Dimensionality Reduction / PCA

feature matrix

n samples / rows
p features / columns

$$X = \begin{pmatrix} | & | & & | \\ x^{(1)} & x^{(2)} & \cdots & x^{(p)} \\ | & | & & | \end{pmatrix} \begin{array}{l} n \\ \text{rows} \end{array}$$

p columns

p column vectors of length n:

$$x^{(j)} = \begin{pmatrix} x_{1j} \\ \vdots \\ x_{nj} \end{pmatrix}$$

variances & covariances

$$\mathrm{Var}(x_j) = \frac{1}{n}\sum_{k=1}^{n}\left(x_k^{(j)} - \cancel{\mu_{x^{(j)}}}\right)^2 = \sigma_j^2 = \mathrm{Cov}(x_j, x_j) = \sigma_{j,j}^2$$

$$\mathrm{Cov}(x_i, x_j) = \frac{1}{n}\sum_{k=1}^{n}\left(x_k^{(i)} - \cancel{\mu_{x^{(i)}}}\right)\left(x_k^{(j)} - \cancel{\mu_{x^{(j)}}}\right) = \sigma_{i,j}^2$$

for the sake of simplicity, let's assume that X was column centered (all column vectors are centered: $\mu_{x^{(j)}} = 0 \ \forall j$)

$$\sigma_{i,j}^2 = \frac{1}{n}\sum_{k=1}^{n} x_k^{(i)} x_k^{(j)} = \frac{1}{n}\sum x^{(i)T} \cdot x^{(j)}$$

that's the covariance matrix of X

$$\begin{pmatrix} \sigma_1^2 & \sigma_{1,2}^2 & & \\ \sigma_{2,1}^2 & \sigma_2^2 & & \\ & & \ddots & \\ & & & \sigma_p^2 \end{pmatrix} = \frac{1}{n} X^T \cdot X \longrightarrow \text{shape } (p, p)$$

X^T: shape (p, n); X: (n, p)

we want a new base V (a new matrix), which when applied to X:

$$X' = XV$$

gives us a covariance matrix for X' without covariance between variables

$$X'^T \cdot X' = \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_p \end{pmatrix} = \Lambda$$

as an additional constraint, we want to choose V to be orthonormal

if V is the form $V = \begin{pmatrix} | & & | \\ u_1 & \dots & u_p \\ | & & | \end{pmatrix}$, $u_j^2 = 1$, $u_i u_j = 0$ if $i \neq j$

we can express it as

$$V^T \cdot V = I$$

$$\Lambda = X'^T \cdot X' = (XV)^T (XV)$$

$$= (V^T X^T)(XV)$$

$$= V^T (X^T X) V$$

let's left multiply by V on both sides

$$V\Lambda = V(V^T X^T X V) = \underbrace{(VV^T)}_{I}(X^T X)V$$

or $\boxed{(X^T X)V = V\Lambda}$

$$(X^TX)\begin{pmatrix} | & & | \\ u_1 & \cdots & u_p \\ | & & | \end{pmatrix} = \begin{pmatrix} | & & | \\ u_1 & \cdots & u_p \\ | & & | \end{pmatrix}\begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_p \end{pmatrix}$$

$$A = (a_{ij})$$
$$B = (b_{ij}) \quad 1 \leq i,j \leq p :$$
$$C = (c_{ij})$$
$$C = AB \Longrightarrow c_{ij} = \sum_{k=1}^{p} a_{ik} b_{kj}$$

let's focus on the right side

$$a_{ij} = u_{ji}$$
$$b_{ij} = \begin{cases} \lambda_i = \lambda_j & \text{if } i=j \\ 0 & \text{otherwise} \end{cases}$$

$$c_{ij} = \underbrace{\sum_{k=1}^{p} a_{ik} b_{kj}}_{\text{only one term remains when } k=j}$$

$$= \underbrace{a_{ij}}_{u_{ji}} \underbrace{b_{jj}}_{\lambda_j} = \lambda_j u_{ji}$$

the right side is

$$\begin{pmatrix} | & & | \\ \lambda_1 u_1 & \cdots & \lambda_p u_p \\ | & & | \end{pmatrix}$$

on the right side, each column is made of

$$(X^T X)\begin{pmatrix} | \\ u_j \\ | \end{pmatrix} = (X^T X) \cdot u_j$$

$$(p \times p) \quad (p \times 1) \longrightarrow (p \times 1)$$

$$\begin{pmatrix} | & & | \\ (X^T X) u_1 & \dots & (X^T X) u_p \\ | & & | \end{pmatrix}$$

identifying the columns on each side, we get:

$$\boxed{(X^T X) u_j = \lambda_j u_j}$$

To perform PCA, we are looking for the eigenvalues λ_j and eigenvectors u_j of $X^T \cdot X$