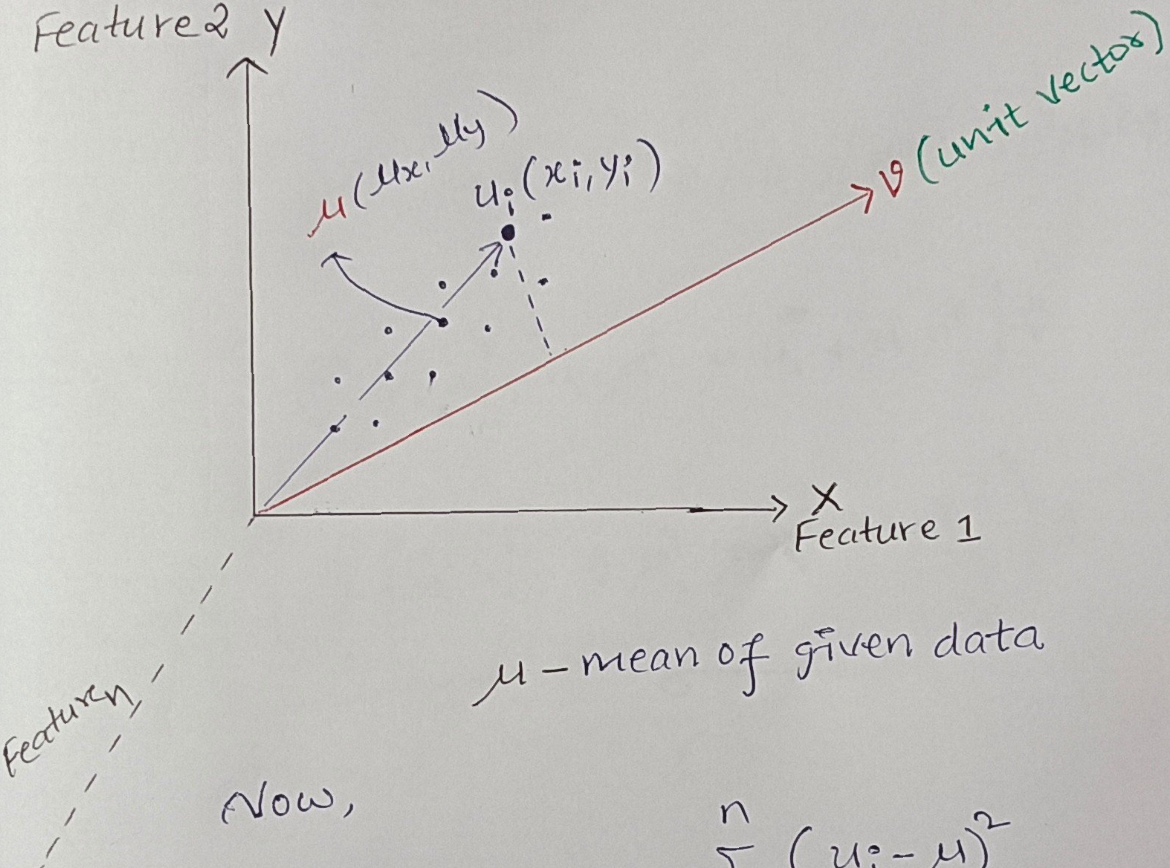
PCA

Aim:- PCA aims to find directions (unit vectors) along which the projected data exhibits the highest possible Variance.

The problem Formulation:-



μ – mean of given data

Now,

$$\text{Variance given data} = \frac{\sum_{i=1}^{n} (u_i - \mu)^2}{n}$$

Variance of projected data =

$$\boxed{V = \frac{1}{n} \sum_{i=1}^{n} \left(u_i^T \cdot v - \mu^T \cdot v \right)^2}$$

* Now PCA aims to maximize this variance ($\mathcal{V}$)

Let's simplify $\mathcal{V}$

$$\mathcal{V} = \frac{1}{n}\sum_{i=1}^{n}(\underbrace{u_i^T \cdot \vartheta}-\underbrace{\mu^T \cdot \vartheta}).(u_i^T \cdot \vartheta - \mu^T \cdot \vartheta)$$

Just interchanged

$$= \frac{1}{n}\sum_{i=1}^{n}(\vartheta^T \cdot u_i - \vartheta^T \cdot \mu) \cdot (u_i^T \vartheta - \mu^T \cdot \vartheta)$$

$$= \frac{1}{n}\sum_{i=1}^{n}\left[\vartheta^T u_i \cdot u_i^T \vartheta - \vartheta^T u_i \cdot \mu^T \vartheta - \vartheta^T \mu \cdot u_i^T \vartheta + \vartheta^T \mu \mu^T \vartheta\right]$$

$$= \frac{1}{n}\sum_{i=1}^{n}\vartheta^T\left[u_i \cdot u_i^T - u_i \cdot \mu^T - \mu \cdot u_i^T + \mu \cdot \mu^T\right]\vartheta$$

$$= \vartheta^T \Big(\underbrace{\frac{1}{n}\sum_{i=1}^{n}\left[u_i \cdot u_i^T - u_i \cdot \mu^T - \mu \cdot u_i^T + \mu \cdot \mu^T\right]}_{\text{'}C\text{'}}\Big)\vartheta$$

$$= \vartheta^T C \vartheta$$

Therefore $\boxed{\mathcal{V} = \vartheta^T C \vartheta}$ → Now our goal is to maximize this variance $\mathcal{V}$ with a constraint $\|\vartheta\| = 1$ ($\because$ ϑ is a unit vector) we know $||v|| = 1$

$\Rightarrow v^T \cdot v = |v^T||v| \cos\theta$

$= |v|^T |v| \cos(0)$

$= 1 \cdot 1 = 1$

$\therefore$ our constraint is $v^T \cdot v = 1$

* our objective is to maximize variance V subject to a constraint $v^T \cdot v = 1$. Such problems of constrained optimization might be reformulated as unconstrained optimization problems via use of Lagrangian multipliers.

Lagrangian multipliers:-

If we would like to maximize $f(x)$ subject to $g(x) = c$, we introduce the Lagrange multiplier λ and construct the Lagrangian

$\mathcal{L}(x, \lambda)$

$$\boxed{\mathcal{L}(x, \lambda) = f(x) - \lambda(g(x) - c)}$$

* The sign of λ doesn't make any difference.

we then solve the System of equations:

$$\left\{ \frac{\partial \mathcal{L}(x,\lambda)}{\partial x} = 0, \; \frac{\partial \mathcal{L}(x,\lambda)}{\partial \lambda} = 0 \right\}$$

The Solution:-

In our case, we want to maximize Variance $\underbrace{v}_{f(x)}$ subject to a constraint $\underbrace{v^T . v = 1}_{g(x)=c}$.

our Lagrangian is:

$$\mathcal{L}(v,\lambda) = v^T C v - \lambda (v^T . v - 1)$$

We solve for the stationary points:

$$\frac{\partial \mathcal{L}(v,\lambda)}{\partial v} = \frac{\partial}{\partial v}\left[v^T C v - \lambda (v^T . v - 1)\right]$$

$$0 = C \frac{\partial}{\partial v}(v^T . v) - \lambda \frac{\partial}{\partial v}(v^T . v)$$

$$\Rightarrow C \frac{\partial}{\partial v}(|v|^2) = \lambda \frac{\partial}{\partial v}(|v|^2) \quad \left[v^T . v = |v||v| \right]$$

$\because |v^T| = |v|$

$$C(\cancel{x}v) = \lambda(\cancel{x}v)$$

$$\Rightarrow \boxed{Cv = \lambda v}$$

It is an Eigen Vector Equation

* The vector We are searching for is an eigen vector, Guys!!

Now,

$$\frac{\partial L(v,\lambda)}{\partial \lambda} = \frac{\partial}{\partial \lambda}\left[v^T C v - \lambda(v^T v - 1)\right]$$

$$0 = v^T v - 1 \rightarrow$$ We already known it

Let's Decode what is C ?

$$C = \frac{1}{n}\sum_{i=1}^{n}\left[u_i \cdot u_i^T - u_i \cdot \mu^T - \mu \cdot u_i^T + \mu \cdot \mu^T\right]$$

$$u_i = \begin{bmatrix} x_i \\ y_i \end{bmatrix} \quad \mu = \begin{bmatrix} \mu_x \\ \mu_y \end{bmatrix}$$ → matrix representation of a vector.

μ_x - Mean feature 1 (x)

μ_y = Mean of fature 2 (y)

Now,

$$u_i \cdot u_i^T = \underset{2\times 1}{\begin{bmatrix} x_i \\ y_i \end{bmatrix}} \underset{1\times 2}{\begin{bmatrix} x_i & y_i \end{bmatrix}} = \underset{2\times 2}{\begin{bmatrix} x_i^2 & x_i y_i \\ y_i x_i & y_i^2 \end{bmatrix}}$$

$$u_i \cdot \mu^T = \begin{bmatrix} x_i \\ y_i \end{bmatrix} \begin{bmatrix} \mu_x & \mu_y \end{bmatrix} = \underset{2\times 2}{\begin{bmatrix} x_i \mu_x & x_i \mu_y \\ y_i \mu_x & y_i \mu_y \end{bmatrix}}$$

$$\mu \cdot u_i^T = \begin{bmatrix} \mu_x \\ \mu_y \end{bmatrix} \begin{bmatrix} x_i & y_i \end{bmatrix} = \underset{2\times 2}{\begin{bmatrix} \mu_x x_i & \mu_x y_i \\ \mu_y x_i & \mu_y y_i \end{bmatrix}}$$

$$\mu \cdot \mu^T = \begin{bmatrix} \mu_x \\ \mu_y \end{bmatrix} \begin{bmatrix} \mu_x & \mu_y \end{bmatrix} = \underset{2\times 2}{\begin{bmatrix} \mu_x^2 & \mu_x \mu_y \\ \mu_y \mu_x & \mu_y^2 \end{bmatrix}}$$

$$\therefore C = \frac{1}{n} \sum_{i=1}^{n} \begin{bmatrix} x_i^2 - x_i \mu_x - \mu_x x_i + \mu_x^2 & x_i y_i - x_i \mu_y - \mu_x y_i + \mu_x \mu_y \\ y_i x_i - y_i \mu_x - \mu_y x_i + \mu_x \mu_y & y_i^2 - 2\mu_y y_i + \mu_y^2 \end{bmatrix}$$

$$C = \begin{bmatrix} \frac{1}{n} \sum_{i=1}^{n} (x_i - \mu_x)^2 & \frac{1}{n} \sum_{i=1}^{n} (x_i - \mu_x)(y_i - \mu_y) \\ \frac{1}{n} \sum_{i=1}^{n} (x_i - \mu_x)(y_i - \mu_y) & \frac{1}{n} \sum_{i=1}^{n} (y_i - \mu_y)^2 \end{bmatrix}$$

Covariance :- It measures the relationship between two variables.

* A positive covariance indicates that variables tend to change together (both increase or both decrease), while Negative covariance means they tend to change in opposite directions.

Covariance-Matrix

$$[\mathrm{cov}(X,Y)]_{\text{matrix}} = \begin{bmatrix} \mathrm{cov}(X,X) & \mathrm{cov}(X,Y) \\ \mathrm{cov}(Y,X) & \mathrm{cov}(Y,Y) \end{bmatrix}$$

↑ For 2-D

$$= \begin{bmatrix} \mathrm{Var}(X) & \mathrm{cov}(X,Y) \\ \mathrm{cov}(Y,X) & \mathrm{Var}(Y) \end{bmatrix}$$

we know

$$\mathrm{cov}(X,Y) = \mathrm{cov}(Y,X) = \frac{1}{n}\sum_{i=1}^{n}(x_i - \mu_x)(y_i - \mu_y)$$

Covariance matrix =

$$\begin{bmatrix} \frac{1}{n}\sum_{i=1}^{n}(x_i-\mu_x)^2 & \frac{1}{n}\sum_{i=1}^{n}(x_i-\mu_x)(y_i-\mu_y) \\ \frac{1}{n}\sum_{i=1}^{n}(x_i-\mu_x)(y_i-\mu_y) & \frac{1}{n}\sum_{i=1}^{n}(y_i-\mu_y)^2 \end{bmatrix}$$

Very Very clearly,

Covariance Matrix = C

I am Very happy

Guys. I hope you can recollect we use to find the eigen value and eigen vectors of covariance matrix. This is the Reason!!!