PCA & SVD

Note Title 5/15/2012

Recall the centered data matrix

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

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

and the sample covariance matrix

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

Then, PCA is nothing but the eigendecomposition of S

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

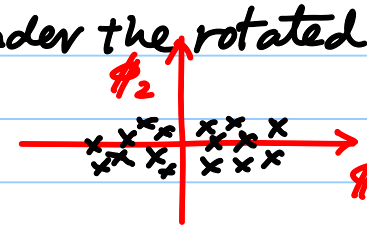
$\lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_d \geq 0.$

$\Phi := [\boldsymbol{\phi}_1 \cdots \boldsymbol{\phi}_d] \in \mathbb{R}^{d\times d}$ is an ortho. matrix, and $\{\boldsymbol{\phi}_1, \cdots, \boldsymbol{\phi}_d\}$ form an ONB of $\mathbb{R}^d$.

$\boldsymbol{\phi}_j^T \tilde{X}$ 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 $\boldsymbol{\phi}_j$.

If $\tilde{X}$ forms a "cigar" shape, then $\boldsymbol{\phi}_j^T \tilde{X}$ 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.,

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

$$\mathbb{R}^d \ni \tilde{x}_j \longmapsto \Phi_k^T \tilde{x}_j \in \mathbb{R}^k$$

top k PCA coordinates or top k Principal components of $\tilde{x}_j$.

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 $\mathbb{x}_j$'s are linearly indep. So, after the first $n-1$ eigenvectors are useless!

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

So looks like $\text{rank}(S) = n$.

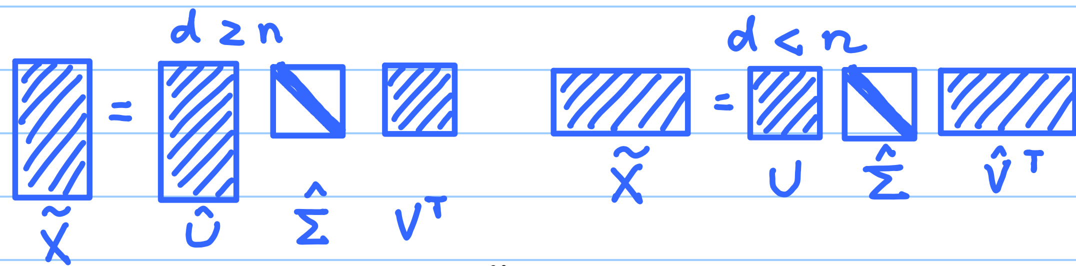
But since $\tilde{\mathbb{x}}_1 + \cdots + \tilde{\mathbb{x}}_n = 0$ because the mean $\bar{\mathbb{x}}$ is subtracted from each data vector $\mathbb{x}_j$ (i.e., $\tilde{\mathbb{x}}_j = \mathbb{x}_j - \bar{\mathbb{x}}$)

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:

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

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

Now $\hat{\Sigma} = \mathrm{diag}(\sigma_1, \cdots, \sigma_{n-1}, \underline{\underline{0}})$ if $\mathbf{x}_1, \cdots, \mathbf{x}_n$ are linearly indep.

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

Finally, S can be written as

$$S = \hat{U}\underbrace{\left(\frac{1}{n}\hat{\Sigma}^2\right)}_{= \mathrm{diag}(\sigma_1^2/n, \cdots, \sigma_{n-1}^2/n, 0)}\hat{U}^T$$

$\uparrow$ columns are orthonormal.

Comparing this with the eigendecomposition

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

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

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.

<u>Note</u>: $\tilde{X} V = \hat{U} \hat{\Sigma} V^T V = \hat{U} \hat{\Sigma}$

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

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

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., $d = 16384$, $n = 143$.