# Linear algebra for computational statistics III

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### Things to know

- basic operation of matrix
- spanning space, null space
- projection and geometry
- linear map and matrix

# Decomposition of matrix

Decomposition of linear maps

#### Step 3

행렬이 대응시키는 변환을 분해하는 과정을 소개한다. 먼저 내적을 도입하여, 벡터공간 위에서 거리와 각도가 자연스럽게 정의되는 과정을 살펴본다. 다음으로 대칭인 반양정치행렬의 분해를 특별한 직교 선형변환의 분해로 이해할 수 있으며, 이를 통해 행렬의 대응을 분해하여 해석한다. 여기서는 내적공간(inner product space)와 정사형(projection), Spectral Decomposition, Singular Value Decomposition을 배운다.

Inner product An inner product space is a vector space V with an inner product:

$$\langle \cdot, \cdot \rangle : V \times V \to \mathbb{R}$$

that satisfies the following three properties for all vectors  $x, y, z \in V$  and all scalars  $a \in \mathbb{R}$ .

- Symmetry:  $\langle x, y \rangle = \langle y, x \rangle$
- Linearity:

$$\langle ax, y \rangle = a \langle x, y \rangle$$
  
 $\langle x + y, z \rangle = \langle x, z \rangle + \langle y, z \rangle$ 

• Positive-definite:  $\langle x, x \rangle > 0, x \in V - \{0\}$ 

#### example

Suppose that  $a,b \in \mathbb{R}^p$ 

- Let  $\langle a, b \rangle = a^{\top}b$ . Then the  $\langle \cdot, \cdot \rangle$  is inner product?
- Let  $H \in \mathbb{R}^{p \times p}$  is symmetric and  $\langle a, b \rangle = a^{\top} H b$ . Then the  $\langle \cdot, \cdot \rangle$  is inner product?
- ullet If H is positive definite, ...

(NOTE) Vector space에는 Addition과 scalar multiplication 연산만 정의되어 있다. Vector space 위에 inner production 연산을 정의해놓으면, Vector space 위에 각도를 정의할 수 있다. 한편 inner production 연산이 주어지면 원소의 길이(norm) 혹은 두 원소간의 거리 (distance)를 정의할 수 있다.

- For  $x,y \in V$  define  $\langle x,y \rangle = x^{\top}y$ . If  $x^{\top}y = 0$  we write  $x \perp y$
- We define the norm of  $x \in V$  by  $||x|| = \sqrt{x^{\top}x}$
- We can define the distance between x and y by d(x,y) = ||x-y||

Hereafter, we use the above definition of the inner product and the norm in our vector space V.

### angle and inner product (law of cosine)

- Let a point A, B, C in  $\mathbb{R}^2$  and C is the origin and B is a point on x-axis.
- Let the length of  $\overline{AB}$ ,  $\overline{BC}$  and  $\overline{CA}$  be c, a, and b, respectively.
- Let the angle  $\angle C$  be  $\theta$ .
- The point A is  $(b\cos\theta, b\sin\theta)$ , and the point B=(a,0). Thus,

$$c^{2} = (b\cos\theta - a)^{2} + b^{2}\sin^{2}\theta$$
$$= a^{2} + b^{2} - 2ab\cos\theta$$

### angle and inner product

Because the law of cosine is the fact derived only from geometry, we can apply the law of cosine to a Euclidean space.

Consider a vector u, v, and u-v and denote the norms of the vectors by  $\|u\|$ ,  $\|v\|$ , and  $\|u-v\|$ , respectively. Note that  $\|u\|$ ,  $\|v\|$ , and  $\|u-v\|$  correspond to b, a, and c. By the law of cosine

$$||u - v||^2 = ||u||^2 + ||v||^2 - 2||u|| ||v|| \cos(\theta),$$

which reduces to

$$u^{\top}v = ||u|||v||\cos(\theta).$$

As a result the angle in  $\mathbb{R}^p$  are defined by the law of cosine.

### angle and inner product Thus,

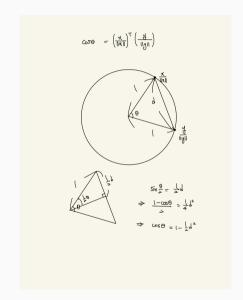
- $\cos(\theta) = u^{\mathsf{T}} v / (\|u\| \|v\|)$
- $u^{\top}v = 0$  is regarded as  $u \perp v$

ch) Let u and v be points on a unit sphere and let d be a Euclidean distance between u and v. Then,

$$u^{\top}v = \cos(\theta) = 1 - \frac{1}{2}d^2.$$

The equation shows the relationships of inner product, cosine similarity, and distance.

### angle and inner product



### Projection

Suppose that V is an inner product vector space. Let  $x,y\in V$  then there exists  $\hat{y}\in\mathcal{C}(x)$  such that  $(y-\hat{y})\perp x$ . That is y is decomposed into  $y=\hat{y}+(y-\hat{y})$  with  $\hat{y}\perp(y-\hat{y})$ .

### Transpose and projection (figure will be corrected!)

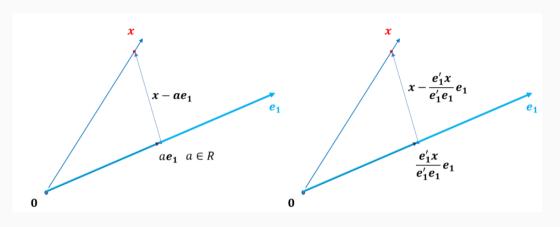


Figure 1: Illustration of projection via transpose operation

$$y = ax + (y - ax)$$
 with  $a = y^{\top}x/\|x\|^2 \in \mathbb{R}$ 

Projection Let  $y, x_1, \cdots, x_k \in V$  and suppose that  $x_1, \cdots, x_k$  are linearly independent. Consider  $X = [x_1, \cdots, x_k]$  and  $\mathcal{C}(X)$ . Then, how can we find  $\hat{y} \in \mathcal{C}(X)$  such that

$$y = \hat{y} + (y - \hat{y})$$

satisfying  $\hat{y} \perp (y - \hat{y})$ ?

The answer is the Projection map (matrix)!

Orthogonal Projection Let  $x, y \in \mathbb{R}^p$  and consider  $\Pi$ , a linear map from  $\mathbb{R}^p$  to  $\mathbb{R}^p$ . The projection map of y onto C(x) satisfies the following properties:

- $\Pi y \in \mathcal{C}(x)$ ;
- $(\Pi y)^{\top} y = y^{\top} (\Pi y) = 0;$
- $\Pi(\Pi y) = \Pi y$

### Orthogonal Projection

Orthogonal projection is a linear map defined by  $\Pi: V \mapsto V$  (in fact, we can understand the P as a matrix) such that  $\Pi = \Pi^2 = \Pi^\top$ .

- Let  $\Pi = x(x^{\top}x)^{-1}x^{\top}$  then  $\Pi = \Pi^2 = \Pi^{\top}$ ?
- $\Pi y \in \mathcal{C}(x)$  for  $x \in V$ ?
- $\langle \Pi y, y \Pi y \rangle = 0$ ?

You can conclude that the  $\Pi$  is the orthogonal projection operator (onto C(x)).

#### Orthogonal Projection

- Let  $x, y \in \mathbb{R}^n$  and compute the projection of y onto  $\mathcal{C}(x)$ . Then, it is given by  $(x(x^\top x)^{-1}x^\top)y$ . Show that  $x(x^\top x)^{-1}x^\top$  is a projection operator.
- Let  $X \in \mathbb{R}^{n \times m}$  and  $y \in \mathbb{R}^n$ . Compute the projection of y onto  $\mathcal{C}(X)$ .
- Write an example and confirm the result numerically.

### 잠깐!

회귀모형의 OLS를 돌이켜보자. Response vector  $Y \in \mathbb{R}^n$ 과 predictor matrix  $X \in \mathbb{R}^{n \times p}$  일때, OLS를 이용한 Y값의 추정량은

$$\hat{Y} = X(X^{\top}X)^{-1}X^{\top}Y \in \mathbb{R}$$

로 주어진다. 여기서  $X(X^\top X)^{-1}X^\top$ 가  $\mathcal{C}(X)$ 에 Projection operator 고  $\hat{Y}\in\mathcal{C}(X)$  이며  $(Y-\hat{Y})\perp\hat{Y}$ 임을 알 수 있다.

Projection은 벡터 성분을 직교분해할 때 흔히 볼 수 있었던 연산이다.

### Basic on undergraduate levels

- Symmetric Matrix
- Orthogonal Matrix

### Orthogonal matrix

ullet Orthogonal matrix E: a square matrix satisfying

$$E=[e_1,\cdots,e_p],$$

where  $e_i^{\top} e_k = 0$  for  $j \neq k$  and  $||e_j|| = 1$  for all j.

- It is easily shown that  $E^{\top}E = I$ .
- Because  $E(E^{\top}E) = E$ ,  $EE^{\top} = I$ .

That is,  $E^{\top}E = EE^{\top} = I$ , and  $E^{\top}$  is the inverse of E.

### Orthogonal matrix (Isometric transformation)

Let  $E \in \mathbb{R}^{p \times p}$  be orthogonal matrix and  $x, y \in \mathbb{R}^p$ . d(x, y) = d(Ex, Ey)?

$$d(x,y)^{2} = (x-y)^{\top}(x-y) = (x-y)^{\top}E^{\top}E(x-y)$$
$$= ||E(x-y)||^{2} = d(Ex, Ey)^{2}$$

The map  $\mathcal{L}_E$  preserves the distance (isometric). Actually, E is understood as the rotation map.

### Orthogonal matrix (Rotation)

What is the geometrical meaning of the first column of an orthogonal matrix?

Let E be the orthogonal and  $a_1 = (1, 0, \dots, 0)$ .

- $Ea_1$  is the first column vector.
- In addition,  $Ea_1$  is the image of a linear map E for  $a_1$ , which is the first coordinate basis vector.
- That is, the first column vector is the transformed image of the first coordinate basis vector.

To sum up, each column of E denotes an image of each coordinate basis transformed by E. Since the transformed image is orthogonal to each other, the map can be regarded as a geometrical rotation.

#### Diagonal matrix

Let  $D = diag(d_1, \dots, d_p) \in \mathbb{R}^{p \times p}$  be diagonal matrix and  $x = (x_1, \dots, x_p) \in \mathbb{R}^p$ . Then,

$$Dx = (d_1x_1, \cdots, d_px_p)^{\top}$$

The map D is called the scaling map.

앞다행, 뒤다열!

### Eigendecomposition

Let  $A \in \mathbb{R}^{p \times p}$  be a symmetric matrix. Then there exists an orthogonal matrix E and a diagonal matrix D (with real-valued elements) such that

$$A = EDE^{\top}$$

• Orthogonality of E: write

$$E = [e_1, \cdots, e_p]$$

then  $e_i^{\top} e_k = 0$  for  $j \neq k$  and  $||e_j|| = 1$  for all j.

 $\bullet$  Projection onto  $\mathcal{C}(e_j)$  is given by  $e_j(e_j^\top e_j)^{-1}e_j^\top = e_je_j^\top$ 

Eigendecomposition Suppose that A be a symmetric matrix. Let  $\lambda_j$  be the jth diagonal element of D, then we can write

$$A = EDE^{\top} = \sum_{j=1}^{p} \lambda_j e_j e_j^{\top}$$

We can know that A is the sum of orthogonal projection operators.  $e_j$ s are eigenvector and  $\lambda_j$  is the associated eigenvalue.  $C(e_j)$  is eigenspace spaned by  $e_j$ .

For simplicity let A be  $2 \times 2$  matrix.

• Let  $D_1 = \operatorname{diag}(\lambda_1, 0)$  and  $D_2 = \operatorname{diag}(\lambda_2, 0)$ , then

$$D_1 E^\top = \lambda_1 \left( \begin{array}{c} e_1^\top \\ 0 \end{array} \right) \text{ and } D_2 E^\top = \lambda_2 \left( \begin{array}{c} 0 \\ e_2^\top \end{array} \right)$$

• We can easily show that

$$\left( \begin{array}{cc} e_1 & e_2 \end{array} \right) \left( \begin{array}{c} e_1^\top \\ e_2^\top \end{array} \right) = e_1 e_1^\top + e_2^\top e_2$$

Thus,

$$A = EDE^{\top} = E(D_1E^{\top} + D_2E^{\top}) = \lambda_1 e_1 e_1^{\top} + \lambda_2 e_2^{\top} e_2$$

### Eigendecomposition

This eigendecomposition can be viewed as the decomposition of a linear map:

$$\mathcal{L}_A = \sum_{j=1}^p \lambda_j \mathcal{L}_{E_j},$$

where  $E_j = e_j e_i^{\top}$ .

Note that

 $\bullet$  projection onto  $\mathcal{C}(e_j)$  is given by  $e_j(e_j^\top e_j)^{-1}e_j^\top = e_je_j^\top$ 

Therefore,

$$\mathcal{L}_A(x) = \sum_{j=1}^p \lambda_j \mathcal{L}_{E_j}(x),$$

where  $\mathcal{L}_{E_j}(x)$  is projection onto the jth eigenspace.

### **Approximation of Linear map**

Let 
$$A^{(k)} = \sum_{j=1}^k \lambda_j e_j e_j^{\top}$$
 then  $A^{(k)}$  approximates  $A$ ?

$$\begin{split} EDE^{\top}\mathbf{x} &= [e_{1}, \cdots, e_{p}] \mathsf{diag}(\lambda_{1}, \cdots, \lambda_{p}) \begin{pmatrix} e_{1}^{\top} \\ \vdots \\ e_{p}^{\top} \end{pmatrix} \mathbf{x} \\ &= [e_{1}, \cdots, e_{p}] \mathsf{diag}(\lambda_{1}, \cdots, \lambda_{p}) \begin{pmatrix} e_{1}^{\top}\mathbf{x} \\ \vdots \\ e_{p}^{\top}\mathbf{x} \end{pmatrix} \\ &= [e_{1}, \cdots, e_{p}] \begin{pmatrix} \lambda_{1}e_{1}^{\top}\mathbf{x} \\ \vdots \\ \lambda_{p}e_{p}^{\top}\mathbf{x} \end{pmatrix} \\ &= \sum_{i=1}^{p} e_{j}(\lambda_{j}e_{j}^{\top}\mathbf{x}) = (\sum_{i=1}^{p} \lambda_{j}e_{j}e_{j}^{\top})\mathbf{x}, \end{split}$$

Eigendecomposition shows the linear map of a symmetric matrix as the composition of three operations:

$$Ax = EDE^{\top}x$$

$$x \mapsto E^{\top}x$$
 (rotation)  $\mapsto D(E^{\top}x)$  (scaling)  $\mapsto E(DE^{\top}x)$  (reverse rotation)

#### Inverse matrix of positive definite matrix

Let A be symmetric and nonnegative definite matrix. Then the minimum eigenvalue is positive if and only if A is positive definite.

pf) Let  $\lambda_{min}$  be the minumum eigenvalue of  $\mathbf{A}$ . Assume that  $\lambda_{min} > 0$ . Let  $\mathbf{x} = \sum_{j=1} a_j e_j \neq 0$ , then

$$\mathbf{x}^{\top} \mathbf{A} \mathbf{x} = \sum_{j=1}^{p} \lambda_j (e_j^{\top} \mathbf{x})^2 = \sum_{j=1}^{p} \lambda_j a_j^2 > 0.$$

Assume that **A** is pd matrix. WLOG, let  $\lambda_p$  be the minimum eigenvalue of **A**. Then,

$$e_p^{\top} \mathbf{A} e_p = \sum_{j=1} \lambda_j (e_j^{\top} e_p)^2 = \lambda_p > 0.$$

#### Inverse matrix of positive definite matrix

The inverse matrix of such A is given by

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

$$\mathsf{pf}) \; \mathbf{E} D^{-1} \mathbf{E}^{\top} \mathbf{A} = \mathbf{E} D^{-1} \underbrace{\mathbf{E}^{\top} \mathbf{E}}_{=I} D \mathbf{E}^{\top} = I$$

and  $\mathbf{A}\mathbf{E}D^{-1}\mathbf{E}^{\top} = \mathbf{E}D\underbrace{\mathbf{E}^{\top}\mathbf{E}}_{=I}D^{-1}\mathbf{E}^{\top} = I$ . By definition of the inverse matrix, we obtain the result.

### 잠깐!

특별히 pd matrix  $A \in \mathbb{R}^{p \times p}$ 에 대해서

$$\lambda_{\min} = \min_{x} \frac{x^{\top} A x}{\|x\|^2}, \quad \lambda_{\max} = \max_{x} \frac{x^{\top} A x}{\|x\|^2}$$

라 놓으면  $\lambda_{\max} \geq \lambda_{\min} > 0$  이며,  $\lambda_{\max}, \lambda_{\min}$  각각 A의 maximum eigenvalue, minimum eigenvalue에 해당한다. 한편 pd matrix A에서 Eigenmatrix의 열  $e_1, \cdots e_p$ 는 다음과 같이 구할 수 있다.

- $\bullet \ e_1 = \operatorname{argmax}_{x \in \mathbb{R}^p} \frac{x^{\top} A x}{\|x\|^2}$
- $e_2 = \operatorname{argmax}_{x \in \mathbb{R}^p : x \perp e_1} \frac{x^{\top} A x}{\|x\|^2}$
- $\bullet \ \ e_3 = \mathrm{argmax}_{x \in \mathbb{R}^p: x \perp \mathcal{C}([e_1, e_2])} \frac{x^{\top} A x}{\|x\|^2}$
- ...

### **Singular Value Decomposition**

Let  $\mathbf{X} \in \mathbb{R}^{n \times p}$  (p < n) denote a (row-centered) data matrix whose rows are observations and columns are variables. The *singular value decomposition* (SVD) factorises  $\mathbf{X}$  as

$$\mathbf{X} = \mathbf{U} \, \mathbf{\Sigma} \, \mathbf{V}^{\top},$$

where

- $\mathbf{U} = [U_1, \dots, U_p] \in \mathbb{R}^{n \times p}$  contains the left singular vectors  $(\mathbf{U}^\top \mathbf{U} = \mathbf{I}_p)$ ;
- $\mathbf{V} = [V_1, \dots, V_p] \in \mathbb{R}^{p \times p}$  contains the right singular vectors  $(\mathbf{V}^\top \mathbf{V} = \mathbf{I}_p)$ ;
- $\Sigma = \operatorname{diag}(\sigma_1, \dots, \sigma_p)$  with singular values  $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_p > 0$ ;
- $r = \operatorname{rank}(\mathbf{X}) \le \min\{n, p\}.$

# Singular Value Decomposition: Example i

Let

$$\mathbf{A} = \begin{bmatrix} 3 & 1 \\ 2 & 2 \\ 1 & 3 \end{bmatrix} \in \mathbb{R}^{3 \times 2}$$

be a real matrix with rank p=2. The **reduced singular value decomposition** (SVD) of  ${\bf A}$  is given by

$$\mathbf{A} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^{\top}$$

where

• 
$$\mathbf{U} = \begin{bmatrix} -0.5026 & 0.7746 \\ -0.5740 & -0.6325 \\ -0.6464 & 0.0000 \end{bmatrix} \in \mathbb{R}^{3\times 2}$$
 contains the left singular vectors (orthonormal:  $\mathbf{U}^{\mathsf{T}}\mathbf{U} = \mathbf{I}_2$ ).

# Singular Value Decomposition: Example ii

- $\Sigma = \begin{bmatrix} 5.1962 & 0 \\ 0 & 1.7321 \end{bmatrix} \in \mathbb{R}^{2 \times 2}$  is the diagonal matrix of singular values,
- $\mathbf{V} = \begin{bmatrix} -0.7071 & -0.7071 \\ -0.7071 & 0.7071 \end{bmatrix} \in \mathbb{R}^{2\times 2}$  contains the right singular vectors (orthonormal:  $\mathbf{V}^{\top}\mathbf{V} = \mathbf{I_2}$ ).

Thus, the matrix A can be approximately reconstructed as

$$\mathbf{A} pprox \mathbf{U} \mathbf{\Sigma} \mathbf{V}^{ op} = egin{bmatrix} 3 & 1 \ 2 & 2 \ 1 & 3 \end{bmatrix}.$$

### **Data and representation**

 $(A)_{ij}$  denotes the entry of A in the row i and the column j. For  $i=1,\cdots,n$ ,

$$x_i = (X)_{i1}e_1 + \dots + (X)_{ip}e_p,$$

where  $\{e_1, \ldots, e_p\}$  forms the standard basis of  $\mathbb{R}^p$ .

- Coordinate system:  $(e_1, \dots, e_p)$
- Scaling factor:  $(1, \ldots, 1) \in \mathbb{R}^p$
- Representation of  $x_i$  w.r.t the  $(e_1,\cdots,e_p)$ :  $((X)_{i1},\cdots,(X)_{ip})\in\mathbb{R}^p$ .

How to obtain low dimensional representation of  $x_i$  effectively?

### **SVD: Definition & Structure**

### Full SVD (rank p)

$$\mathbf{X} = \underbrace{\mathbf{U}}_{n \times p} \underbrace{\mathbf{\Sigma}}_{p \times p} \underbrace{\mathbf{V}}_{p \times p}^{\top} = \sum_{i=1}^{p} \sigma_{i} U_{i} V_{i}^{\top}, \quad \sigma_{1} \ge \dots \ge \sigma_{p} > 0.$$

$$\mathbf{U}\mathbf{\Sigma} = \begin{bmatrix} U_1 & \cdots & U_p \end{bmatrix} \begin{bmatrix} \sigma_1 & & & \\ & \ddots & & \\ & & \sigma_p \end{bmatrix} = \begin{bmatrix} \sigma_1 U_1 & \cdots & \sigma_p U_p \end{bmatrix}$$

### SVD: Definition & Structure

$$\mathbf{X} = \begin{bmatrix} \sigma_1 U_1 & \cdots & \sigma_p U_p \end{bmatrix} \begin{bmatrix} V_1^\top \\ V_2^\top \\ \vdots \\ V_p^\top \end{bmatrix} = \sigma_1 \ U_1 V_1^\top + \cdots + \sigma_p U_p V_p^\top$$

The example below helps understanding the above equation:

$$\underbrace{\begin{bmatrix} u_{11} & u_{21} \\ u_{12} & u_{22} \\ u_{13} & u_{23} \end{bmatrix}}_{\mathbf{U} \in \mathbb{R}^{3 \times 2}} \underbrace{\begin{bmatrix} \sigma_1 v_{11} & \sigma_1 v_{21} \\ \sigma_2 v_{12} & \sigma_2 v_{22} \end{bmatrix}}_{\mathbf{\Sigma} \mathbf{V}^\top \in \mathbb{R}^{2 \times 2}} = \begin{bmatrix} \begin{bmatrix} U_1 & U_2 \end{bmatrix} \begin{bmatrix} \beta_{11} & \beta_{12} \\ \beta_{21} & \beta_{22} \end{bmatrix} \\ & = \begin{bmatrix} \beta_{11} U_1 + \beta_{21} U_2 & \beta_{12} U_1 + \beta_{22} U_2 \end{bmatrix} \\ & = \begin{bmatrix} \beta_{11} U_1 & \beta_{12} U_1 \end{bmatrix} + \begin{bmatrix} \beta_{21} U_2 & \beta_{22} U_2 \end{bmatrix} \\ & = \underbrace{U_1 \begin{bmatrix} \beta_{11} & \beta_{12} \end{bmatrix} + U_2 \begin{bmatrix} \beta_{21} & \beta_{22} \end{bmatrix}}_{\text{Linear algebra for computational statistics III}}$$

### **SVD:** Definition & Structure

Our conclusion is that a data matrix  $\mathbf{X} \in \mathbb{R}^{n \times p}$  has the following representation,

$$\mathbf{X} = \underbrace{\mathbf{U}}_{n \times p} \underbrace{\mathbf{\Sigma}}_{p \times p} \underbrace{\mathbf{V}}_{p \times p}^{\top} = \sum_{i=1}^{p} \sigma_{i} U_{i} V_{i}^{\top}, \quad \sigma_{1} \ge \dots \ge \sigma_{p} > 0.$$

### **SVD** and representation

Denote the *i*th row vector of  $\mathbf{X}$  by  $x_i^{\mathsf{T}}$ . Then,

$$\mathbf{X} = \begin{bmatrix} x_1^\top \\ \vdots \\ x_n^\top \end{bmatrix} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^\top = \begin{bmatrix} U_1 & \cdots & U_p \end{bmatrix} \underbrace{\begin{bmatrix} \sigma_1 V_1^\top \\ \cdots \\ \sigma_p V_p^\top \end{bmatrix}}_{=\mathbf{\Sigma} \mathbf{V}^\top}.$$

By taking transpose operator on  ${f X}$ 

$$\begin{bmatrix} x_1 & \cdots & x_n \end{bmatrix} = \begin{bmatrix} \sigma_1 V_1 & \cdots & \sigma_p V_p \end{bmatrix} \mathbf{U}^\top.$$

Thus,  $x_1 = \sigma_1 V_1 \times (U^\top)_{11} + \sigma_2 V_2 \times (U^\top)_{21} + \dots + \sigma_k V_k \times (U^\top)_{p1}$ , which implies  $(\sigma_1(U^\top)_{11}, \dots, \sigma_p(U^\top))_{p1}$  is a representation of  $x_1$  with respect to  $(V_1, \dots, V_p)$ .

### **SVD** and representation

For  $i = 1, \dots, n$ ,

$$x_i = \sigma_1(U^{\top})_{1i} \times V_1 + \sigma_2(U^{\top})_{2i} \times V_2 + \dots + \sigma_p(U^{\top})_{pi} \times V_p$$

and  $(U^{\top})_{ji} = U_{ij}$ , the following interpretations are derived from SVD.

- New (orthonormal) coordinate system:  $(V_1, \cdots, V_p)$
- Scaling factor:  $(\sigma_1, \cdots, \sigma_p)$
- Representation of  $x_i$  w.r.t the  $(V_1, \dots, V_p)$ :  $(\sigma_1 U_{i1}, \dots, \sigma_p U_{ip})$ .

# Singular Value Decomposition: Example i

$$\mathbf{A} = \begin{bmatrix} 3 & 1 \\ 2 & 2 \\ 1 & 3 \end{bmatrix} \in \mathbb{R}^{3 \times 2}$$

There is three observation in  $\mathbb{R}^2$ .  $x_1^{\top}=(3,1)$ , the representation of the ith obs with respect to  $(1,0)^{\top},(0,1)^{\top}$ .

$$\mathbf{U} = \begin{bmatrix} -0.5026 & 0.7746 \\ -0.5740 & -0.6325 \\ -0.6464 & 0.0000 \end{bmatrix} \in \mathbb{R}^{3 \times 2}$$

The first row of U, (-0.5026, 0.7746) is the representation of  $x_1$  with respect to (-0.7071, -0.7071) and (-0.7071, 0.7071).

### Rank-k Truncated SVD: Definition & Structure

### Full SVD (rank p)

$$\mathbf{X} = \sum_{i=1}^{p} \sigma_i U_i V_i^{\top}, \quad \sigma_1 \ge \dots \ge \sigma_p > 0.$$

If  $\sigma_j \simeq 0$  for all j > k, then  $\mathbf{X} \simeq \sum_{i=1}^k \sigma_i U_i V_i^{\top}$ . That is,  $x_i$  is represented based on the basis  $\{V_1, \cdots, V_k\}$  of a k-dimensional subspace and  $(U_{i1}, \cdots, U_{ik}) \in \mathbb{R}^k$  is the rank-reduced representation of  $x_i$ .

#### Rank-2 Truncated SVD: Visualization

Let  $\mathbf{X}_k = \sum_{i=1}^k \sigma_i U_i V_i^{\mathsf{T}}$ . and the denote ith row vector of  $\mathbf{X}_k$  by  $\tilde{x}_i^{\mathsf{T}}$ .

- Axis:  $V_1$  (horizontal) and  $V_2$  (vertical)
- Interpretations of the Axis:

$$V_1 = (v_{11}, \cdots, v_{1p})^{\top} = \sum_{j=1}^p v_{1j}e_j$$
 and  $V_2 = (v_{21}, \cdots, v_{2p})^{\top} = \sum_{j=1}^p v_{1j}e_j$ , where  $e_j$ s are the standard basis.  $V_j$  is explained by the covariates's names of the data and the associated coefficients  $(v_{j1}, \cdots, v_{jp})$ .

- (ex) Suppose that  $V_1=(0.7101,-0.7101,0,\cdots,0)$ ,  $X_1$ : GDP,  $X_2$ : interest rate, then  $V_1$  is the weighted sum of GDP and interest rate with the weight (0.7101,-0.7101).
- Poisiton of  $\tilde{x}_i^{\top}$ :  $(\sigma_1 U_{i1}, \sigma_2 U_{i2})$ .