PRINCIPAL COMPONENTS ANALYSIS

(pre-class notes page 1)

* DIAGONALIZING A MATRIX

$A \leftarrow$ matrix $\lambda_1, \lambda_2 \leftarrow$ eigenvalues $\vec{x}_1, \vec{x}_2 \leftarrow$ e'vectors

$$\underbrace{A\begin{bmatrix}\vec{x}_1 & \vec{x}_2\end{bmatrix}}_{V} = \begin{bmatrix}A\vec{x}_1 & A\vec{x}_2\end{bmatrix} = \begin{bmatrix}\lambda_1\vec{x}_1 & \lambda_2\vec{x}_2\end{bmatrix} = \underbrace{\begin{bmatrix}\vec{x}_1 & \vec{x}_2\end{bmatrix}}_{V}\underbrace{\begin{bmatrix}\lambda_1 & 0\\ 0 & \lambda_2\end{bmatrix}}_{\Lambda}$$

↑ matrix of eigenvectors eigenvalue matrix

$$\Rightarrow \boxed{AV = V\Lambda}$$

$$V^{-1}AV = V^{-1}V\Lambda = \Lambda$$

$$\Rightarrow \boxed{V^{-1}AV = \Lambda}$$

← A is diagonalized

or A can be rewritten as

$$\boxed{A = V\Lambda V^{-1}}$$

A can be broken into eigenvectors & eigenvalues

* makes it easy to compute powers of A!

$$A^2 = (V\Lambda \cancel{V^{-1})(V}\Lambda V^{-1}) = V\Lambda^2 V^{-1}$$

$$\Rightarrow A^n = V\Lambda^n V^{-1}$$

As $n \to \infty$, $\lambda > 1$ will dominate

* SIMILAR MATRICES

$$B = M^{-1}AM$$

same e'values

let $\boxed{B\vec{x} = \lambda\vec{x}}$

$$B\vec{x} = M^{-1}AM\vec{x} = \lambda\vec{x} \Rightarrow$$

$$\cancel{M(M^{-1}}AM\vec{x}) = M(\lambda\vec{x}) \Rightarrow (AM)\vec{x} = \lambda(M\vec{x})$$

$\Rightarrow$ same e'values as B, $\vec{x}$ is ~~rotated~~ transformed

* any diagonal matrix is <u>similar</u> (because $A = V\Lambda V^{-1}$)

~~de~~ SYMMETRIC MATRICES $A = A^T$

Recall $A = \begin{bmatrix} -1 & 2 \\ 2 & -1 \end{bmatrix}$ from last class
we found $\lambda = \{-3, +1\}$, $\vec{v} = \left\{ \begin{bmatrix} 1 \\ -1 \end{bmatrix}, \begin{bmatrix} 1 \\ +1 \end{bmatrix} \right\}$

$A = A^T$, $\vec{v}_1^{\,T} \vec{v}_2 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}^T \begin{bmatrix} 1 \\ 1 \end{bmatrix} = (1) + (-1) = 0$

$\Rightarrow$ eigenvectors are orthogonal

Another definition: ~~A~~ $V = [\vec{v}_1 \ \vec{v}_2]$ is an orthogonal matrix if $\boxed{V^T = V^{-1}}$

Lets show that for this matrix:

I normalized the columns

$V = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \Rightarrow V^{-1} = \frac{1}{\sqrt{2} \cdot \cancel{\ }} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} = V^T$

$\det = (\frac{1}{\sqrt{2}})(\frac{1}{\sqrt{2}}) - (\frac{1}{\sqrt{2}})(-1/\sqrt{2})$
$= 1/2 + 1/2 = 1$

THM: Symmetric matrices have real eigenvalues and orthogonal eigenvectors

PROOF: Rewrite A as $A = V^{-1} \Lambda V$ (diagonalization)

$\Rightarrow A^T = (V^{-1} \Lambda V)^T = V^T \Lambda (V^{-1})^T$

By defintion $A = A^T$

$\Rightarrow V^{-1} \Lambda V = V^T \Lambda (V^{-1})^T$

For this to be true, $V^{-1} = V^T$

$\hookrightarrow V^{-1} \Lambda V = V^{-1} \Lambda (V^T)^T = V^{-1} \Lambda V$ ✓

Since $V^{-1} = V^T$, eigenvectors V are orthogonal

(all positive semidefinite matrices are SYMMETRIC)

* POSITIVE SEMIDEFINITE MATRICES

S is positive semidefinite if $S = A^T A$

THM: Positive semidefinite matrices have all $\lambda \geq 0$.

PROOF: Let $\lambda, \vec{v}$ be eigenvalues & eigenvectors of S

$$\Rightarrow \underbrace{(A^T A)}_{S}\vec{v} = \lambda \vec{v}$$
$$\vec{v}^T (A^T A \vec{v}) = \vec{v}^T (\lambda \vec{v})$$
$$\Rightarrow (A\vec{v})^T (A\vec{v}) = \lambda \vec{v}^T \vec{v}$$
$$\Rightarrow \|A\vec{v}\|^2 = \lambda \|\vec{v}\|^2$$

norm always ≥ 0

$\Rightarrow \lambda \geq 0 \quad \forall S = A^T A$

When will $\lambda = 0$?

* If S does not have independent columns *

Ex: $S = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \Rightarrow \det\left(\begin{bmatrix} 1-\lambda & 1 \\ 1 & 1-\lambda \end{bmatrix}\right) = \lambda^2 - 2\lambda + \cancel{1} - \cancel{1} = 0$

$\Rightarrow \lambda(\lambda - 2) = 0$

$\Rightarrow \lambda = \{0, 2\}$

eigenvectors: $\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = 2\begin{bmatrix} a \\ b \end{bmatrix} \Rightarrow \vec{v}_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$

$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = 0\begin{bmatrix} a \\ b \end{bmatrix} \Rightarrow \vec{v}_2 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}$

Rewrite S as diagonalization

$$S = V^T \Lambda V = \frac{1}{2}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}^T \begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$$

column of zeros, $\vec{v}_2$ $\emptyset$ matter

can write S as

$$S = \frac{1}{2}\begin{bmatrix} 1 \\ 1 \end{bmatrix}^T (2) \begin{bmatrix} 1 \\ 1 \end{bmatrix} \overset{\checkmark}{=} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

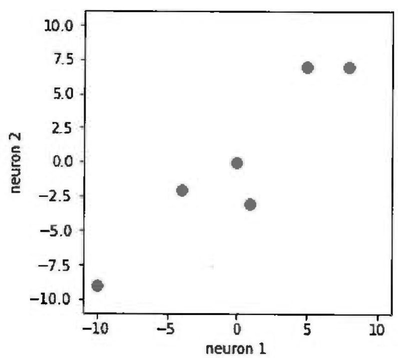
S is a RANK ONE matrix

$\boxed{\text{Now let's look @ a "newer" example}}$

In [1]:

```
import numpy as np
import matplotlib.pyplot as plt
%matplotlib inline

n1 = np.array([5,-4,8,-10,1,0])
n2 = np.array([7,-2,7,-9,-3,0])

A = np.concatenate((n1[np.newaxis,:], n2[np.newaxis,:]), axis=0)
print(A.shape)

# plot neuron activity
fig = plt.figure(figsize=(4,4))
ax = fig.add_subplot(111)
ax.scatter(n1,n2,s=60)
ax.set_xlabel('neuron 1')
ax.set_ylabel('neuron 2')
ax.set_xlim(-11,11)
ax.set_ylim(-11,11)
plt.show()
```

```
(2, 6)
```



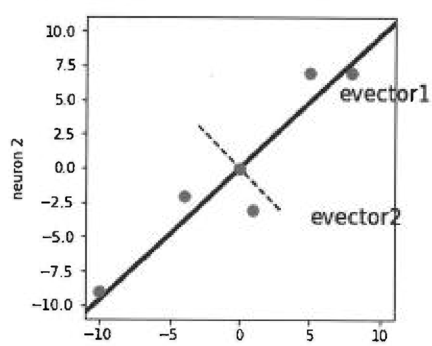
In [2]:

```
print('covariance matrix')
print(A @ A.T)

# find eigenvalues and eigenvectors of covariance matrix
lam, v = np.linalg.eig(A @ A.T)

print('eigenvalues: %2.0f, %2.0f'%(lam[0],lam[1]))
print('eigenvectors: [%2.2f,%2.2f], [%2.2f,%2.2f]'%(v[0,0],v[1,0],v[0,1],v[1,1]))
```

```
covariance matrix
[[206 186]
 [186 192]]
eigenvalues: 385, 13
eigenvectors: [0.72,0.69], [-0.69,0.72]
```

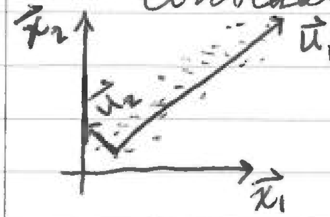
In [3]:

```
# plot EIGENVECTOR on top
fig = plt.figure(figsize=(4,4))
ax = fig.add_subplot(111)
ax.scatter(n1,n2,s=60)
ax.plot(np.array([-11,11]), np.array([-11,11])*v[1,0]/v[0,0],color='k', zorder=0, lw=3)
ax.text(7,5,'evector1',fontsize=15)
ax.plot(np.array([-3,3]), np.array([-3,3])*v[1,1]/v[0,1],'--',color='k', zorder=0)
ax.text(5,-4,'evector2',fontsize=15)
ax.set_xlabel('neuron 1')
ax.set_ylabel('neuron 2')
ax.set_xlim(-11,11)
ax.set_ylim(-11,11)
plt.show()
```



* PRINCIPAL COMPONENTS ANALYSIS

- LINEAR dimensionality reduction ~~technique~~ technique
  - (most data is HIGH-dimensional)
  - ↳ constrain points to lower-dimensional space



Find $\vec{u}_1$ that captures the MOST variance in the data

In other words, find a low-dimensional space that preserves as much of the variance in the original data as possible.

Why? • hard to work w/ high-D data, may want a low-D summary that is more interpretable

• can use as a "pre-processing" step before doing classification or regression
  — reduces dimensionality ⇒ fewer parameters
  ⇒ "regularization"

DERIVATION: $X = \left[\vec{x}_1 \cdots \vec{x}_n \right]_{d \times n}$ $\quad \vec{x}_i \in \mathbb{R}^d$

can think of $\vec{x}_i$ as ~~neurons~~ stimuli
& d as ~~stimuli~~ neurons

If $\vec{x}_i$ is mean 0, then covariance $S = \underbrace{X X^T}_{d \times d}$
(if its not, subtract mean NOW!)

want to maximize variance of projection of data onto $\vec{u}_1$

⇓

$$\max_{\vec{u}_1} \operatorname{var}_i(\vec{u}_1^T \vec{x}_i) = \sum_i (\vec{u}_1^T \vec{x}_i)(\vec{u}_1^T \vec{x}_i)^T = \sum_i \vec{u}_1^T(\vec{x}_i \vec{x}_i^T)\vec{u}_1$$

$$= \vec{u}_1^T S \vec{u}_1$$

if $\vec{u}_1 \to \infty$, variance $\to \infty$

★ PCA DERIVATION

$\max_{\vec{u}_1} \ \vec{u}_1^T S \vec{u}_1$ need a constraint on $\vec{u}_1$

– force $\|\vec{u}_1\|^2 = 1 \equiv \vec{u}_1^T \vec{u}_1 = 1$

Lagrangian $\mathcal{L}(\vec{u}_1, \lambda) = \vec{u}_1^T S \vec{u}_1 - \lambda(\vec{u}_1^T \vec{u}_1 - 1)$

$$\frac{\partial \mathcal{L}}{\partial \vec{u}_1} = 2S\vec{u}_1 - 2\lambda\vec{u}_1 = 0$$

$$\Rightarrow S\vec{u}_1 = \lambda\vec{u}_1$$

What is $\vec{u}_1$ then?

let $\vec{u}_1 = \vec{v}$ ← eigenvector of S

$$\max_{\vec{v}} \ \vec{v}^T(S\vec{v}) = \vec{v}^T(\lambda\vec{v}) = \lambda\underbrace{\vec{v}^T\vec{v}}_{1}$$

plug in $\lambda\vec{v}$

$$= \lambda$$

To maximize variance, we need LARGEST λ

Will $\lambda \geq 0$? Yes, S is positive semi-definite

EQUIVALENCE W/ SINGULAR VALUE DECOMPOSITION

Suppose $X = U\Sigma V^T$ where U & V orthogonal

$$XX^T = (U\Sigma V^T)(U\Sigma V^T)^T = U\Sigma \cancel{V^T} V \Sigma^T U^T$$

$$= U\Sigma^2 U^T$$

↑ U are eigenvectors of $S = XX^T$

So eigenvectors of covariance S are LEFT singular vectors

RIGHT singular vectors: $\boxed{\Sigma^{-1}U^T X = V}$

PROVE THIS