11/7/2023: PCA continued

Goal: Choose unit vector w to maximize $\frac{1}{n}\sum_{i=1}^{n}(w^T x^{(i)})^2$

$$= \frac{1}{n}\sum_{i=1}^{n}\underbrace{(w^T x^{(i)})}_{1\times 1}\underbrace{(x^{(i)T} w)}_{1\times 1}$$

matrix multiplication is associative

$$= \frac{1}{n}\sum_{i=1}^{n}\underbrace{w^T}_{1\times d}\underbrace{(x^{(i)} x^{(i)T})}_{d\times d}\underbrace{w}_{d\times 1}$$

$$xx^T = \begin{bmatrix} x_1^2 & x_1x_2 & x_1x_3 \dots \\ x_2x_1 & \ddots & \\ & & \ddots \end{bmatrix}$$

$$= \frac{1}{n} w^T \left(\sum_{i=1}^{n} x^{(i)} x^{(i)T}\right) w$$

Recall: Covariance matrix $\Sigma = \frac{1}{n}\sum_{i=1}^{n}(x^{(i)}-\mu)(x^{(i)}-\mu)^T$

AND: in PCA we ensure $\mu=0$ for data

$$= w^T \Sigma w$$

↑ covariance matrix of our data

this is symmetric

Every symmetric matrix Σ can be written as

$$\Sigma = UDU^T \quad \text{where} \quad D = \begin{bmatrix} \lambda_1 & & 0 \\ & \lambda_2 & \\ 0 & & \ddots \\ & & & \lambda_d \end{bmatrix}$$

eigenvalues, is diagonal

and U is orthonormal

$$U = \begin{bmatrix} u_1 & u_2 & \dots & u_d \end{bmatrix}$$

eigenvectors

Each column u_i has $\|u_i\| = 1$ AND $u_i^T u_j = 0$ for $i \neq j$ (i.e. orthogonal)

$$\underset{w}{\text{maximize}} \quad w^T \Sigma w = \underbrace{w^T U}_{a^T} D \underbrace{U^T w}_{a}$$

Define: $a = U^T w$. NOTE: $\|a\| = \|w\| = 1$ because U is orthonormal

So now: $\underset{a}{\text{maximize}} \quad a^T D a$

$$= \sum_{j=1}^{d} \lambda_j a_j^2$$

Subject to $\sum_{j=1}^{d} a_j^2 = 1$

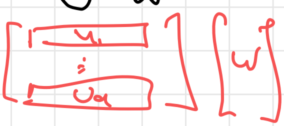
Optimal solution: Choose $a_j = 1$ when λ_j is largest eigenvalue

Choose $a_j = 0$ else

Alternatively: Order λ's so that $\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_d$

Then choose $a = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix}$

$a = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \end{bmatrix} = U^T w$ Solve for w: $\boxed{w = u_1}$!



We know

$u_1^T u_1 = 1$

$u_j^T u_1 = 0$

for any $j \neq 1$

$$\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} u_1^T w \\ u_2^T w \\ \vdots \\ u_d^T w \end{bmatrix}$$ ✓ ✓ ✓ ✓

Takeaways for PCA: Given data $\{x^{(1)}, \dots, x^{(n)}\}$:

1. Mean-center data
2. Compute $\Sigma = \frac{1}{n} \sum_{i=1}^{n} x^{(i)} x^{(i)T}$
3. Decompose Σ into UDU^T
4. Choose w to be eigenvector corresponding to largest eigenvalue

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What if we want >1 dimension

e.g. 2-dimensional visualizations

Solution: Use top k eigenvectors to get k dimensions