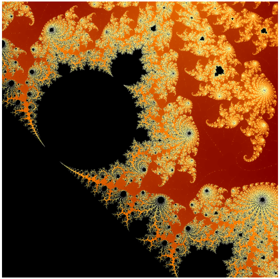
Your turn

Application: Mandelbrot set

$$z_{n+1} = z_n^2 + c, \quad z_0 = 0$$

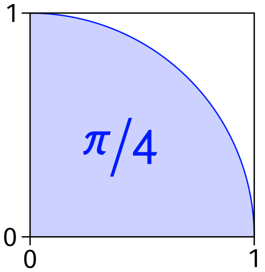
Mandelbrot set contains the points for which z remains bounded.





Your turn

Application: π from random numbers

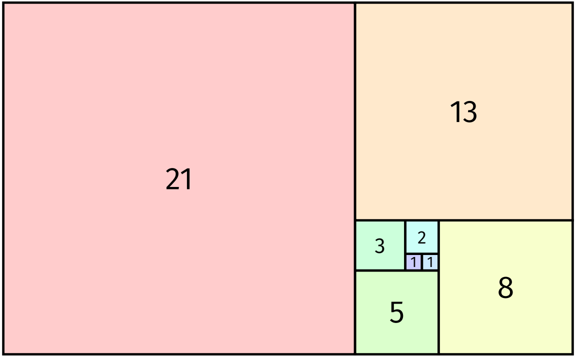


1. Create pairs of random numbers and determine the fraction of pairs which has a distance from the origin less than one.
2. Multiply the result by four to obtain an approximation of π.

hint: `count_nonzero(a)` counts the number of non-zero values in the array a and also works for Boolean arrays. Remember that `np.info(...)` can be helpful.

Your turn

Fibonacci series and linear algebra



Fibonacci series:

1, 1, 2, 3, 5, 8, 13, 21, ...

$$F_{n+1} = F_n + F_{n-1}, \quad F_1 = F_2 = 1$$

$$\text{or}: \quad \begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} F_n \\ F_{n-1} \end{pmatrix} = \begin{pmatrix} F_{n+1} \\ F_n \end{pmatrix}$$

What is the limit of F_{n+1}/F_n for large n?

Eigenvalue problems

$$\begin{pmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nn} \end{pmatrix} \begin{pmatrix} v_1^{(k)} \\ \vdots \\ v_n^{(k)} \end{pmatrix} = \lambda^{(k)} \begin{pmatrix} v_1^{(k)} \\ \vdots \\ v_n^{(k)} \end{pmatrix} \qquad k = 1, \ldots, n$$

eigenvalue $\lambda^{(k)}$ eigenvector $\begin{pmatrix} v_1^{(k)} \\ \vdots \\ v_n^{(k)} \end{pmatrix}$

for our Fibonacci problem:

$$\begin{pmatrix} 1 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} F_n \\ F_{n-1} \end{pmatrix} = \lambda \begin{pmatrix} F_{n+1} \\ F_n \end{pmatrix}$$

We are looking for the eigenvalue larger than one.

Linear algebra in NumPy

```
import numpy.linalg as LA
```

Matrix and vector products

dot, vdot, inner, outer, matmul, tensordot, einsum, LA.matrix_power, kron

Decompositions

LA.cholesky, LA.qr, LA.svd

Matrix eigenvalues

LA.eig, LA.eigh, LA.eigvals, LA.eigvalsh

Norms and other numbers

LA.norm, LA.cond, LA.det, LA.matrix_rank, LA.slogdet, trace

Solving equations and inverting matrices

LA.solve, LA.tensorsolve, LA.lstsq, LA.inv, LA.pinv, LA.tensorinv

hint: see also the methods for linear algebra in SciPy

Statistics in NumPy

Order statistics

amin, amax, nanmin, nanmax, ptp, percentile, nanpercentile

Averages and variances

median, average, mean, std, var, nanmedian, nanmean, nanstd, nanvar

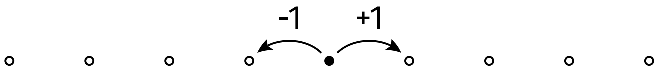
Correlating

corrcoef, correlate, cov

Histograms

histogram, histogram2d, histogramdd, bincount, digitize

Application: Brownian motion



1. Simulate several trajectories for a one-dimensional Brownian motion
   hint: `np.random.choice`
2. Plot the mean distance from the origin as a function of time
3. Plot the variance of the trajectories as a function of time

Sorting, searching, and counting in NumPy

Sorting

sort, lexsort, argsort, ndarray.sort, msort, sort_complex, partition, argpartition

Searching

argmax, nanargmax, argmin, nanargmin, argwhere, nonzero, flatnonzero, where, searchsorted, extract

Counting

count_nonzero

Application: identify entry closest to 1/2

$$\begin{pmatrix} 0.05344164 & 0.37648768 & 0.80691163 & 0.71400815 \\ 0.60825034 & 0.35778938 & 0.37393356 & 0.32615374 \\ 0.83118547 & 0.33178711 & 0.21548027 & 0.42209291 \end{pmatrix}$$

$$\Downarrow$$

$$\begin{pmatrix} 0.37648768 \\ 0.60825034 \\ 0.42209291 \end{pmatrix}$$

hint: use `np.argsort`

Polynomials in NumPy

Power series: `numpy.polynomial.polynomial`

Polynomial Class

Polynomial

Basics

polyval, polyval2d, polyval3d, polygrid2d, polygrid3d, polyroots, polyfromroots

Fitting

polyfit, polyvander, polyvander2d, polyvander3d

Calculus

polyder, polyint

Algebra

polyadd, polysub, polymul, polymulx, polydiv, polypow

Miscellaneous

polycompanion, polydomain, polyzero, polyone, polyx, polytrim, polyline

also: Chebyshev, Legendre, Laguerre, Hermite polynomials

Some examples

```
P.Polynomial([24, -50, 35, -10, 1])
```

$$p_4(x) = x^4 - 10x^3 + 35x^2 - 50x + 24 = (x-1)(x-2)(x-3)(x-4)$$

```
p4.deriv()
```

$$\frac{\mathrm{d}p_4(x)}{\mathrm{d}x} = 4x^3 - 30x^2 + 70x - 50$$

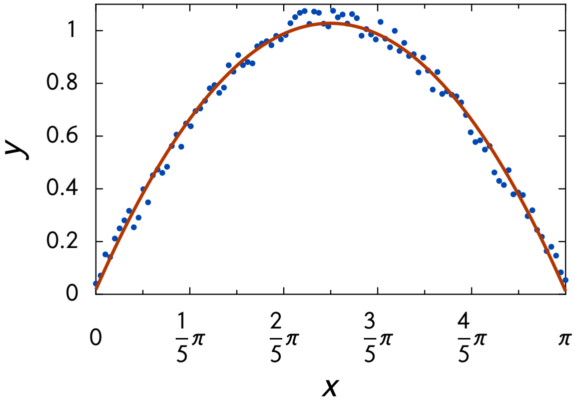
```
p4.integ()
```

$$\int p_4(x)\mathrm{d}x = \frac{1}{5}x^5 - \frac{5}{2}x^4 + \frac{35}{3}x^3 - 25x^2 + 24x + C$$

```
p4.polydiv()
```

$$\frac{p_4(x)}{2x+1} = \frac{1}{2}x^3 - \frac{21}{4}x^2 + \frac{161}{8}x - \frac{561}{16} + \frac{945}{16p_4(x)}$$

Application: polynomial fit



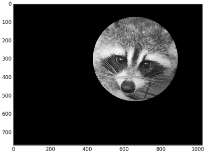
Your turn

add some noise to a function and fit it to a polynomial

see `scipy.optimize.curve_fit` for general fit functions

Application: image manipulation

```python
from scipy import misc
face = misc.face(gray=True)
```



Your turn