Singular value decomposition

Victor Kitov

Table of Contents

SVD decomosition[1][2]

Every matrix $X \in \mathbb{R}^{NxD}$, rank $X = R$, can be decomposed into the product of three matrices:

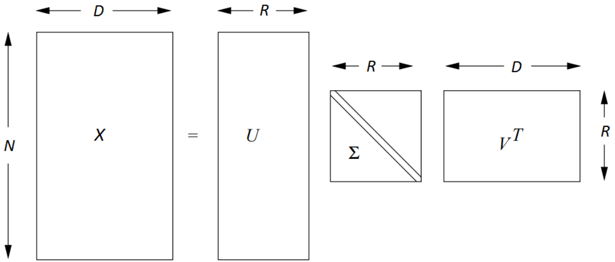
$$X = U\Sigma V^T$$

where

- $U \in \mathbb{R}^{NxR}$, $\Sigma \in \mathbb{R}^{RxR}$, $V^T \in \mathbb{R}^{RxD}$
- $\Sigma = diag\{\sigma_1, \sigma_2, ...\sigma_R\}$, $\sigma_1 \geq \sigma_2 \geq ... \geq \sigma_R \geq 0$,
- $U^T U = I$, $V^T V = I$, where $I \in \mathbb{R}^{RxR}$ is identity matrix.

[1] Prove it
[2] Is it unique?

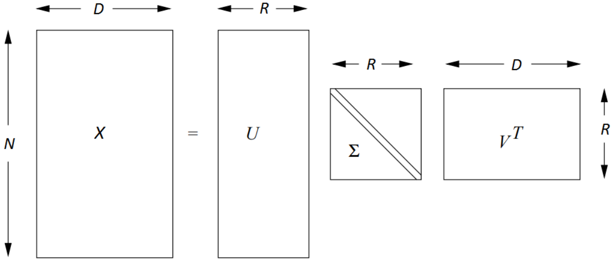
Interpretation of SVD



For X_{ij} let i denote objects and j denote properties.

- Columns of U - orthonormal basis of columns of X
- Rows of V^T- orthonormal basis of rows of X
- Σ - scaling.
- Efficient representations of low-rank matrix!

Interpretation of SVD



For X_{ij} let i denote objects and j denote properties.

- Rows of U are normalized coordinates of rows in V^T
- $\Sigma = diag\{\sigma_1, ...\sigma_R\}$ shows the magnitudes of presence of each row from V^T.

Finding U and V

- **Finding U:**
  $XX^T = U\Sigma V^T \left(U\Sigma V^T\right)^T = U\Sigma V^T V\Sigma U^T = U\Sigma^2 U^T$. So
  $$XX^T U = U\Sigma^2 U^T U = U\Sigma^2.$$
  So U consists of eigenvectors of $XX^T$with corresponding eigenvalues $\sigma_1^2, \sigma_2^2, ...\sigma_R^2$.

Finding U and V

- **Finding** U:
  $XX^T = U\Sigma V^T \left(U\Sigma V^T\right)^T = U\Sigma V^T V\Sigma U^T = U\Sigma^2 U^T$. So
  $$XX^T U = U\Sigma^2 U^T U = U\Sigma^2.$$
  So U consists of eigenvectors of $XX^T$with corresponding eigenvalues $\sigma_1^2, \sigma_2^2, ...\sigma_R^2$.
- **Finding** V
  $X^T X = \left(U\Sigma V^T\right)^T U\Sigma V^T = (V\Sigma U^T)U\Sigma V^T = V\Sigma^2 V^T$. It follows that
  $$X^T XV = V\Sigma^2 V^T V = V\Sigma^2$$
  So V consists of eigenvectors of $X^T X$ with corresponding eigenvalues $\sigma_1^2, \sigma_2^2, ...\sigma_R^2$ - **these are top** R **principal components!**

SVD: existence

Theorem 1

For any matrix $X \in \mathbb{R}^{NxD}$ SVD decomposition exists.

Proof. Consider arbitrary $X = [x_1^T, ...x_N^T]^T \in \mathbb{R}^{NxD}$ with $\text{rg}\, X = R$. For rows $x_1^T, ...x_N^T$ find principal components $v_1, ...v_R$.
Define $V^T = [v_1^T, ...v_R^T] \in \mathbb{R}^{RxD}$. By definition of principal coomponents $V^T V = I$. Consider B with rows=coordinates of $x_1, ...x_N$ in principal components, then $X = BV^T$.
Let $b_1, ..b_D$ be columns of B, satisfying $b_i = Xv_i$. Then $b_i^T b_j = v_i^T X^T X v_j = \lambda_j v_i^T v_j = \lambda_j \mathbb{I}[i=j]$, because v_j is an eigenvector of $X^T X$ with eigenvalue λ_j. Also $\lambda_j \ge 0$ because $X^T X \succeq 0$. So $b_1, ...b_D$ are orthogonal.
If we consider $\Sigma = \text{diag}\{\sqrt{\lambda_1}, ...\sqrt{\lambda_D}\}$ $B = U\Sigma$ we will obtain that $U^T U = I$. So SVD decomposion $X = U\Sigma V^T$ exists. □

SVD: uniqueness

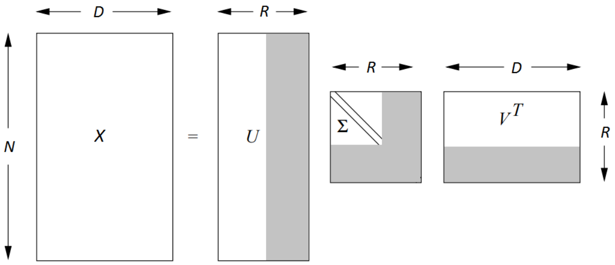
Theorem

SVD decomposition is unique if and only if all eigenvalues of $X^T X$ are unique.

- Unique set of eigenvalues mean that eigenvectors are uniquely defined (up to multiplicative constant).
- If two eigenvalues are equal we may change the order of respective eigenvectors.
- Sometimes condition $\sigma_1 \geq \sigma_2 \geq ... \geq \sigma_R \geq 0$ is not required.
    - Then we can freely change ordering of $u_1, ...u_R$; $\sigma_1, ...\sigma_R$; $v_1, ...v_R$.

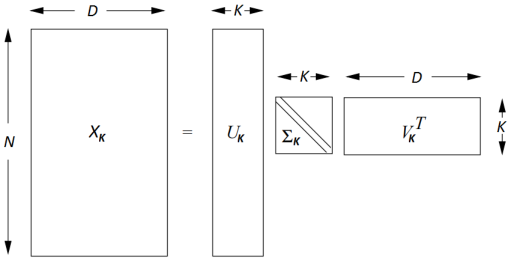
Table of Contents

Reduced SVD decomposition



$$\Sigma = diag\{\sigma_1, \sigma_2, ...\sigma_K, \sigma_{K+1}, ...\sigma_R\} \longrightarrow$$
$$diag\{\sigma_1, \sigma_2, ...\sigma_K, 0, 0, ..0\} = \Sigma_K$$

Reduced SVD decomposition



Simplification to rank $K \leq R$:

$$X_K = U_K \Sigma_K V_K$$

$$\Sigma = diag\{\sigma_1, \sigma_2, ...\sigma_K, \sigma_{K+1}, ...\sigma_R\} \longrightarrow diag\{\sigma_1, \sigma_2, ...\sigma_K\} = \Sigma_K$$
$$U = [u_1, u_2, ...u_K, u_{K+1}, ...u_R] \longrightarrow [u_1, u_2, ...u_K] = U_K$$
$$V = [v_1, v_2, ...v_K, v_{K+1}, ...v_R] \longrightarrow [v_1, v_2, ...v_K] = V_K$$

- Now rows of U give reduced representation of rows of X.

Properties of reduced SVD decomposition

Frobenius norm of matrix

$$\|X\|_F^2 = \sum_{n=1}^{N}\sum_{d=1}^{D} x_{nd}^2$$

- For matrix X and its approximation $\widehat{X}$ we can measure

$$\text{approximation error} = \left\|\widehat{X} - X\right\|_F^2$$

Theorem 2

Suppose $X \in \mathbb{R}^{NxD}$, is approximated with $\widehat{X}_K = U_K \Sigma_K V_K$. Then:

1. $\operatorname{rank} X_K = K$.
2. $X_K = \arg\min_{B:\operatorname{rank} B \le K} \|X - B\|_F^2$

Proof of theorem 2

1. rg U_K = rg $U_K\Sigma_K = K$, rg $V_K = K$, so rg $\widehat{X}_K$ = rg $[U_K\Sigma_K V_K] = K$
2. Let $X = [x_1, ...x_N]^T$, $B = [b_1, ...b_N]^T$, $D = U\Sigma$, $D_K = U_K\Sigma_K$, so $X = DV$, $\widehat{X}_K = D_K V_K$
    1. consider subspace L spanned by $b_1, ...b_N$. Since rg $B \le K, dim(L) \le K$.
    2. $\|X - B\|_F^2 = \sum_{n=1}^N \|x_n - b_n\|^2 \le \sum_{n=1}^N \left\|x_n - \tilde{b}_n\right\|^2$, where $\tilde{b}_n$ is projection of x_n on L.
    3. Since rows of V_K are top K principal components, rows of D_K are coordinates in first K principal components, and $\widehat{X}_K = [p_1, ...p_N]^T$ consists of projections onto K best fit subspace.
    4. $\left\|X - \widehat{X}_K\right\|_F^2 = \|[x_1 - p_1, ...x_N - p_N]^T\|_F^2 = \sum_{n=1}^N \|x_n - p_n\|^2 \le \sum_{n=1}^N \left\|x_n - \tilde{b}_n\right\|^2 \le \sum_{n=1}^N \|x_n - b_n\|^2 = \|X - B\|_F^2$

Which K to choose for approximation?

- Suppose $X = U\Sigma V^T$, $\Sigma = diag\{\sigma_1, ...\sigma_R\}$
- Approximation $\widehat{X}_K = U\Sigma_K V^T$, $\Sigma = diag\{\sigma_1, ...\sigma_K, 0, 0, ...0\}$.
- Then error of approximation $E_K = X - \widehat{X}_K = U\tilde{\Sigma}V^T$, where $\tilde{\Sigma} = diag\{0, 0, ...0, \sigma_{K+1}, ...\sigma_R\}$

Which K to choose for approximation?

Select K giving relative error below some threshold t:

$$K = \arg\min_K \left\{ \frac{\|E_K\|_F^2}{\|X\|_F^2} = \frac{\sum_{i=K+1}^R \sigma_i^2}{\sum_{i=1}^R \sigma_i^2} < t \right\}$$

We used theorem 3 for calculation of Frobenius matrix norm.

Frobenius norm

Theorem 3

for any matrix X and its singular value decomposition $A = U\Sigma V^T$, $\Sigma = diag\{\sigma_1, ...\sigma_R\}$:

$$\|X\|_F^2 = \sum_{i=1}^{R} \sigma_i^2$$

Proof. Using lemmas 1 and 2, we obtain:

$$\begin{aligned} \|X\|_F^2 &= \text{tr}[U\Sigma V^T V\Sigma U^T] = \text{tr}[U(\Sigma^2 U^T)] = \\ &= \text{tr}[(\Sigma^2 U^T)U] = \text{tr}[\Sigma^2] = \sum_{r=1}^{R} \sigma_r^2 \end{aligned}$$

□

Lemmas

Lemma 1

For any $X \in \mathbb{R}^{NxD}$ $||X||_F^2 = \text{tr}\, XX^T$

Proof. $\left\{XX^T\right\}_{i,j} = \sum_{k=1}^{D} x_{ik}x_{kj}^t = \sum_{k=1}^{D} x_{ik}x_{jk}$. So

$$\text{tr}\, XX^T = \sum_{i=1}^{N}\{XX^T\}_{i,i} = \sum_{i=1}^{N}\sum_{k=1}^{D} x_{ik}x_{ik} = \|X\|_F^2$$

□

Lemmas

Lemma 2

For any $A \in \mathbb{R}^{NxD}$ *and* $B \in \mathbb{R}^{DxN}$

$$\text{tr}\, AB = \text{tr}\, BA$$

Proof. $\{AB\}_{n,n} = \sum_{d=1}^{D} a_{n,d} b_{d,n}$, so

$$\text{tr}\, AB = \sum_{n=1}^{N} \{AB\}_{n,n} = \sum_{n=1}^{N} \sum_{d=1}^{D} a_{n,d} b_{d,n}$$

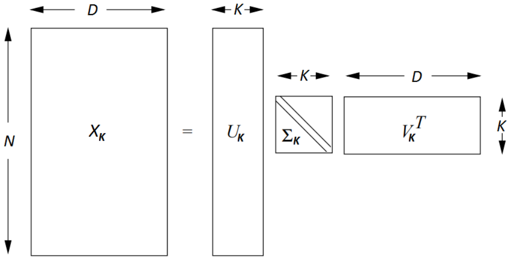
$\{BA\}_{d,d} = \sum_{n=1}^{N} b_{d,n} a_{n,d}$, so

$$\text{tr}\, BA = \sum_{d=1}^{D} \{BA\}_{d,d} = \sum_{d=1}^{D} \sum_{n=1}^{N} b_{d,n} a_{n,d} =$$

$$= \sum_{n=1}^{N} \sum_{d=1}^{D} a_{n,d} b_{d,n} = \text{tr}\, AB$$

Table of Contents

Dimensionality reduction



- rows of U give reduced representation of rows of X.
- $x_n \in \mathbb{R}^D \longrightarrow u_n \in \mathbb{R}^K$

Memory efficiency

Storage costs of $X \in \mathbb{R}^{NxD}$, assuming $N \geq D$ and each element taking 1 byte:

Memory storage costs

representation of X	memory requirements
original X	?
fully SVD decomposed	?
reduced SVD to rank K	?

Performance efficiency

- Multiplication Xq
    - X - normalized documents representation
    - q - normalized search query

representation of X	Xq complexity
original X	?
reduced SVD to rank K	?

Table of Contents

Example

	Terminator	Gladiator	Rambo	Titanic	Love story	A walk to remember
Andrew	4	5	5	0	0	0
John	4	4	5	0	0	0
Matthew	5	5	4	0	0	0
Anna	0	0	0	5	5	5
Maria	0	0	0	5	5	4
Jessika	0	0	0	4	5	4

Example

$$U = \begin{pmatrix} 0. & 0.6 & -0.3 & 0. & 0. & -0.8 \\ 0. & 0.5 & -0.5 & 0. & 0. & 0.6 \\ 0. & 0.6 & 0.8 & 0. & 0. & 0.2 \\ 0.6 & 0. & 0. & -0.8 & -0.2 & 0. \\ 0.6 & 0. & 0. & 0.2 & 0.8 & 0. \\ 0.5 & 0. & 0. & 0.6 & -0.6 & 0. \end{pmatrix}$$

$$\Sigma = \text{diag}\{\begin{pmatrix} 14. & 13.7 & 1.2 & 0.6 & 0.6 & 0.5 \end{pmatrix}\}$$

$$V^T = \begin{pmatrix} 0. & 0. & 0. & 0.6 & 0.6 & 0.5 \\ 0.5 & 0.6 & 0.6 & 0. & 0. & 0. \\ 0.5 & 0.3 & -0.8 & 0. & 0. & 0. \\ 0. & 0. & 0. & -0.2 & 0.8 & -0.6 \\ -0. & -0. & -0. & 0.8 & -0.2 & -0.6 \\ 0.6 & -0.8 & 0.2 & 0. & 0. & 0. \end{pmatrix}$$

Example (excluded insignificant concepts)

$$U_2 = \begin{pmatrix} 0. & 0.6 \\ 0. & 0.5 \\ 0. & 0.6 \\ 0.6 & 0. \\ 0.6 & 0. \\ 0.5 & 0. \end{pmatrix}$$

$$\Sigma_2 = \text{diag}\{\begin{pmatrix} 14. & 13.7 \end{pmatrix}\}$$

$$V_2^T = \begin{pmatrix} 0. & 0. & 0. & 0.6 & 0.6 & 0.5 \\ 0.5 & 0.6 & 0.6 & 0. & 0. & 0. \end{pmatrix}$$

Concepts may be

- patterns among movies (along j) - action movie / romantic movie
- patterns among people (along i) - boys / girls

Dimensionality reduction case: patterns along j axis.

Applications

- Example: new movie rating by new person
$$x = \begin{pmatrix} 5 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$
- **Dimensionality reduction:** map x into concept space:
$$y = V_2^T x = \begin{pmatrix} 0 & 2.7 \end{pmatrix}$$
- **Recommendation system:** map y back to original movies space:
$$\widehat{x} = yV_2^T = \begin{pmatrix} 1.5 & 1.6 & 1.6 & 0 & 0 & 0 \end{pmatrix}$$