01/26/2023 <u>Dimensionality Reduction (Principal Component Analysis)</u>

- row is a sample

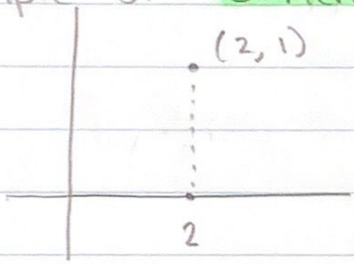
$$A = \begin{bmatrix} — a_1 — \\ — a_2 — \\ \vdots \\ — a_n — \end{bmatrix}_{n \times d}$$

$a_1, a_2, \ldots, a_n \sim P$ - should be similar

n is number of samples

d is number of elements in sampe

- example of dimensionality reduction



- dimensionality reduction
  - want to minimize coordinates needed while maximizing variance captured

$$A = \begin{bmatrix} — a_1 — \\ — a_2 — \\ \vdots \\ — a_n — \end{bmatrix}_{n \times d} \Rightarrow A' = \begin{bmatrix} - a_1' - \\ - a_2' - \\ \vdots \\ - a_n' - \end{bmatrix}_{n \times 2 \text{ or } 3}$$

  - procedure of principal component analysis (PCA)
    1.) Center the data

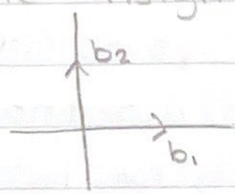
$$\bar{a} = \frac{1}{n} \sum_{i=1}^{n} a_i \qquad B = \begin{bmatrix} — a_1 - \bar{a} — \\ — a_2 - \bar{a} — \\ \vdots \\ — a_n - \bar{a} — \end{bmatrix}_{n \times d}$$

2.) Compute the Covariance matrix (C)

$$\underset{d\times d}{C} = \underset{d\times n}{B^T} \underset{n\times d}{B}$$

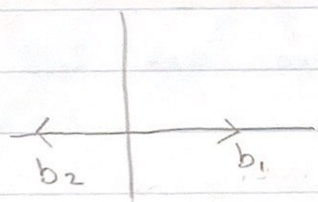
B^TB tells us how these values are related to each other

- some insight



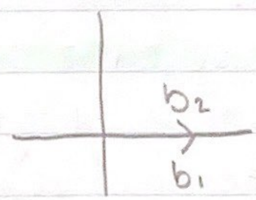
$b_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ $b_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$

$b_1^T b_2 = 0$ ← b_1 doesn't tell us anything about b_2



$b_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ $b_2 = \begin{bmatrix} -1 \\ 0 \end{bmatrix}$

$b_1^T b_2 = -1$ ← b_1 and b_2 are perfectly negatively correlated



$b_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ $b_2 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$

$b_1^T b_2 = 1$ ← b_1 and b_2 are perfectly correlated

- Side note: linear algebra review
  - eigen vectors with respect to different eigenvalues will be orthogonal

$\lambda_1 \geq \lambda_2 \geq \lambda_3 \geq \ldots \geq \lambda_n$

$$V = \begin{bmatrix} | & | & | \\ x_1 & x_2 & x_3 \\ | & | & | \end{bmatrix} \quad \Lambda = \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix} \Rightarrow \underset{3\times 3}{C} V = V\Lambda$$

$$\Rightarrow C = V\Lambda V^T$$

3.) Eigendecomposition of C (covariance matrix)

$$\underset{d\times d}{C} = \underset{d\times d}{V}\,\underset{d\times d}{D}\,\underset{d\times d}{V^T}$$

V is matrix containing columns of eigenvectors

D is diagonal matrix of eigenvalues

4.) Principal Component

$$T_{n\times 2} = \underset{n\times d}{B}\,\underset{d\times 2}{V}[:, [\underset{\text{most info}}{1}, \underset{\text{2nd most info}}{2}]]$$

for linear model

- why does this work?
  - each centered sample in B (row) is a linear combination of V^T rows
  - for orthogonal basis set, to find the projection of a vector $(a_j - \bar{a})$ on a basis vector (v_i) or function, you just do their inner product
    - example

$$a_j - \bar{a} = [3, 1]$$

$$V = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad v_1 = [1, 0] \quad v_2 = [0, 1]$$

$$(a_j - \bar{a})^T v_1 = 3$$

$$(a_j - \bar{a})^T v_2 = 1 \quad \therefore a_j - \bar{a} = 3v_1 + 1v_2$$

$$B^TB = \underbrace{V}_{Q} D V^T$$

orthogonal

$$\underbrace{Q^TB^T}_{\text{weights}} \begin{bmatrix} - a_1 - \bar{a} - \\ \vdots \\ - a_n - \bar{a} - \end{bmatrix} = \begin{bmatrix} v_1^T \\ v_2^T \\ \vdots \\ v_d^T \end{bmatrix}$$

- hence if PCA is converting $n \times d$ data into $n \times 2$ data, that just means the 2 coordinates in $n \times 2$ data are just the weights of v_1^T and v_2^T