PCA & SVD

Note Title

Recall the **centered data matrix**

$$\tilde{X} := [\tilde{x}_1 \ \cdots \ \tilde{x}_n] \in \mathbb{R}^{d \times n}$$

$$\tilde{x}_j := x_j - \bar{x}, \quad \bar{x} := \frac{1}{n} \sum_{j=1}^{n} x_j,$$

and the **sample covariance matrix**

$$S := \frac{1}{n} \tilde{X} \tilde{X}^T$$

Then, **PCA** is nothing but **the eigendecomposition of S**

$$S = \Phi \Lambda \Phi^T, \quad \Lambda = \mathrm{diag}(\lambda_1, \cdots, \lambda_d)$$

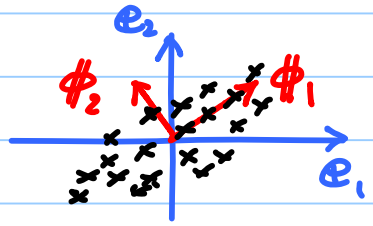
$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_d \geq 0.$

$\Phi := [\phi_1 \ \cdots \ \phi_d] \in \mathbb{R}^{d \times d}$ is an ortho. matrix, and $\{\phi_1, \cdots, \phi_d\}$ form an ONB of $\mathbb{R}^d$.

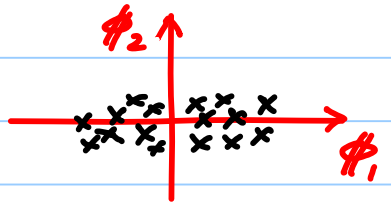
$\phi_j^T \tilde{X}$ is said to be **the jth principal components** of $\tilde{X}$.

These are nothing but the expansion coefficients of $\tilde{X}$ w.r.t. the ONB vector ϕ_j.

If $\tilde{X}$ forms a "cigar" shape,



then $\phi_j^T \tilde{X}$ are the coordinate values of $\tilde{X}$ under the rotated axes



- Hence viewing the given dataset under the principal axes $\phi_1, \phi_2, \cdots$, provides us better interpretations of the data than viewing them under the original axes $e_1, e_2, \cdots$.
- PCA is also often used as a tool to do dimension reduction and feature extraction by keeping only top k PCA coordinates where $k \ll d$, i.e.,

$$\Phi_k := [\phi_1 \cdots \phi_k] \in \mathbb{R}^{d \times k}$$

$$\mathbb{R}^d \ni \tilde{x}_j \longmapsto \underbrace{\Phi_k^T \tilde{x}_j}_{\text{top } k \text{ PCA coordinates or top } k \text{ Principal components of } \tilde{x}_j} \in \mathbb{R}^k$$

Note that using these top k principal components, we can approximate the original data x_j by

$$x_j \approx \bar{x} + \Phi_k \Phi_k^T \tilde{x}_j$$

Of course the approximation gets better and better as k increases. In fact, if $k = d$, then x_j is recovered exactly (within machine ε).

Now we'll face the problem when we compute the eigendecomposition of $S = \Phi \Lambda \Phi^T$:

(1) If d is large, we cannot compute this eigendecomposition because we cannot hold $\Phi \in \mathbb{R}^{d \times d}$ in computer memory, and its computational cost is $O(d^3)$, i.e., too expensive to compute.

(2) Fortunately, we often do not need all d eigenvectors, most likely, only first k eigenvectors $k \ll d$.

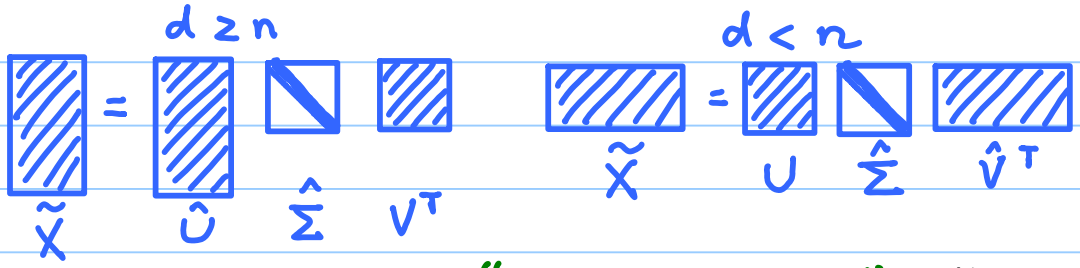
(3) Moreover if $d > n$, then $\text{rank}(S) = n-1$ if x_j's are linearly indep. So, after the first $n-1$ eigenvectors are useless !

Why? $S = \frac{1}{n} \tilde{X} \tilde{X}^T = \frac{1}{n} \{ \underbrace{\tilde{x}_1 \tilde{x}_1^T}_{\text{rank 1}} + \cdots + \underbrace{\tilde{x}_n \tilde{x}_n^T}_{\text{rank 1}} \}$

So looks like $\text{rank}(S) = n$.
But since $\tilde{x}_1 + \cdots + \tilde{x}_n = 0$ because the mean $\bar{x}$ is subtracted from each data vector x_j (i.e., $\tilde{x}_j = x_j - \bar{x}$)
Hence, S loses 1 rank.
So, $\text{rank}(S) = n-1$.

Now, let's consider the reduced SVD of $\tilde{X}$:

$$\tilde{X} = \hat{U} \hat{\Sigma} V^T$$



Just consider the "neo-classical" setting, i.e., $d \geq n$ (e.g., the face image database)

Then consider the sample covariance matrix S using the above SVD:

$$S = \frac{1}{n} \tilde{X} \tilde{X}^T = \frac{1}{n} \hat{U} \hat{\Sigma} V^T V \hat{\Sigma}^T \hat{U}^T$$

$$= \frac{1}{n} \hat{U} \hat{\Sigma} \hat{\Sigma}^T \hat{U}^T = \frac{1}{n} \hat{U} \hat{\Sigma}^2 \hat{U}^T$$

Now $\hat{\Sigma} = \text{diag}(\sigma_1, \cdots, \sigma_{n-1}, 0)$ if $x_1, \cdots, x_n$ are linearly indep.

So, $\hat{\Sigma}^2 = \text{diag}(\sigma_1^2, \cdots, \sigma_{n-1}^2, 0)$.

Finally, S can be written as

$$S = \hat{U} \left(\frac{1}{n} \hat{\Sigma}^2 \right) \hat{U}^T$$

$\hat{U}$: columns are orthonormal.

$\frac{1}{n}\hat{\Sigma}^2 = \text{diag}(\sigma_1^2/n, \cdots, \sigma_{n-1}^2/n, 0)$

Comparing this with the eigendecomposition

$S = \Phi \Lambda \Phi^T$, we can conclude that

$$\begin{cases} \Phi(:, 1:n) = \hat{U} \\ \Lambda(1:n, 1:n) = \frac{1}{n}\hat{\Sigma}^2 = \text{diag}(\sigma_1^2/n, \cdots, \sigma_n^2/n, 0) \end{cases}$$

In fact, only the $1:n-1$ portion is useful since $\sigma_n = 0$.

Hence, we should use the reduced SVD of $\tilde{X}$ (not S) for computing PCA!! Do not use the eigendecomposition of S unless d is small.

Note: $\tilde{X} V = \hat{U} \hat{\Sigma} V^T V = \hat{U} \hat{\Sigma}$

$= [\sigma_1 u_1, \cdots \sigma_{n-1} u_{n-1}, 0]$

$= [\tilde{X} v_1, \cdots, \tilde{X} v_n]$

So, $u_j = \frac{1}{\sigma_j} \tilde{X} v_j$, $j = 1, \cdots, n-1$.

In other words, each principal axis u_j is just a linear combination of the (centered) input vectors $\tilde{x}_1, \cdots, \tilde{x}_n$!

Now let's do MATLAB experiments using the face image database consisting of 143 faces each of which has $128 \times 128 = 16384$ pixels, i.e., $d = 16384$, $n = 143$.