Consider a simple case: $\min_{u} \underbrace{u^T C u \quad \text{s.t.} \quad u^T u = 1}_{\text{constrained optimization problem}} \iff 1 - u^T u = 0$

Lagrangian $L(u, \lambda) = u^T C u + \lambda(1 - u^T u)$

u: primal variable; λ: Lagrange multiplier

$$\nabla_u L(u, \lambda) = 0 \implies Cu = \lambda u \quad \text{(or)} \quad \boxed{u^T C u = \lambda}$$

So, $\min_{u} u^T C u$ s.t. $u^T u = 1$ is the smallest eigenvalue λ of C.

$$C = \frac{1}{n} \sum_{i=1}^{n} (x_i - \bar{x})(x_i - \bar{x})^T \leftarrow \text{real-symmetric matrix}$$

$\Downarrow$

all eigenvalues are real ⊕

there exists a orthonormal basis of eigenvectors

Let this basis be $\{u_1, \dots u_m, u_{m+1}, \dots u_d\}$

Corresponding to eigenvalues $\{\lambda_1, \dots \lambda_m, \lambda_{m+1}, \dots \lambda_d\}$ where

$\lambda_1 \geq \lambda_2 \dots \geq \lambda_d$

To minimize $J^* = \sum_{j=m+1}^{d} u_j^T C u_j$ over $\{u_{m+1}, \dots, u_d\}$

Choose $u_{m+1}, \dots, u_d$ to be the $(d-m)$ eigenvectors corresponding to the "$d-m$" least eigenvalues $\{\lambda_{m+1}, \dots, \lambda_d\}$

The remaining $u_1 \dots u_m$ are chosen to be the top-m eigenvectors of C.

PCA:

1. Data: $\{x_1, \dots, x_n\}$ $x_i \in \mathbb{R}^d$ $\forall i$
2. Let $\bar{x} = \frac{1}{n} \sum_{i=1}^{n} x_i$ and $C = \frac{1}{n} \sum_{i=1}^{n} (x_i - \bar{x})(x_i - \bar{x})^T$
3. Find eigenvalues $\{\lambda_1, \dots, \lambda_d\}$ $\lambda_1 \geq \lambda_2 \dots \geq \lambda_d$ with corresponding eigenvectors $\{u_1, \dots, u_d\}$
4. Projected data formed as follows:

$$\tilde{x}_i = \sum_{j=1}^{m} (x_i^T u_j) u_j + \sum_{j=m+1}^{d} (\bar{x}^T u_j) u_j$$

Example:

Consider the dataset $\mathcal{D} = \left\{ \underbrace{\begin{pmatrix} -1 \\ -1 \end{pmatrix}}_{x_1}, \underbrace{\begin{pmatrix} 0 \\ 0 \end{pmatrix}}_{x_2}, \underbrace{\begin{pmatrix} 1 \\ 1 \end{pmatrix}}_{x_3} \right\}$

Let us project $\mathcal{D}$ onto a "m=1"-dimensional subspace

$$\bar{x} = \frac{1}{3} \sum_{i=1}^{3} x_i = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$C = \frac{1}{3} \sum_{i=1}^{3} (x_i - \bar{x})(x_i - \bar{x})^T = \frac{1}{3} \sum_{i=1}^{3} x_i x_i^T$$

$$= \frac{1}{3} \left[\begin{pmatrix} -1 \\ -1 \end{pmatrix} (-1 \ -1) + 0 + \begin{pmatrix} 1 \\ 1 \end{pmatrix} (1 \ 1) \right] = \frac{2}{3} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}$$

Eigenvalues of C: $\lambda_1 = \frac{4}{3}, \quad \lambda_2 = 0$

Eigenvectors of C: $u_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad u_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$

Best 1d-space is spanned by $u_1 = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$

The projected data:

$$\tilde{x}_i = (x_i^T u_1)u_1 + (\bar{x}^T u_2)u_2 = (x_i^T u_1)u_1$$

$$\tilde{x}_1 = \frac{1}{2}(-1 \ -1)\begin{pmatrix}1\\1\end{pmatrix}\begin{pmatrix}1\\1\end{pmatrix} = \begin{pmatrix}-1\\-1\end{pmatrix}, \quad \tilde{x}_2 = 0$$

$$\tilde{x}_3 = \frac{1}{2}(1 \ 1)\begin{pmatrix}1\\1\end{pmatrix}\begin{pmatrix}1\\1\end{pmatrix} = \begin{pmatrix}1\\1\end{pmatrix}$$

Note! $\tilde{x}_1 = x_1$, $\tilde{x}_2 = x_2$, $\tilde{x}_3 = x_3$

Reconstruction error: $J^* = \frac{1}{3}\sum_{i=1}^{3} \|x_i - \tilde{x}_i\|^2 = 0$ (why?)