8. Component Analysis

8.1 Singular Matrix Decomposition

If **A** is a square matrix, then we can perform eigenvector-eigenvalue decomposition for **A**:

$$\mathbf{A} = \mathbf{E}\mathbf{D}\mathbf{E}^{-1}$$

$$\mathbf{A} = \lambda_1 \mathbf{e_1} \mathbf{f_1^H} + \lambda_2 \mathbf{e_2} \mathbf{f_2^H} + \cdots + \lambda_{N-1} \mathbf{e_{N-1}} \mathbf{f_{N-1}^H} + \lambda_N \mathbf{e_N} \mathbf{f_N^H}$$

where

$$\mathbf{E} = \begin{bmatrix} \mathbf{e_1} & \mathbf{e_2} & \cdots & \mathbf{e_N} \end{bmatrix}, \quad \mathbf{E}^{-1} = \begin{bmatrix} \mathbf{f_1} & \mathbf{f_2} & \cdots & \mathbf{f_N} \end{bmatrix}^{\mathbf{H}}$$

$$\mathbf{A}\mathbf{e_m} = \lambda_m \mathbf{e_m}$$

If $|\lambda_m|$ is the largest, then

$$\lambda_m \mathbf{e_m} \mathbf{f_m^H}$$

is the most important component of **A**.

8.1.1 Singular Value Decomposition Process

Q: How do we perform eigenvector-eigenvalue decomposition for **A** if **A** is not a square matrix?

$$size(\mathbf{A}) = M \times N, \quad M \neq N$$

We can apply the singular value decomposition (SVD) process as follows.

(1) Generate **B** and **C**

$$\mathbf{B} = \mathbf{A}^{\mathbf{H}}\mathbf{A} \qquad\qquad \mathbf{C} = \mathbf{A}\mathbf{A}^{\mathbf{H}}$$

(Note): Since **B** is an NxN square matrix,
C is an MxM square matrix,
therefore, it is possible to derive the eigenvector sets for **B** and **C**.

$$\mathbf{B} = \mathbf{A}^{\mathbf{H}}\mathbf{A} \qquad \mathbf{C} = \mathbf{A}\mathbf{A}^{\mathbf{H}}$$

(2) Perform Eigenvector-Eigenvalue Decomposition for **B** and **C**

$$\mathbf{B} = \mathbf{V}\mathbf{D}\mathbf{V}^{-1} \qquad \mathbf{C} = \tilde{\mathbf{U}}\boldsymbol{\Omega}\tilde{\mathbf{U}}^{-1}$$

(Note): Since $\mathbf{B}^{\mathbf{H}} = \mathbf{B}$, $\mathbf{C}^{\mathbf{H}} = \mathbf{C}$, **B** and **C** have orthogonal eigenvector sets and $\tilde{\mathbf{U}}$ and **V** are orthogonal matrices.

(i) It is proper to normalize $\tilde{\mathbf{U}}$ and **V** properly such that

$$\mathbf{V}^{\mathbf{H}}\mathbf{V} = \mathbf{I} \qquad \tilde{\mathbf{U}}^{\mathbf{H}}\tilde{\mathbf{U}} = \mathbf{I}$$

then

$$\mathbf{B} = \mathbf{V}\mathbf{D}\mathbf{V}^{\mathbf{H}} \qquad \mathbf{C} = \tilde{\mathbf{U}}\boldsymbol{\Omega}\tilde{\mathbf{U}}^{\mathbf{H}}$$

(ii) It is proper to sort the eigenvalues of **B** and **C** from large to small.

The eigenvectors are also sorted according to eigenvalues.

(3) Then, we calculate

$$\mathbf{S_1} = \tilde{\mathbf{U}}^{\mathbf{H}}\mathbf{AV}$$

$\mathbf{S_1}$ will be an *M*x*N* diagonal matrix

$$S_1[m,n] = 0 \quad if\ m \neq n$$

(4) Varying the sign of $\mathbf{S_1}$ and $\tilde{\mathbf{U}}$

$$S[m,n] = |S_1[m,n]|$$

$$U[m,n] = \tilde{U}[m,n] \quad \text{if } S_1[n,n] \geq 0,$$

$$U[m,n] = -\tilde{U}[m,n] \quad \text{if } S_1[n,n] < 0,$$

(Note): With sign change,

$$\mathbf{S} = \mathbf{U}^{\mathbf{H}}\mathbf{AV} \quad \text{and} \quad \mathbf{C} = \mathbf{U\Omega U}^{-1}$$

are still satisfied.

(5) Then, the SVD of **A** is

$$\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^{\mathbf{H}}$$

eigenvector matrix of $\mathbf{A}\mathbf{A}^{\mathbf{H}}$, size: MxM

diagonal matrix, size: MxN

eigenvector matrix of $\mathbf{A}^{\mathbf{H}}\mathbf{A}$, size: NxN

If

$$\mathbf{U} = \begin{bmatrix} \mathbf{u_1} & \mathbf{u_2} & \cdots & \mathbf{u_M} \end{bmatrix}, \quad \mathbf{V} = \begin{bmatrix} \mathbf{v_1} & \mathbf{v_2} & \cdots & \mathbf{v_N} \end{bmatrix}$$

then

$$\mathbf{A} = s_1 \mathbf{u_1} \mathbf{v_1^H} + s_2 \mathbf{u_2} \mathbf{v_2^H} + \cdots + s_{K-1} \mathbf{u_{K\text{-}1}} \mathbf{v_{K\text{-}1}^H} + s_K \mathbf{u_K} \mathbf{v_K^H}$$

where $K = \min(M, N)$

$$s_n = S[n, n]$$

$$\mathbf{S}=\begin{bmatrix} s_1 & 0 & \cdots & 0 \\ 0 & s_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & s_N \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}$$

if $M > N$

$$\mathbf{S}=\begin{bmatrix} s_1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & s_2 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & s_M & 0 & \cdots & 0 \end{bmatrix}$$

if $M < N$

s_k is call the singular value

[Example 1] Perform the SVD for the following matrix

$$\mathbf{A} = \begin{bmatrix} 2 & 2 \\ -1 & 1 \\ -1 & 1 \end{bmatrix}$$

(Solution): First, we determine

$$\mathbf{B} = \mathbf{A}^{\mathbf{H}}\mathbf{A} = \begin{bmatrix} 6 & 2 \\ 2 & 6 \end{bmatrix} \qquad \mathbf{C} = \mathbf{A}\mathbf{A}^{\mathbf{H}} = \begin{bmatrix} 8 & 0 & 0 \\ 0 & 2 & 2 \\ 0 & 2 & 2 \end{bmatrix}$$

Then, we perform eigenvector-eigenvalue decomposition for **B** and **C**:

$$\mathbf{B} = \mathbf{V}\mathbf{D}\mathbf{V}^{\mathbf{H}} \quad \text{where} \quad \mathbf{V} = \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{bmatrix} \qquad \mathbf{D} = \begin{bmatrix} 8 & 0 \\ 0 & 4 \end{bmatrix}$$

$$\mathbf{C} = \tilde{\mathbf{U}}\boldsymbol{\Omega}\tilde{\mathbf{U}}^{\mathbf{H}}$$

where $\tilde{\mathbf{U}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1/\sqrt{2} & 1/\sqrt{2} \\ 0 & 1/\sqrt{2} & -1/\sqrt{2} \end{bmatrix}$ $\quad \boldsymbol{\Omega} = \begin{bmatrix} 8 & 0 & 0 \\ 0 & 4 & 0 \\ 0 & 0 & 0 \end{bmatrix}$

Note: The eigenvalues should be (i) normalized and (ii) sorted according to the magnitudes of the eigenvalues.

Then,

$$\mathbf{S_1} = \tilde{\mathbf{U}}^{\mathbf{H}}\mathbf{AV} = \begin{bmatrix} \sqrt{8} & 0 \\ 0 & -2 \\ 0 & 0 \end{bmatrix}$$

Then,

$$\mathbf{S} = \begin{bmatrix} |\sqrt{8}| & 0 \\ 0 & |-2| \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} \sqrt{8} & 0 \\ 0 & 2 \\ 0 & 0 \end{bmatrix}$$

Since $S_1[2, 2] < 0$, we change the sign of the 2nd column of $\tilde{\mathbf{U}}$ and obtain

$$\mathbf{U} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1/\sqrt{2} & 1/\sqrt{2} \\ 0 & -1/\sqrt{2} & -1/\sqrt{2} \end{bmatrix}$$

Therefore,

$$\mathbf{A} = \mathbf{USV^H} \quad \text{where}$$

$$\mathbf{U} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1/\sqrt{2} & 1/\sqrt{2} \\ 0 & -1/\sqrt{2} & -1/\sqrt{2} \end{bmatrix} \quad \mathbf{S} = \begin{bmatrix} \sqrt{8} & 0 \\ 0 & 2 \\ 0 & 0 \end{bmatrix} \quad \mathbf{V} = \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & -1/\sqrt{2} \end{bmatrix}$$

Note that

$$\mathbf{A} = s_1 \mathbf{u_1} \mathbf{v_1^H} + s_2 \mathbf{u_2} \mathbf{v_2^H}$$

$$\mathbf{A} = \sqrt{8} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{bmatrix} + 2 \begin{bmatrix} 0 \\ -1/\sqrt{2} \\ -1/\sqrt{2} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{2}} & \frac{-1}{\sqrt{2}} \end{bmatrix}$$

principal component

minor component

(Note):

(1) In fact, the eigenvalues of **B** and **C** has a close relation to the singular values of **A**.

$$\mathbf{S}^{\mathbf{H}}\mathbf{S} = \mathbf{D} \qquad \mathbf{S}\mathbf{S}^{\mathbf{H}} = \mathbf{\Omega}$$

$$S^2[n,n] = D[n,n] = \Omega[n,n]$$

Since

$$\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^{\mathbf{H}}$$

$$\mathbf{B} = \mathbf{A}^{\mathbf{H}}\mathbf{A} = \mathbf{V}\mathbf{S}^{\mathbf{H}}\mathbf{U}^{\mathbf{H}}\mathbf{U}\mathbf{S}\mathbf{V}^{\mathbf{H}} = \mathbf{V}\mathbf{S}^{\mathbf{H}}\mathbf{S}\mathbf{V}^{\mathbf{H}}$$

(Note):

(2) Even when $M = N$ (i.e., **A** is a square matrix), the SVD may not be the same as the eigenvector-eigenvalue decomposition.

For the SVD, **U** and **V** are both orthonormal matrices and the singular values are non-negative.

However, for a square matrix, the eigenvectors may not be orthogonal and the eigenvalues can be negative (even complex).

(3) Moreover, since **U** and **V** are usually different and $\mathbf{V}^{\mathbf{H}} \neq \mathbf{U}^{-1}$, one cannot use the SVD to compute the power of a matrix.

[Example 2] Determine the eigenvector-eigenvalue decomposition and the SVD of **A**.

$$\mathbf{A} = \begin{bmatrix} 2 & -1 \\ 0 & -1 \end{bmatrix}$$

(Solution): The eigenvalues of **A** are 2 and -1.

The eigenvectors corresponding to 2 is $[1\ 0]^T$
The eigenvectors corresponding to -1 is $[1, 3]^T$

Therefore,

$$\mathbf{A} = \begin{bmatrix} 1 & 1 \\ 0 & 3 \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & -1/3 \\ 0 & 1/3 \end{bmatrix}$$

To perform SVD for **A**,

$$\mathbf{B} = \mathbf{A}^{\mathbf{H}}\mathbf{A} = \begin{bmatrix} 4 & -2 \\ -2 & 2 \end{bmatrix} \qquad \mathbf{C} = \mathbf{A}\mathbf{A}^{\mathbf{H}} = \begin{bmatrix} 5 & 1 \\ 1 & 1 \end{bmatrix}$$

$$\mathbf{B} = \begin{bmatrix} 0.8507 & 0.5257 \\ -0.5257 & 0.8507 \end{bmatrix} \begin{bmatrix} 5.2361 & 0 \\ 0 & 0.7639 \end{bmatrix} \begin{bmatrix} 0.8507 & -0.5257 \\ 0.5257 & 0.8507 \end{bmatrix}$$

$$\mathbf{C} = \begin{bmatrix} 0.9732 & -0.2298 \\ 0.2298 & 0.9732 \end{bmatrix} \begin{bmatrix} 5.2361 & 0 \\ 0 & 0.7639 \end{bmatrix} \begin{bmatrix} 0.9732 & 0.2298 \\ -0.2298 & 0.9732 \end{bmatrix}$$

$$\begin{bmatrix} 0.9732 & -0.2298 \\ 0.2298 & 0.9732 \end{bmatrix}^{\mathbf{H}} \mathbf{A} \begin{bmatrix} 0.8507 & 0.5257 \\ -0.5257 & 0.8507 \end{bmatrix} = \begin{bmatrix} 2.2882 & 0 \\ 0 & -0.8740 \end{bmatrix}$$

$$\mathbf{A} = \begin{bmatrix} 0.9732 & 0.2298 \\ 0.2298 & -0.9732 \end{bmatrix} \begin{bmatrix} 2.2882 & 0 \\ 0 & 0.8740 \end{bmatrix} \begin{bmatrix} 0.8507 & -0.5257 \\ 0.5257 & 0.8507 \end{bmatrix}$$

8.1.2 Generalized Inverse Using the SVD

Suppose that the SVD of **A** is

$$\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^{\mathbf{H}}$$

Then the generalized inverse of **A** is

$$\mathbf{A}^{+} = \mathbf{V}\mathbf{S}^{+}\mathbf{U}^{\mathbf{H}}$$

where

$$S^{+}[n,n] = 1/S[n,n] \quad \text{if } S[n,n] \neq 0$$

$$S^{+}[n,n] = 0 \quad \text{if } S[n,n] = 0$$

$$size\left(\mathbf{S}^{+}\right) = N \times M \quad \text{if } size\left(\mathbf{S}\right) = M \times N$$

(Proof):

$$\mathbf{AA^{+}A = USV^{H}VS^{+}U^{H}USV^{H} = USS^{+}SV^{H}}$$

If

$$\mathbf{S_2 = S^{+}S}$$

then

$$S_2[n,n] = 1 \quad if \; S[n,n] \neq 0 \qquad\qquad S_2[n,n] = 0 \quad if \; S[n,n] = 0$$

Therefore,

$$\mathbf{S = SS^{+}S}$$

$$\mathbf{AA^{+}A = USV^{H} = A}$$

(1) $\mathbf{AA^{+}A = A}$ is satisfied.

Note: The generalized inverse derived from the SVD is in fact the pseudo inverse since

$$(2)\quad \mathbf{A}^{+}\mathbf{A}\mathbf{A}^{+} = \mathbf{A}^{+}$$

$$(3)\quad \left(\mathbf{A}\mathbf{A}^{+}\right)^{H} = \mathbf{A}\mathbf{A}^{+}$$

$$(4)\quad \left(\mathbf{A}^{+}\mathbf{A}\right)^{H} = \mathbf{A}^{+}\mathbf{A}$$

are all satisfied.

(Try to prove them)

[Example 3] Determine the generalized inverse of the following matrix

$$\mathbf{A} = \begin{bmatrix} 2 & 2 & 2 \\ 2 & 2 & 2 \\ 1 & -2 & 1 \\ -1 & 2 & -1 \end{bmatrix}$$

Note: Since the 1st and the 3rd columns are dependent, we cannot use the method of

$$(\mathbf{A}^{\mathbf{T}}\mathbf{A})^{-1}\mathbf{A}^{\mathbf{T}}$$

to determine the generalized inverse. Instead, we should apply the SVD method.

$$\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^{\mathbf{H}} \qquad \mathbf{A}^{+} = \mathbf{V}\mathbf{S}^{+}\mathbf{U}^{\mathbf{H}}$$

(Solution): Since

$$\mathbf{A} = \begin{bmatrix} 2 & 2 & 2 \\ 2 & 2 & 2 \\ 1 & -2 & 1 \\ -1 & 2 & -1 \end{bmatrix}$$

$$\mathbf{B} = \mathbf{A}^{\mathbf{H}}\mathbf{A} = \begin{bmatrix} 10 & 4 & 10 \\ 4 & 16 & 4 \\ 10 & 4 & 10 \end{bmatrix} \qquad \mathbf{C} = \mathbf{A}\mathbf{A}^{\mathbf{H}} = \begin{bmatrix} 12 & 12 & 0 & 0 \\ 12 & 12 & 0 & 0 \\ 0 & 0 & 6 & -6 \\ 0 & 0 & -6 & 6 \end{bmatrix}$$

$$\mathbf{B} = \mathbf{V}\mathbf{D}\mathbf{V}^{\mathbf{H}}$$

where $\mathbf{V} = \begin{bmatrix} 1/\sqrt{3} & 1/\sqrt{6} & 1/\sqrt{2} \\ 1/\sqrt{3} & -2/\sqrt{6} & 0 \\ 1/\sqrt{3} & 1/\sqrt{6} & -1/\sqrt{2} \end{bmatrix}$ $\quad \mathbf{D} = \begin{bmatrix} 24 & 0 & 0 \\ 0 & 12 & 0 \\ 0 & 0 & 0 \end{bmatrix}$

$\mathbf{C} = \tilde{\mathbf{U}}\boldsymbol{\Lambda}\tilde{\mathbf{U}}^{\mathbf{H}}$ where

$$\tilde{\mathbf{U}} = \begin{bmatrix} 1/\sqrt{2} & 0 & 0 & 1/\sqrt{2} \\ 1/\sqrt{2} & 0 & 0 & -1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & -1/\sqrt{2} & 1/\sqrt{2} & 0 \end{bmatrix} \qquad \boldsymbol{\Lambda} = \begin{bmatrix} 24 & 0 & 0 & 0 \\ 0 & 12 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

Then

$$\mathbf{S_1} = \tilde{\mathbf{U}}^{\mathbf{H}}\mathbf{AV} = \begin{bmatrix} \sqrt{24} & 0 & 0 \\ 0 & \sqrt{12} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Since all entries of $\mathbf{S_1}$ are non-negative,

$$\mathbf{S} = \mathbf{S_1} \qquad \mathbf{U} = \tilde{\mathbf{U}}^{\mathbf{H}}$$

$$\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^{\mathbf{H}} \qquad \mathbf{U} = \begin{bmatrix} 1/\sqrt{2} & 0 & 0 & 1/\sqrt{2} \\ 1/\sqrt{2} & 0 & 0 & -1/\sqrt{2} \\ 0 & 1/\sqrt{2} & 1/\sqrt{2} & 0 \\ 0 & -1/\sqrt{2} & 1/\sqrt{2} & 0 \end{bmatrix}$$

$$\mathbf{S} = \begin{bmatrix} \sqrt{24} & 0 & 0 \\ 0 & \sqrt{12} & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \qquad \mathbf{V} = \begin{bmatrix} 1/\sqrt{3} & 1/\sqrt{6} & 1/\sqrt{2} \\ 1/\sqrt{3} & -2/\sqrt{6} & 0 \\ 1/\sqrt{3} & 1/\sqrt{6} & -1/\sqrt{2} \end{bmatrix}$$

$$\mathbf{A}^{+} = \mathbf{V}\mathbf{S}^{+}\mathbf{U}^{\mathbf{H}} \qquad \mathbf{S}^{+} = \begin{bmatrix} 1/\sqrt{24} & 0 & 0 & 0 \\ 0 & 1/\sqrt{12} & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}$$

$$\mathbf{A}^{+} = \begin{bmatrix} 1/12 & 1/12 & 1/12 & -1/12 \\ 1/12 & 1/12 & -1/6 & 1/6 \\ 1/12 & 1/12 & 1/12 & -1/12 \end{bmatrix}$$

8.2 Principal Component Analysis

Principal component analysis (PCA) is to find the principal component of a set of data.

Principal components: Corresponding to larger singular values for SVD

[Process of PCA]

Suppose that there is a set of data. The number of data is M and each data has the length of N.

$$\mathbf{x_m} = \begin{bmatrix} x_{m,1} & x_{m,2} & x_{m,3} & \cdots & x_{m,N} \end{bmatrix}$$

$m = 1, 2, \ldots, M$

(In usual, $M >> N$)

(1) First, we subtract each entry by $\bar{x}_n = \frac{1}{M}\sum_{m=1}^{M} x_{m,n}$

$$\mathbf{a_m} = \begin{bmatrix} a_{m,1} & a_{m,2} & a_{m,3} & \cdots & a_{m,N} \end{bmatrix}$$

where $a_{m,n} = x_{m,n} - \bar{x}_n$, $\quad \bar{x}_n = \frac{1}{M}\sum_{m=1}^{M} x_{m,n}$

(2) Then, construct an *M*x*N* matrix **A**:

$$\mathbf{A} = \begin{bmatrix} \mathbf{a_1} \\ \mathbf{a_2} \\ \vdots \\ \mathbf{a_M} \end{bmatrix} = \begin{bmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,n} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m,1} & a_{m,2} & \cdots & a_{m,n} \end{bmatrix}$$

(3) Then, perform SVD for **A**

$$\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^{\mathbf{H}}$$

(4) Then

second important

(N-1)th important

Nth important

$$\mathbf{A} = s_1\mathbf{u_1}\mathbf{v_1^H} + s_2\mathbf{u_2}\mathbf{v_2^H} + \cdots + s_{N-1}\mathbf{u_{N-1}}\mathbf{v_{N-1}^H} + s_N\mathbf{u_N}\mathbf{v_N^H}$$

most important

where $s_n = S[n,n]$

$$\mathbf{U} = [\mathbf{u_1} \quad \mathbf{u_2} \quad \cdots \quad \mathbf{u_M}], \quad \mathbf{V} = [\mathbf{v_1} \quad \mathbf{v_2} \quad \cdots \quad \mathbf{v_N}]$$

If we want to reduce the component from N to L due to the consideration of compression or feature selection, then

$$\mathbf{A} \cong \mathbf{A_1} = s_1\mathbf{u_1}\mathbf{v_1^H} + s_2\mathbf{u_2}\mathbf{v_2^H} + \cdots + \mathbf{s_L}\mathbf{u_L}\mathbf{v_L^H}$$

Note:

$$\mathbf{x_m} \cong c_{m,1}\mathbf{v_1^H} + c_{m,2}\mathbf{v_2^H} + \cdots + c_{m,L}\mathbf{v_L^H} + \begin{bmatrix} x_{0,1} & x_{0,2} & \cdots & x_{0,L} \end{bmatrix}$$

where

$$c_{m,n} = s_n u_n[m]$$

← m^{th} entry of $\mathbf{u_n}$

$\mathbf{v_1^H}, \mathbf{v_2^H}, \cdots, \mathbf{v_L^H}$ can be viewed as the most important L axes

Main Applications of the PCA

(1) Dimensionality reduction (i.e., feature selection) for pattern recognition and machine learning

(2) Data compression

(3) Data mining

(4) Identifying the principal axis of an object in an image

(5) Line approximation

Example of PCA

3. 在處理二維數據時，有種方法是將數據垂直投影到某一直線，並以該直線為數線，進而了解投影點所成一維數據的變異。下圖的一組二維數據，試問投影到哪一選項的直線，所得之一維投影數據的變異數會是最小？

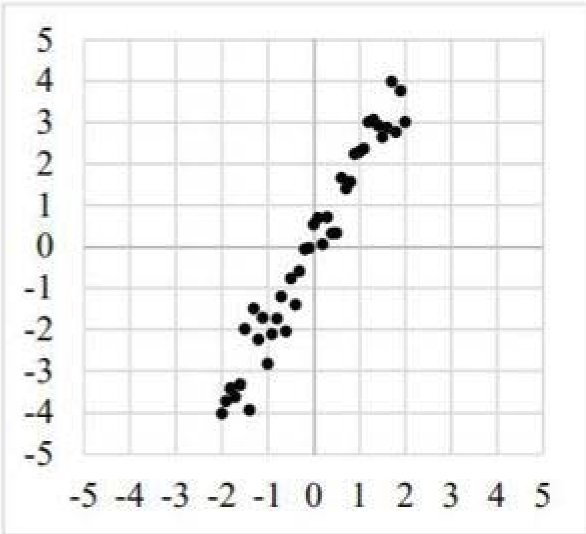
(1) $y=2x$

(2) $y=-2x$

(3) $y=-x$

(4) $y=\frac{x}{2}$

(5) $y=-\frac{x}{2}$



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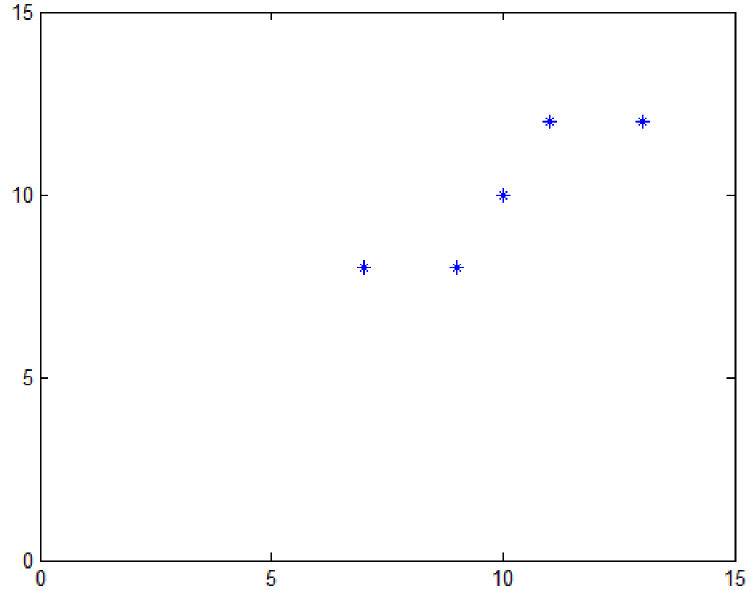
[Example 1] Suppose that there are 5 points in a 2-D space and their coordinates are

$$(7,8),\ (9,8),\ (10, 10),\ (11,12),\ (13,12)$$

Try to find a line that can approximate these points.

(Note): $M = 5$, $N = 2$



(Solution):

First, since the mean of these 5 points is

$$(10, 10),$$

we subtract these points by (10, 10) and obtain

$$(-3, -2),\ (-1\ -2),\ (0, 0),\ (1, 2),\ (3, 2)$$

(-3, -2), (-1 -2), (0, 0), (1, 2), (3, 2)

Then, we construct a 5x2 matrix **A**:

$$\mathbf{A} = \begin{bmatrix} -3 & -2 \\ -1 & -2 \\ 0 & 0 \\ 1 & 2 \\ 3 & 2 \end{bmatrix}$$

Then, we perform SVD for **A**:

$$\mathbf{A} = \mathbf{U}\mathbf{S}\mathbf{V}^{\mathbf{H}}$$

$$\mathbf{U} = \begin{bmatrix} -0.6116 & 0.3549 & 0 & 0.0393 & 0.7060 \\ -0.3549 & -0.6116 & 0 & 0.7060 & -0.0393 \\ 0 & 0 & 1 & 0 & 0 \\ 0.3549 & 0.6116 & 0 & 0.7060 & -0.0393 \\ 0.6116 & -0.3549 & 0 & 0.0393 & 0.7060 \end{bmatrix}$$

$$\mathbf{S} = \begin{bmatrix} 5.8416 & 0 \\ 0 & 1.3695 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{bmatrix}$$

$$\mathbf{V} = \begin{bmatrix} 0.7497 & -0.6618 \\ 0.6618 & 0.7497 \end{bmatrix}$$

Then, **A** can be expanded by

$$\mathbf{A} = 5.8416\begin{bmatrix}-0.6116\\-0.3549\\0\\0.3549\\0.6116\end{bmatrix}\begin{bmatrix}0.7497 & 0.6618\end{bmatrix}+1.3695\begin{bmatrix}0.3549\\-0.6116\\0\\0.6116\\-0.3549\end{bmatrix}\begin{bmatrix}-0.6618 & 0.7497\end{bmatrix}$$

principal component (5.8416) — secondary component (1.3695)

Therefore,

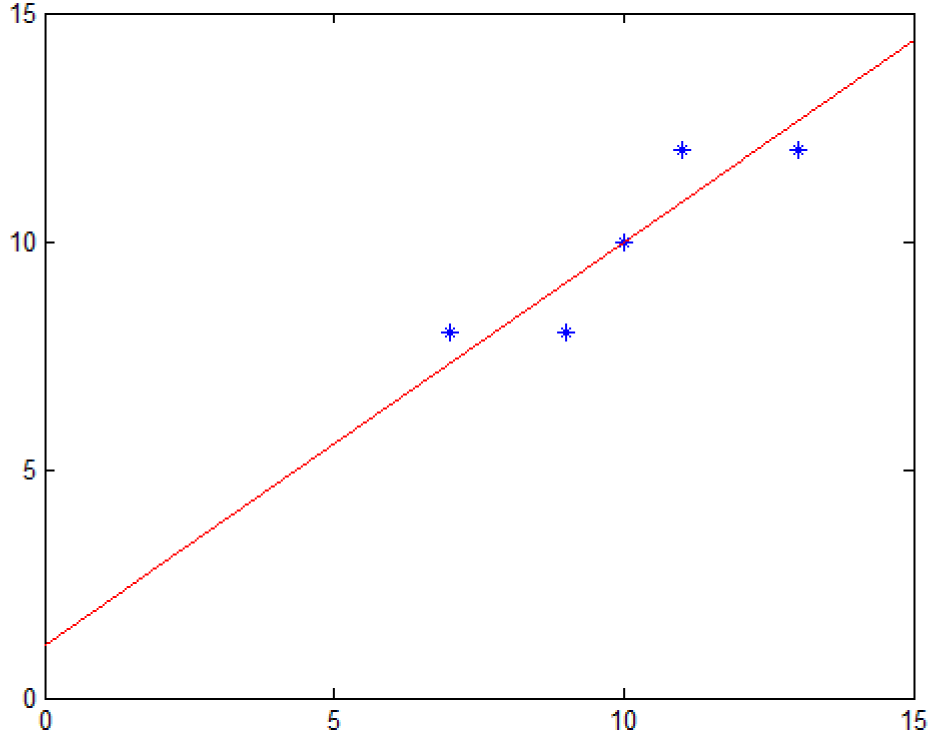
$$\mathbf{A} \cong 5.8416\begin{bmatrix}-0.6116\\-0.3549\\0\\0.3549\\0.6116\end{bmatrix}\begin{bmatrix}0.7497 & 0.6618\end{bmatrix}=\begin{bmatrix}-3.5726\\-2.0733\\0\\2.0733\\3.5726\end{bmatrix}\begin{bmatrix}0.7497 & 0.6618\end{bmatrix}$$

$$\begin{bmatrix} 7 & 8 \\ 9 & 8 \\ 0 & 0 \\ 11 & 12 \\ 13 & 12 \end{bmatrix} \cong \begin{bmatrix} -3.5726 \\ -2.0733 \\ 0 \\ 2.0733 \\ 3.5726 \end{bmatrix} \begin{bmatrix} 0.7497 & 0.6618 \end{bmatrix} + \begin{bmatrix} 10 & 10 \\ 10 & 10 \\ 10 & 10 \\ 10 & 10 \\ 10 & 10 \end{bmatrix}$$

Approximation line:

$$\begin{bmatrix} 10 & 10 \end{bmatrix} + c\begin{bmatrix} 0.7497 & 0.6618 \end{bmatrix}$$

$c \in (-\infty, \infty)$



[Simplification for Computation]

Suppose that we only want to find the most important L axes of the data. (It is usually the case for practical applications).

If M is very large, then the MxM matrix **U is unnecessary to be computed**. One only has to perform eigenvector-eigenvalue decomposition for **B** and obtain the NxN matrix **V**:

$$\mathbf{B} = \mathbf{A}^{\mathbf{H}}\mathbf{A} \qquad\qquad \mathbf{B} = \mathbf{V}\mathbf{D}\mathbf{V}^{-1}$$

If $D[n, n]$ is larger than other diagonal entries of **D**, then the nth column of **V** is the principal axis.

附錄十一 Some Common Mathematical Notations

(1) Commutator

$$[\mathbf{A},\mathbf{B}] = \mathbf{AB} - \mathbf{BA}$$

(2) Trace

$$tr(\mathbf{A}) = \sum_{n=1}^{N} A(n,n)$$

(3) Bras and Kets Notations

$$\langle \mathbf{A} | \mathbf{B} \rangle = \underbrace{\begin{bmatrix} \mathbf{a}_1^* & \mathbf{a}_2^* & \cdots & \mathbf{a}_N^* \end{bmatrix}}_{\mathbf{A}^H} \underbrace{\begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \vdots \\ \mathbf{b}_N \end{bmatrix}}_{\mathbf{B}}$$

A and **B** are column vectors.

$$\langle \mathbf{A} | = \begin{bmatrix} \mathbf{a}_1^* & \mathbf{a}_2^* & \cdots & \mathbf{a}_N^* \end{bmatrix} \qquad | \mathbf{B} \rangle = \begin{bmatrix} \mathbf{b}_1 \\ \mathbf{b}_2 \\ \vdots \\ \mathbf{b}_N \end{bmatrix}$$

(4) sup: supremum (the least upper bound，上確界)

$$\sup\{x \mid 1 < x < 2\} = 2$$

$$\sup\left\{(-1)^n - 1/n \mid n \in N\right\} = 1$$

(5) inf: infimum (the greatest lower bound，下確界)

$$\inf\{x \mid 1 < x < 2\} = 1$$

$$\inf\left\{e^{-x} \mid x \in R\right\} = 0$$

(6) card: the number of elements in a set

$$card(\{x, y\}) = 2$$

$$card\left(\left\{x^2, y^2, xy, x, y, 1\right\}\right) = 6$$