# Computational linear algebra and systems of linear equations

(matrices)

What computational linear algebra is for ←

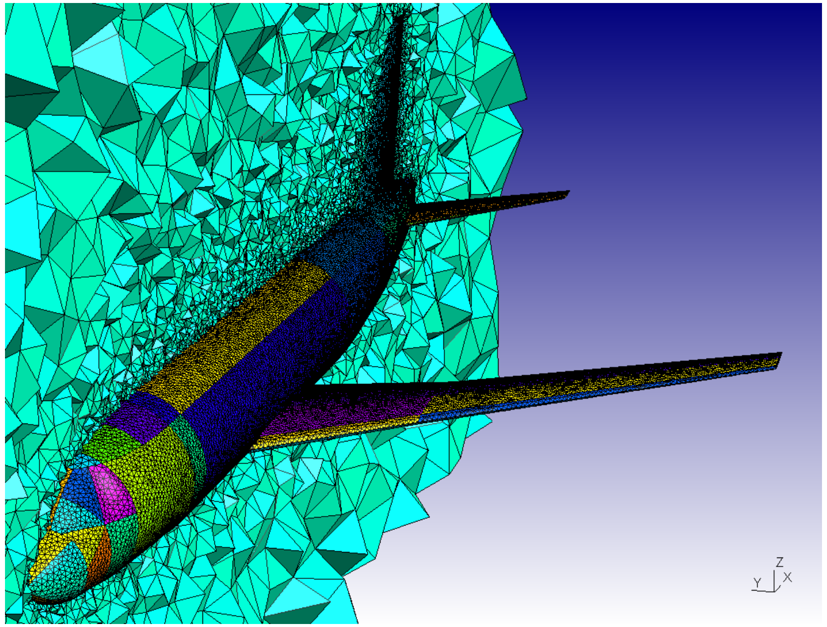
What we do in this section (and what we don't)

Linear algebra in python ←

Solution to the eigenvalue problem

- Finding the largest eigenvalue (basic power method)
- Finding the smallest eigenvalue (inverse power method)
- Finding the complete set of eigenvalues (QR iteration)

Almost all models of physical systems can be expressed as a set of simultaneous equations.



To solve these types of problems we need to numerically solve these (typically very large) matrix equations.

$$\begin{bmatrix} f_{x1} \\ f_{y1} \\ f_{x2} \\ f_{y2} \\ f_{x3} \\ f_{y3} \end{bmatrix} = \begin{bmatrix} k_{x1x1} & k_{x1y1} & k_{x1x2} & k_{x1y2} & k_{x1x3} & k_{x1y3} \\ k_{y1x1} & k_{y1y1} & k_{y1x2} & k_{y1y2} & k_{y1x3} & k_{y1y3} \\ k_{x2x1} & k_{x2y1} & k_{x2x2} & k_{x2y2} & k_{x2x3} & k_{x2y3} \\ k_{y2x1} & k_{y2y1} & k_{y2x2} & k_{y2y2} & k_{y2x3} & k_{y2y3} \\ k_{x3x1} & k_{x3y1} & k_{x3x2} & k_{x3y2} & k_{x3x3} & k_{x3y3} \\ k_{y3x1} & k_{y3y1} & k_{y3x2} & k_{y3y2} & k_{y3x3} & k_{y3y3} \end{bmatrix} \begin{bmatrix} u_{x1} \\ u_{y1} \\ u_{x2} \\ u_{y2} \\ u_{x3} \\ u_{y3} \end{bmatrix}$$

$$\mathbf{f} = \mathbf{K}\mathbf{u}$$

Forces acting at each point (known)

Stiffness matrix (known)

Displacement of each point (unknown)

$$u = K^{-1} f$$

$$KK^{-1} = I.$$

What we will not cover here:

The “under the hood” methods of basic matrix manipulation, including:

- Numerical matrix multiplication
- Gaussian elimination
- Simple matrix inversion
- Matrix decomposition

What we will focus on instead:

Using in-built Python routines to do all the “basic stuff” above

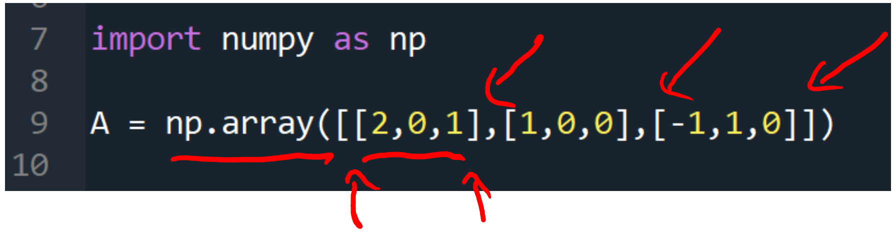
An intro to the more advanced stuff

- the eigenvalue problem
- manipulating sparse matrices

# Matrices in python

The basic form that python uses to store matrices is the numpy array.

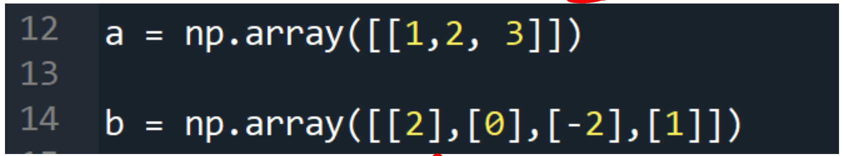
We use *nested square brackets* to define the columns and rows, with commas separating the elements:



```python
import numpy as np

A = np.array([[2,0,1],[1,0,0],[-1,1,0]])
```

$$A = \begin{bmatrix} 2 & 0 & 1 \\ 1 & 0 & 0 \\ -1 & 1 & 0 \end{bmatrix}$$

To define a column vectors and row vectors we need to remember to Keep the nested brackets, e.g.

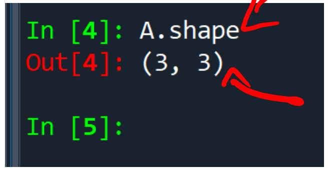


```python
a = np.array([[1,2, 3]])

b = np.array([[2],[0],[-2],[1]])
```

$$\begin{bmatrix} 1 & 2 & 3 \end{bmatrix}$$

$$\begin{bmatrix} 2 \\ 0 \\ -2 \\ 1 \end{bmatrix}$$

The shape attribute returns how many columns and rows the matrix has.



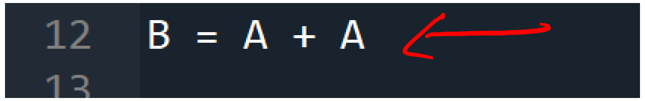
```
In [4]: A.shape
Out[4]: (3, 3)

In [5]:
```

b. shape

(4, 1).

Basic matrix manipulations are built-in to ~~numpy~~ Python:

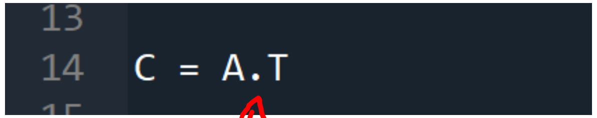
Addition/subraction:



```
B = A + A
```

C = $A^T$

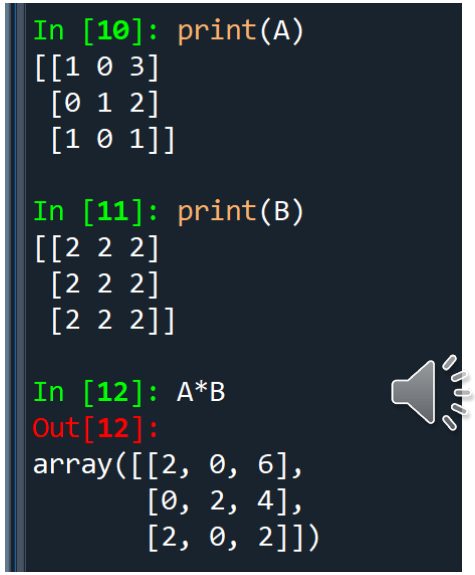
Matrix transpose uses the ".T" attribute:



```
C = A.T
```

(This means don't name a matrix "T" – python will not get confused, but you might)

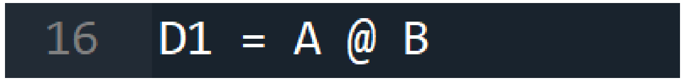
Note that A*B is not matrix multiplication – it just multiplies the two matrices element by element.



```
In [10]: print(A)
[[1 0 3]
 [0 1 2]
 [1 0 1]]

In [11]: print(B)
[[2 2 2]
 [2 2 2]
 [2 2 2]]

In [12]: A*B
Out[12]:
array([[2, 0, 6],
       [0, 2, 4],
       [2, 0, 2]])
```

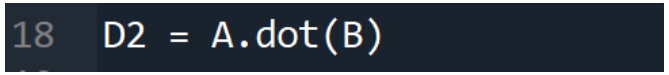
Matrix multiplication can be done in a few ways:

1. using the @ notation



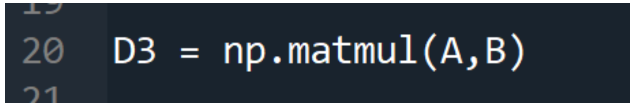
```
D1 = A @ B
```

2. Using the “dot” attribute



```
D2 = A.dot(B)
```

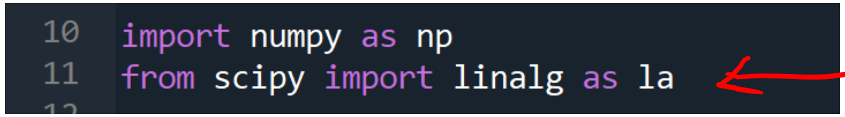
3. Using the inbuilt numpy matmul function



```
D3 = np.matmul(A,B)
```

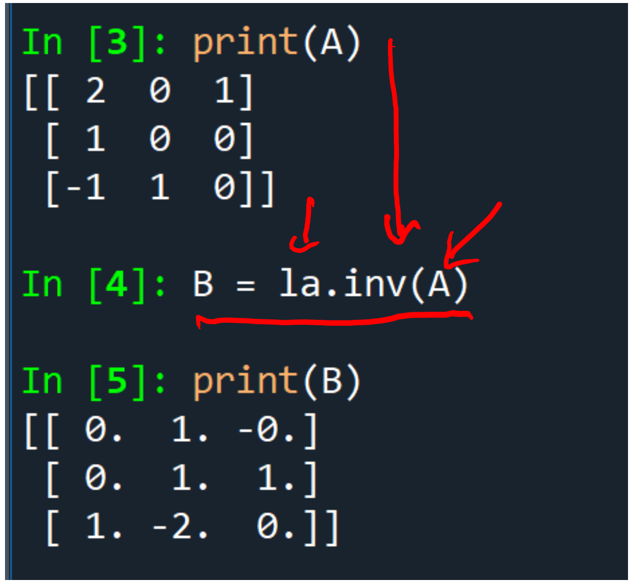
All these ways are equivalent.

For more complex matrix operations we use the linalg package from the scipy module:



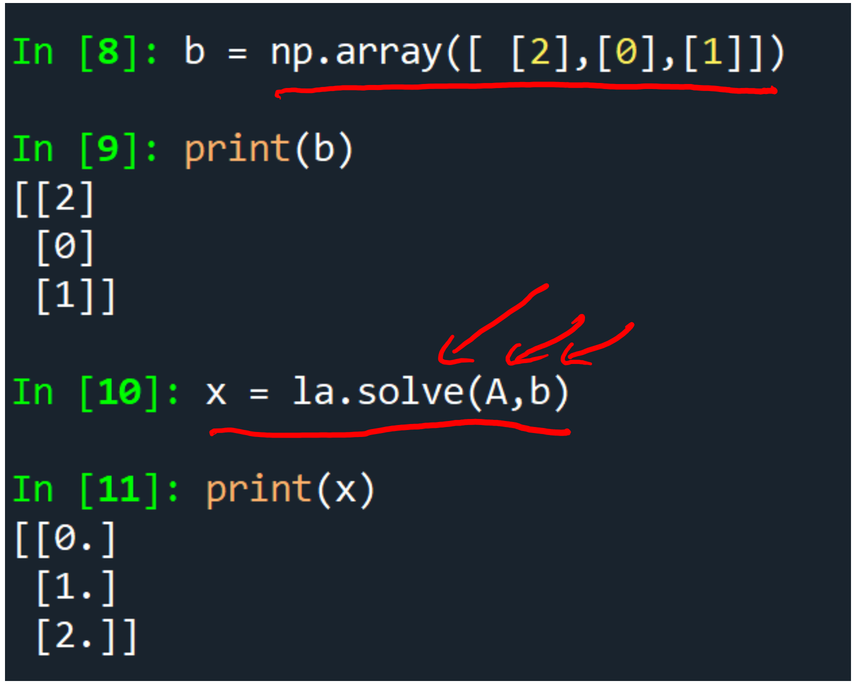
```
import numpy as np
from scipy import linalg as la
```

Using this we can do matrix inversion:



```
In [3]: print(A)
[[ 2  0  1]
 [ 1  0  0]
 [-1  1  0]]

In [4]: B = la.inv(A)

In [5]: print(B)
[[ 0.  1. -0.]
 [ 0.  1.  1.]
 [ 1. -2.  0.]]
```

And solve linear systems directly:



```
In [8]: b = np.array([ [2],[0],[1]])

In [9]: print(b)
[[2]
 [0]
 [1]]

In [10]: x = la.solve(A,b)

In [11]: print(x)
[[0.]
 [1.]
 [2.]]
```

$Ax = b$

find

$x = A^{-1}b$

An important quantity in linear algebra is the *matrix norm*, which expresses the “aggregate size” of the elements in a matrix.

For a matrix A with elements $A_{i,j}$, the $L_p$ norm of A is defined by

$$\boxed{||A||_p = \sqrt[p]{\sum_i \sum_j |A_{i,j}|^p}}$$

pth root

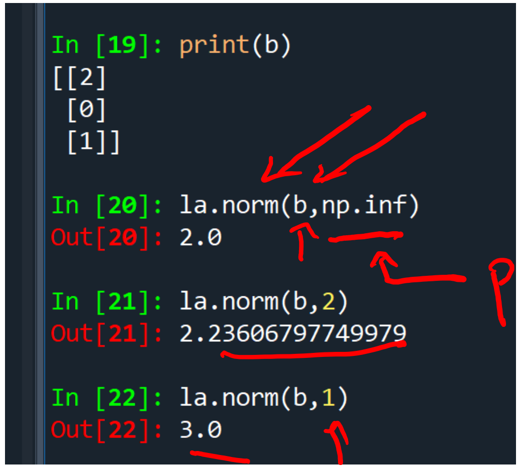
pth power

- The $L_1$ norm (known as the “manhattan distance”) is the sum of the absolute values in the matrix

- The $L_2$ norm (the “Euclidean norm) is the square root of the sum of the squares of all the elements

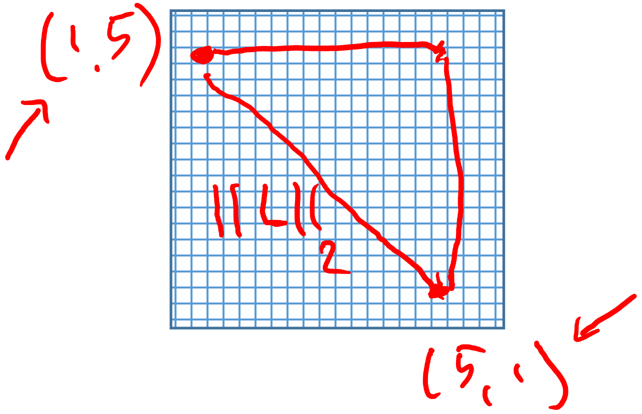
- The $L_\infty$ norm is equal to the *largest value* in the matrix.

In python, norms can be computed using the scipy linalg package:



```
In [19]: print(b)
[[2]
 [0]
 [1]]

In [20]: la.norm(b,np.inf)
Out[20]: 2.0

In [21]: la.norm(b,2)
Out[21]: 2.23606797749979

In [22]: la.norm(b,1)
Out[22]: 3.0
```

p = ∞

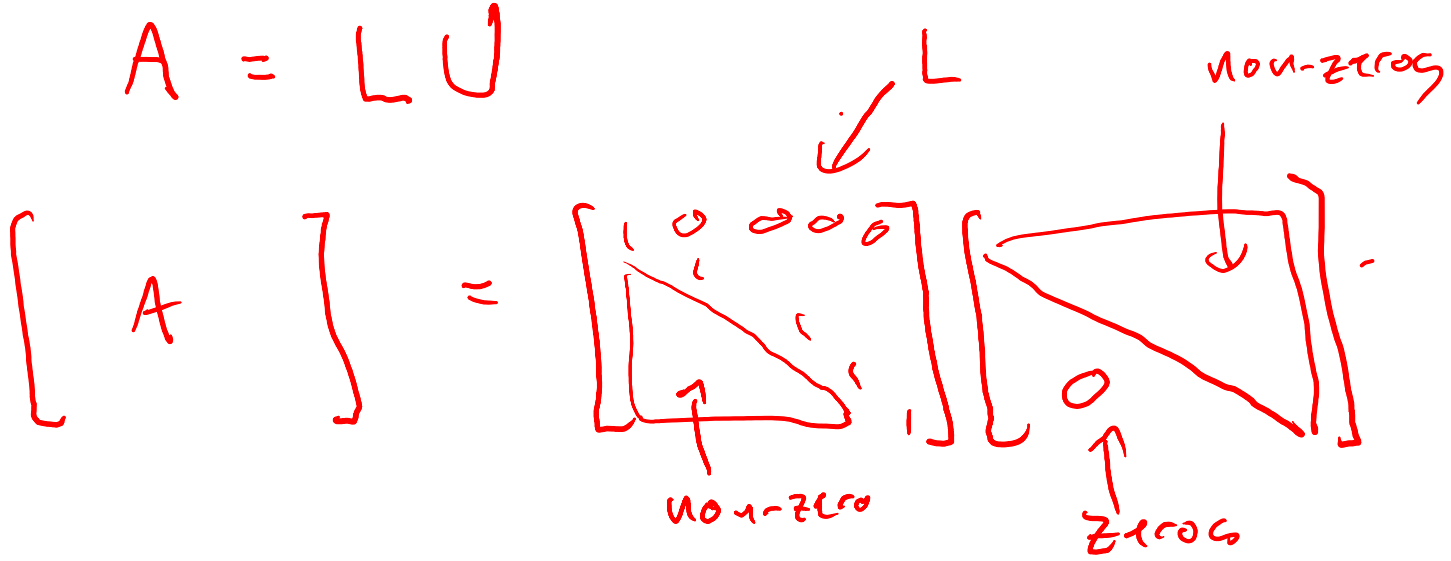


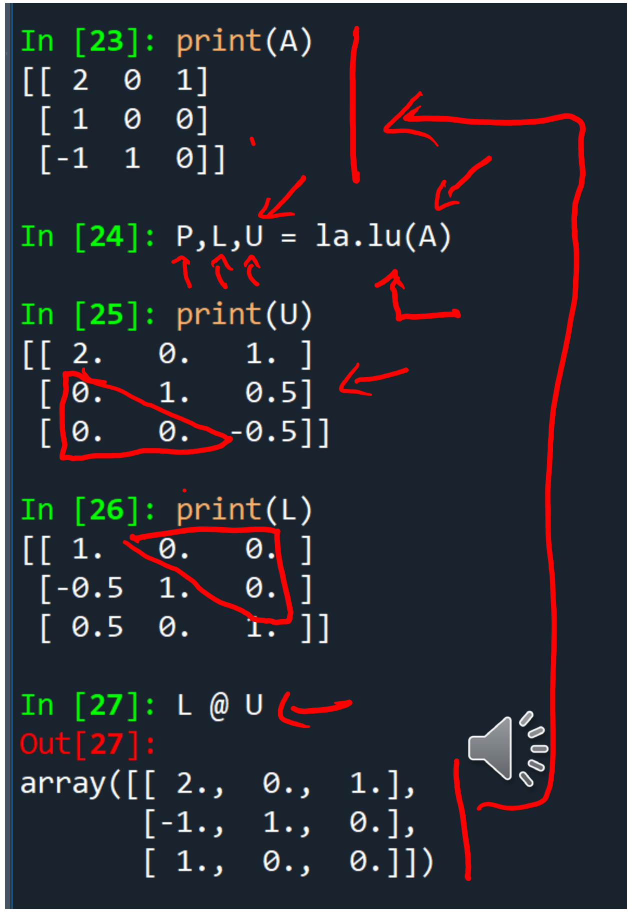
# Matrix decompositions

An important aspect in most computational linear algebra is being able
To decompose a matrix in terms of other, simpler matrices.

The LU decomposition expresses a matrix as the product of two simpler matrices:

$$A = LU$$

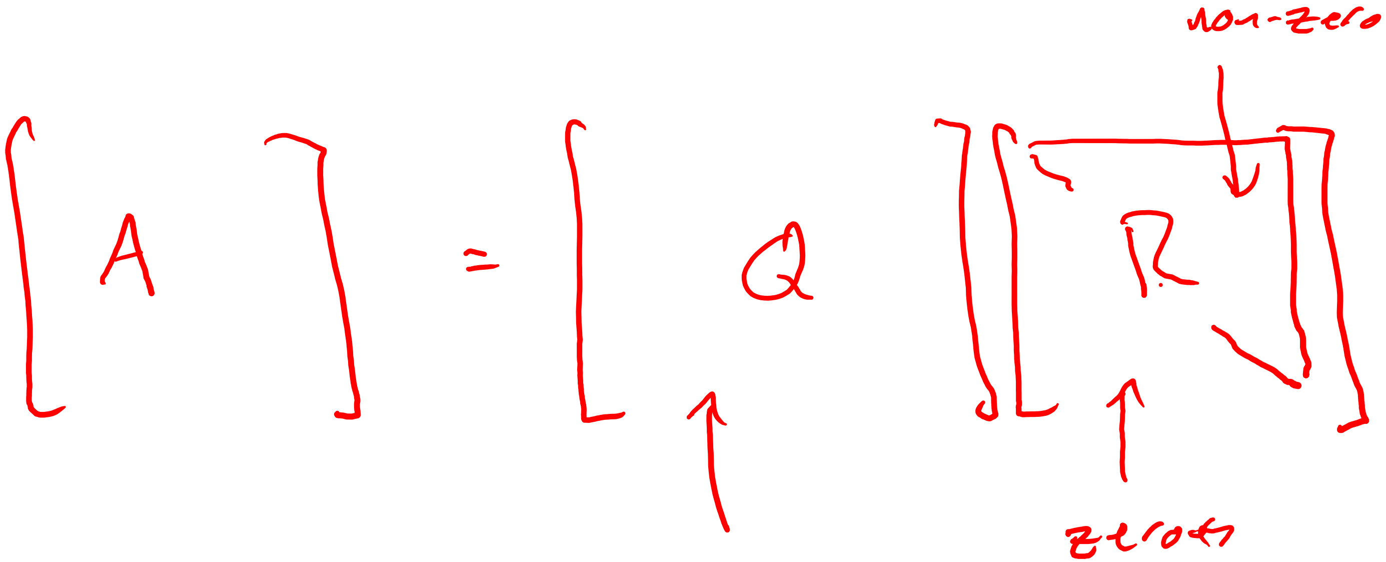




```
In [23]: print(A)
[[ 2  0  1]
 [ 1  0  0]
 [-1  1  0]]

In [24]: P,L,U = la.lu(A)

In [25]: print(U)
[[ 2.   0.   1. ]
 [ 0.   1.   0.5]
 [ 0.   0.  -0.5]]

In [26]: print(L)
[[ 1.   0.   0. ]
 [-0.5  1.   0. ]
 [ 0.5  0.   1. ]]

In [27]: L @ U
Out[27]:
array([[ 2.,  0.,  1.],
       [-1.,  1.,  0.],
       [ 1.,  0.,  0.]])
```

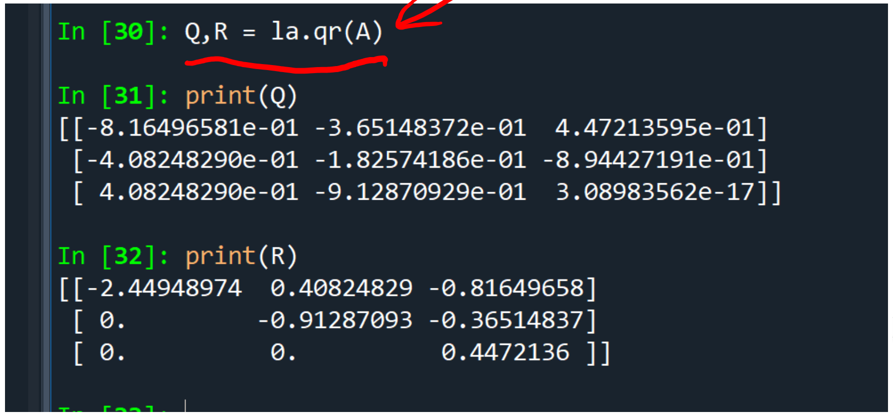
We will outsource the decompositions to the scipy linalg package:

The QR decomposition decomposes a matrix into an *orthogonal matrix* Q and a right-upper-triangular matrix R:



Aside: an orthogonal matrix Q is one for which the Inverse is equal to its own transpose:

$$Q^{-1} = Q^T$$



```
In [30]: Q,R = la.qr(A)

In [31]: print(Q)
[[-8.16496581e-01 -3.65148372e-01  4.47213595e-01]
 [-4.08248290e-01 -1.82574186e-01 -8.94427191e-01]
 [ 4.08248290e-01 -9.12870929e-01  3.08983562e-17]]

In [32]: print(R)
[[-2.44948974  0.40824829 -0.81649658]
 [ 0.         -0.91287093 -0.36514837]
 [ 0.          0.          0.4472136 ]]

In [33]:
```

## Computational expense for basic matrix manipulations

The time taken for a matrix operation (inversion, decomposition, etc) can be characterised by the *computational complexity,* which is related to the size of the matrix.

Here we give the complexity for each of the major operations, for a *dense, unstructured matrix:*

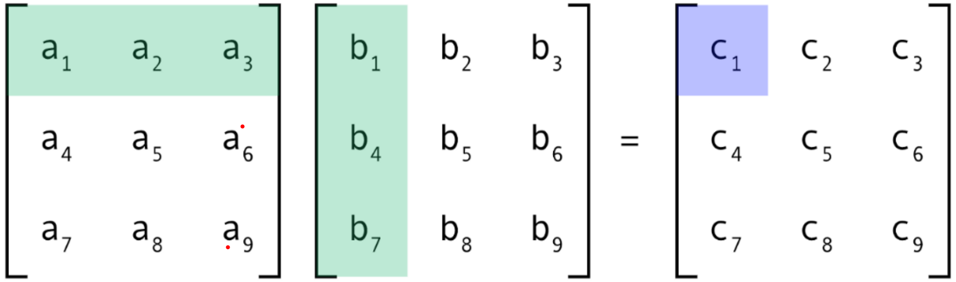
Addition/subtraction of two $n \times m$ matrices $\sim O(nm)$

Multiplication of a $p \times m$ by a $m \times n$ matrix $\sim O(pmn)$

Inversion of an $n \times n$ matrix: $\sim O(n^3)$

LU decomposition of an $n \times n$ matrix: $\sim O(n^3)$

QR decomposition of an $n \times n$ matrix: $\sim O(n^3)$ -



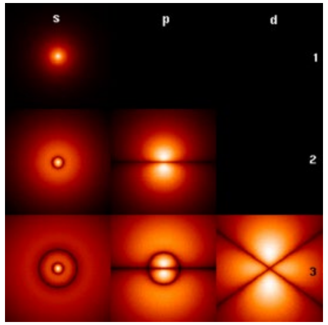
$$\begin{bmatrix} a_1 & a_2 & a_3 \\ a_4 & a_5 & a_6 \\ a_7 & a_8 & a_9 \end{bmatrix} \begin{bmatrix} b_1 & b_2 & b_3 \\ b_4 & b_5 & b_6 \\ b_7 & b_8 & b_9 \end{bmatrix} = \begin{bmatrix} c_1 & c_2 & c_3 \\ c_4 & c_5 & c_6 \\ c_7 & c_8 & c_9 \end{bmatrix}$$

# The eigenvalue problem

This is one of the major computational problems in linear algebra.

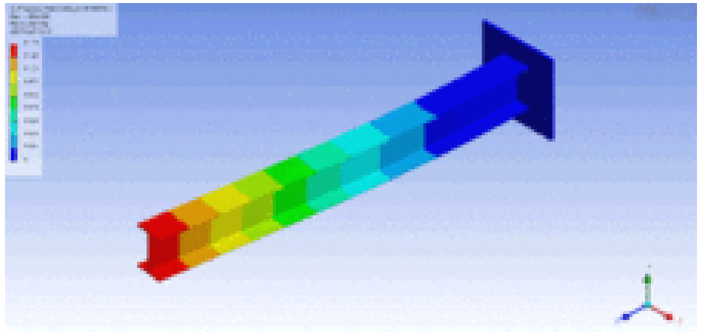
Let **A** be a (square) n x n matrix. A nonzero vector **v** is an *eigenvector* of **A** if,
Recall: For some scalar $\lambda$ , **v** satisfies

$$\boxed{\mathbf{A}\mathbf{v} = \lambda\mathbf{v}}$$



The scalar number $\lambda$ (which may be zero) is called an *eigenvalue of **A**, associated with **v**.*

The set of all eigenvalues of **A** is called the *spectrum* of **A**.

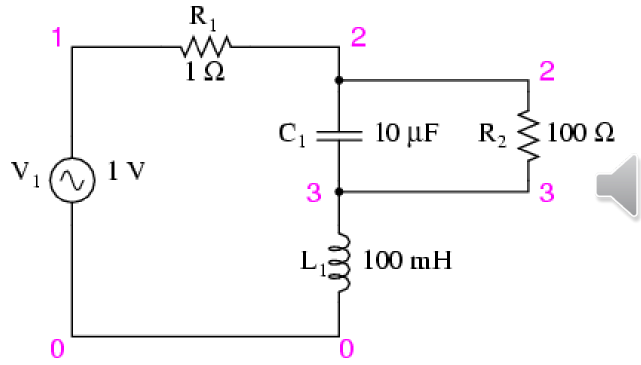


Eigenvalues and Eigenvectors are extremely widely used in all branches of engineering and the physical sciences

Eigenvalue ⟷ Frequency

Eigenvector ⟷ Mode of vibration

*Series LC with resistance in parallel with C*

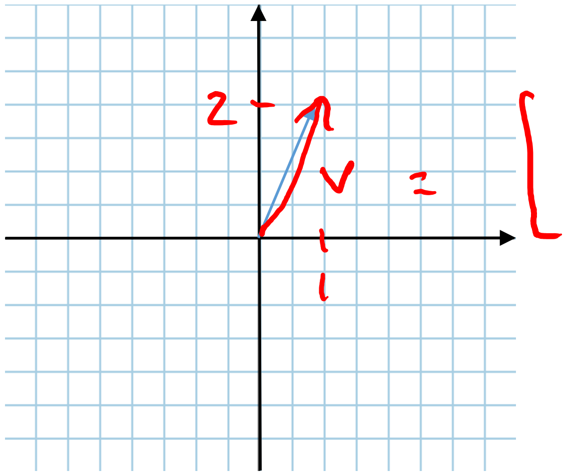


A matrix can be thought of as a *linear transformation of a vector*

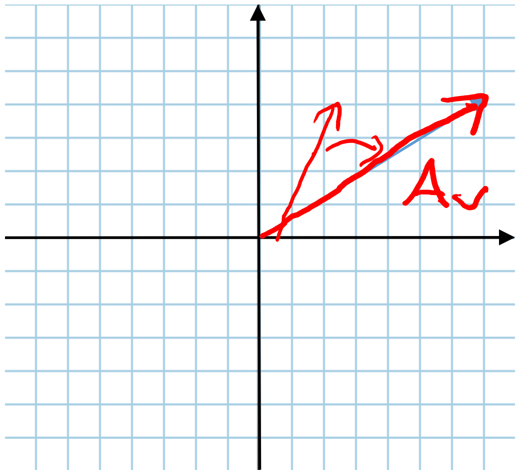
$$\mathrm{u} = Av$$

$$= \begin{bmatrix}3 & 0\\0 & 1\end{bmatrix}\begin{bmatrix}1\\2\end{bmatrix}$$

$$= \begin{bmatrix}3\\2\end{bmatrix}$$

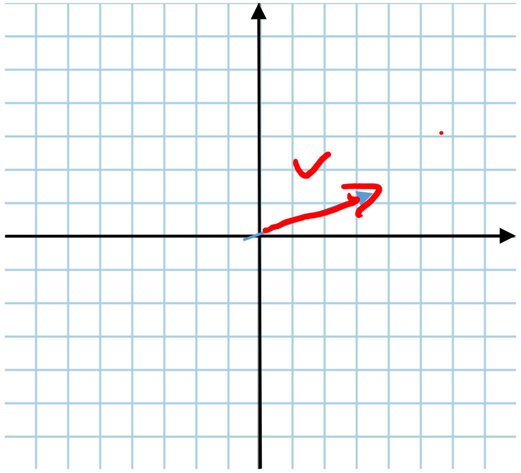


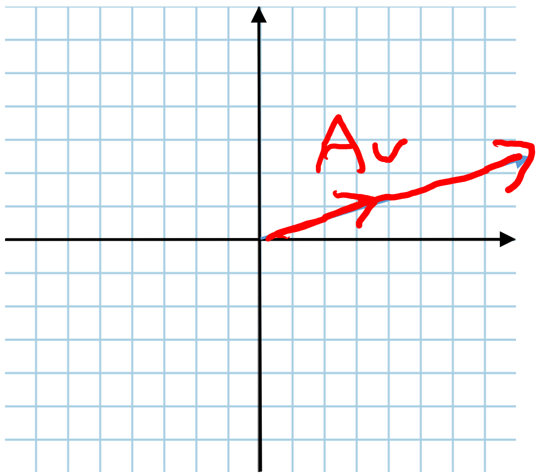
$$= \begin{bmatrix}1\\2\end{bmatrix}$$



Sometimes a linear transformation changes the magnitude of a vector without affecting its “direction”. Such a vector is called an *eigenvector* of the matrix.

$$\mathbf{Av} = \lambda\mathbf{v}$$





For large matrices there will be a lot of eigenvalues, and their computation can be difficult.

$$\underline{\mathbf{Av} = \lambda \mathbf{v}}$$

$$A\underset{\sim}{v} - \lambda \underset{\sim}{v} = 0$$

$$(A - \lambda I)\underset{\sim}{v} = 0$$

$$\Rightarrow \det(\underline{A - \lambda I}) = 0 \Rightarrow \overset{\swarrow}{a_3}\lambda^3 + \overset{\swarrow}{a_2}\lambda^2 + \overset{\swarrow}{a_1}\lambda + \overset{\swarrow}{a_0} = 0.$$

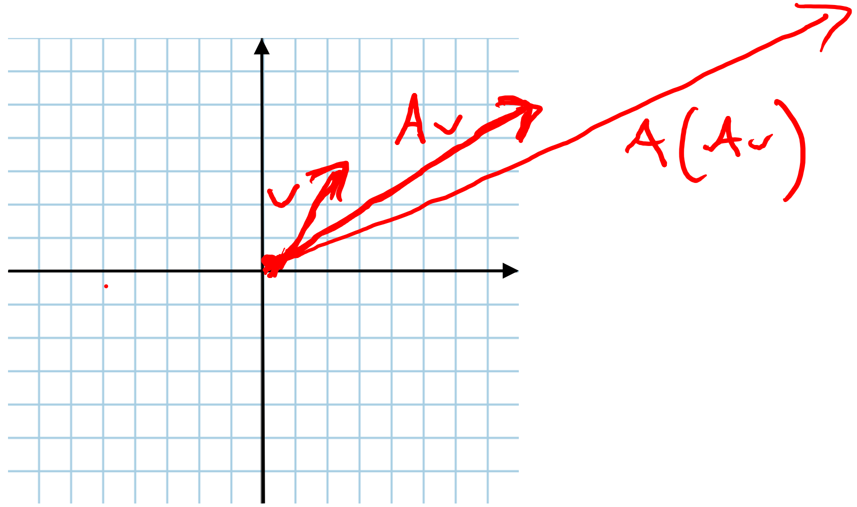
Often we are interested only in the largest eigenvalue, or the smallest eigenvalue.

In this situation *Iterative Power methods* can be used.

# The Basic Power Method

This algorithm computes the largest eigenvalue and eigenvector of a matrix.

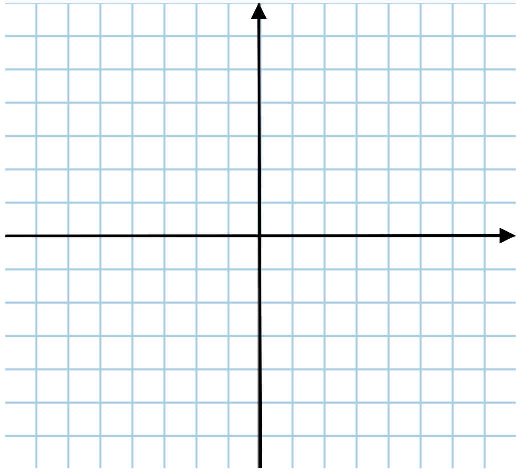
The idea: each transformation by a matrix A *stretches the vector in the* direction of the largest eigenvector* $\mathrm{v}_{\max}$ *of* A.



If we keep on applying A to *any* vector, then eventually this vector will point in the direction of v.

## Basic Power Iteration

1. Start with a vector $\mathrm{v}_k$ (preferably randomized)
2. Apply $\mathrm{u} = \mathrm{A}\mathrm{v}_k$
3. Compute $\mathrm{v}_{k+1} = \dfrac{\mathrm{u}}{\mu_k}$ , where $\mu_k = ||u||_\infty$
4. Repeat from step 2 until converged.



The quantity $\mu_k$ converges to the largest eigenvalue, with eigenvector $v_k$.

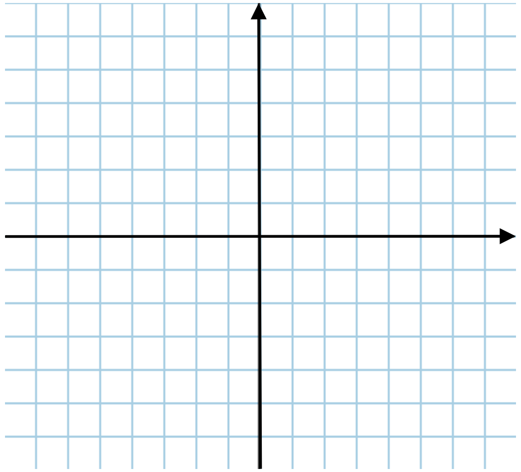
*vector with the largest eigenvalue

## The inverse power method

The idea: the eigenvalues of $A^{-1}$ are the reciprocals of the eigenvalues of A.
We can therefore find the *smallest* eigenvalue of A:

### Inverse Power Iteration

1. Start with a vector $v_k$ (preferably randomized)
2. Apply $u = A^{-1} v_k$
3. Compute $v_{k+1} = \dfrac{u}{\mu_k}$, where $\mu_k = ||u||_\infty$
4. Repeat from step 2 until converged.



The quantity $1/\mu_k$ converges to the smallest eigenvalue of A, with eigenvector $v_k$.

## The QR algorithm

This gives the complete set of eigenvalues of A. The only problem is that it is a bit slow to converge, and is computationally expensive if the matrix is large.

### QR Iteration

1. Form the QR decomposition

$$Q_k R_k = A_k$$

2. Create a new matrix

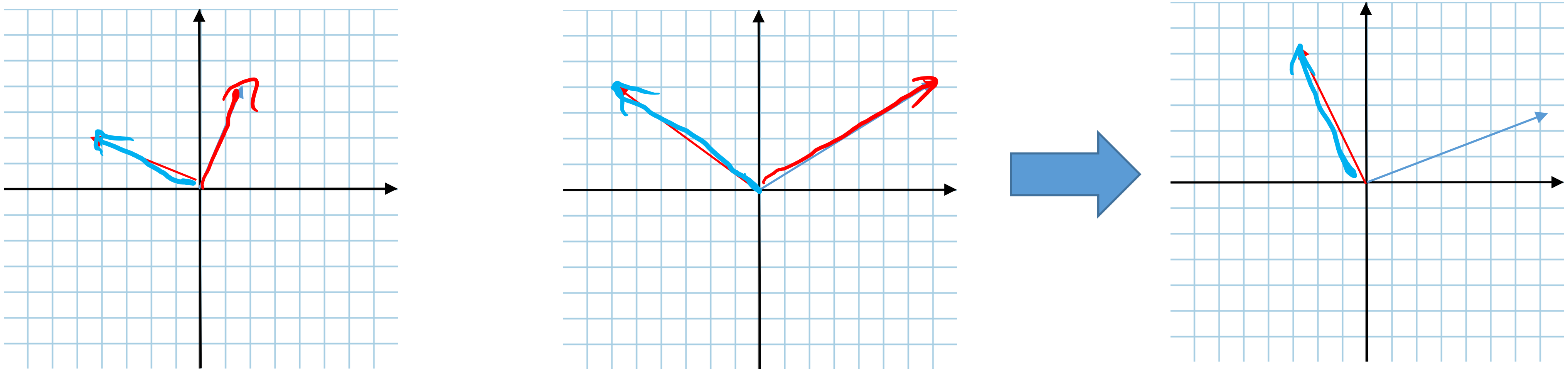
$$A_{k+1} = R_k Q_k$$

3. Repeat from Step 1 until converged.

The eigenvalues are given by the diagonal components of $A_k$.

$$\begin{tikzcd}
\left( \quad A_k \quad \right) \arrow[d] \\
\left( \quad Q_k \quad \right)\left( \quad R_k \quad \right) \arrow[d] \\
A_{k+1} = \left( \quad R_k \quad \right)\left( \quad Q_k \quad \right)
\end{tikzcd}$$

Why does this work? The QR decomposition does a power iteration, but for a set of orthogonal transformations simultaneously



**Other important approaches:**

- Shifted Power method

  - modification of the power method to find the complete spectrum

- The Rayleigh Quotient method

  - A fast iteration method for finding the largest eigenvalue

- The Shifted QR method

  - The convergence of the QR method depends on the ratios between eigenvalues being large. Introducing a “shift” to the eigenvalues improves the convergence

- Arnoldi iteration

  - Combines power iteration with Gram-Schmidt orthogonalisation to compute the full spectrum (very fast for Sparse matrices)