

## LINEAR ALGEBRA: ARRAY INVERSE

- i) Could do it with cofactors and determinant but it's slow.
- ii) Solve a linear system instead:

$$AX = \mathbb{1} \Rightarrow X = A^{-1}$$

Use the methods we saw already, to solve  $n$  linear systems, where  $n$  is the number of columns in  $X$ .  
Implemented in numpy.linalg as  $X = \text{inv}(A)$ .

~~EIGEN~~

## EIGENVALUES AND EIGENVECTORS

- i) For symmetric  $A$ :

$$A\vec{v} = \lambda \vec{v} \rightarrow \text{eigenvector}$$

$\downarrow$   
eigenvalue

If  $A$  is  $N \times N$ , then we have  $N$  eigenvalues and  $N$  eigenvectors. Eigenvectors are orthogonal:

$$\vec{v}_i \cdot \vec{v}_j = 0$$

We also normalize them:  $\vec{v}_i \cdot \vec{v}_i = \|\vec{v}_i\|^2 = 1$

- ii) Consider all the eigenvectors and put them into an array  $V$

$$V \equiv \begin{pmatrix} \vdots & \vdots & \dots & \vdots \\ \vec{v}_1 & \vec{v}_2 & \dots & \vec{v}_N \\ \vdots & \vdots & \dots & \vdots \end{pmatrix}$$

Note that  $V$  is by definition an orthogonal matrix:

$$\rightarrow V^T V = I$$

Now if we also build the diagonal array of eigenvalues  $D \equiv \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_N \end{pmatrix}$ , we can simultaneously get write the eigenvalue equations for all  $N$  eigenvectors as:

$$\boxed{AV = VD}, \text{ or, equivalently, } \boxed{V^T A V = D}$$

We search for an efficient algorithm to compute  $V$  and  $D$ . This is based on the QR decomposition; write  $A$  as

$$A = QR \rightarrow \text{upper triangular.}$$

↓  
orthogonal

It is possible to show (done later) that this is possible for any  $A$ . In iii) we see how to use this decomposition recursively to get  $V$  and  $D$ .

iii) Assume we found  $\boxed{A = Q_1 R_1}$ . Now build:

$$1) \quad \boxed{A_1 = R_1 Q_1} \quad \left( \text{that is, "invert" the order of } Q_1 \text{ and } R_1 \right)$$

It is immediate to see that  $R_1 = Q_1^T A$  (because  $Q_1^T Q_1 = I$ )

Therefore:

$$A_1 = R_1 Q_1 = Q_1^T A Q_1$$

2) Now build the QR decomposition of  $A_1$ :  $\boxed{A_1 = Q_2 R_2}$

and swap again:  $\boxed{A_2 = R_2 Q_2}$

We see that:

$$R_2 = Q_2^T A_1 = Q_2^T Q_1^T A Q_1$$

Now replace  $R_2 = Q_2^T Q_1^T A Q_1$  in  $A_2 = R_2 Q_2$  to get

$$A_2 = Q_2^T Q_1^T A Q_1 Q_2$$

3) Go on recursively. At step  $k$  you build  $A_k = Q_k R_k$  and you know that

$$A_k = (Q_k^T Q_{k-1}^T \dots Q_1^T) A (Q_1 Q_2 \dots Q_k)$$

Then  $A_{k+1} = R_k Q_k$  and so on...

Note that the product of orthogonal matrices is also orthogonal. Therefore  $Q_1 \dots Q_k$  is an orthogonal matrix

4) It can be shown that, for  $k$  large enough,  $\prod_{i=1}^k Q_i$  converges to  $V$ , where  $V$  is the eigenvector matrix. Therefore:

$$\left\{ \begin{array}{l} \lim_{k \rightarrow \infty} \prod_{i=1}^k Q_i = V \\ \lim_{k \rightarrow \infty} \left( \prod_{i=1}^k Q_i^T \right) A \left( \prod_{i=1}^k Q_i \right) = \lim_{k \rightarrow \infty} A_k = V^T A V = D \end{array} \right.$$

The final algorithm to get  $V$  and  $D_k$ , for every  $A$ , is

a) Initialize  $V$  to  $I$

b) Decompose  $A = Q_1 R_1$

c) Swap to get  $A_1 = R_1 Q_1$

d) Set  $A_1 = V$  and compute  $D = V^T A V$ .

e) If  $D$  is diagonal (in the sense that off-diagonal elements are smaller than some  $\epsilon$ ), output  $D$  and ~~the~~  $V$ . Otherwise, go back to step b), finding the QR decomposition of  $A_1$ .

iv) The missing step is showing how to build a QR decomposition of a given array (symmetric)  $A$ .

Start by thinking of  $A$  as a sequence of  $N$  column vectors of length  $N$ :  $\rightarrow$



$$\rightarrow A = \begin{pmatrix} \vec{a}_0 & \vec{a}_1 & \vec{a}_2 & \dots & \vec{a}_N \\ \vdots & \vdots & \vdots & & \vdots \\ \vdots & \vdots & \vdots & & \vdots \end{pmatrix} \quad (A \text{ is a } N \times N \text{ symmetric array})$$

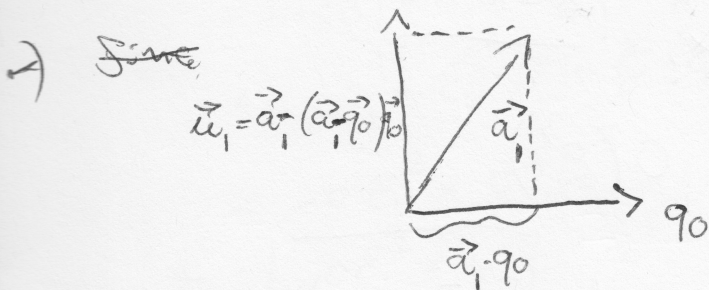
•) We want to build an orthonormal basis, using the vectors  $\{\vec{a}_0, \dots, \vec{a}_N\}$ . We can do this via Gram-Schmidt orthonormalization procedure.

If we call  $\{\vec{q}_0, \dots, \vec{q}_N\}$  the final basis, we can build it like this:

$$\left\{ \begin{array}{l} \vec{u}_0 = \vec{a}_0, \quad \vec{q}_0 = \frac{\vec{u}_0}{|\vec{u}_0|} \\ \vec{u}_1 = \vec{a}_1 - (\vec{a}_1 \cdot \vec{q}_0) \vec{q}_0, \quad \vec{q}_1 = \frac{\vec{u}_1}{|\vec{u}_1|} \\ \vec{u}_2 = \vec{a}_2 - (\vec{a}_2 \cdot \vec{q}_0) \vec{q}_0 - (\vec{a}_2 \cdot \vec{q}_1) \vec{q}_1, \quad \vec{q}_2 = \frac{\vec{u}_2}{|\vec{u}_2|} \\ \vdots \end{array} \right.$$

$$\vec{u}_i = \vec{a}_i - \sum_{k=0}^{i-1} (\vec{a}_i \cdot \vec{q}_k) \vec{q}_k, \quad \vec{q}_i = \frac{\vec{u}_i}{|\vec{u}_i|}$$

The idea is that we project each vector on the previous basis vectors and remove the components along those directions to ~~orthonormalize~~ orthogonalize, we then divide by the modulus to orthonormalize. Graphically:



•) Since  $\{\vec{q}_0, \dots, \vec{q}_N\}$  is a basis, we re-expand  $\{\vec{a}_0, \dots, \vec{a}_N\}$  in this basis to get (invert the Gram-Schmidt above)

$$\left\{ \begin{array}{l} \vec{a}_0 = |\vec{u}_0| \vec{q}_0 \\ \vec{a}_1 = |\vec{u}_1| \vec{q}_1 + (\vec{q}_0 \cdot \vec{a}_1) \vec{q}_0 \\ \vdots \\ \vec{a}_i = |\vec{u}_i| \vec{q}_i + \sum_{k=1}^{i-1} (\vec{q}_{i-1} \cdot \vec{a}_i) \vec{q}_{i-1} \end{array} \right.$$



We can write this last set of equations in matrix form:

$$A = \begin{pmatrix} \vdots & \vdots & \vdots \\ \vec{a}_0 & \vec{a}_1 & \dots & \vec{a}_N \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix} = \underbrace{\begin{pmatrix} \vdots & \vdots & \vdots \\ \vec{q}_0 & \vec{q}_1 & \dots & \vec{q}_N \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix}}_{\text{orthogonal}} \underbrace{\begin{pmatrix} |\vec{u}_0| & \vec{q}_0 \cdot \vec{a}_1 & \vec{q}_0 \cdot \vec{a}_2 & \dots & \vec{q}_0 \cdot \vec{a}_N \\ 0 & |\vec{u}_1| & \vec{q}_1 \cdot \vec{a}_2 & \dots & \vec{q}_1 \cdot \vec{a}_N \\ 0 & 0 & |\vec{u}_2| & \dots & \vec{q}_2 \cdot \vec{a}_N \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \vdots & \vdots & \vdots & \vdots & |\vec{u}_N| \end{pmatrix}}_{\text{upper triangular}}$$

This is the QR decomposition we looked for.

