Singular value decomposition

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SVD decomposition

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

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

where

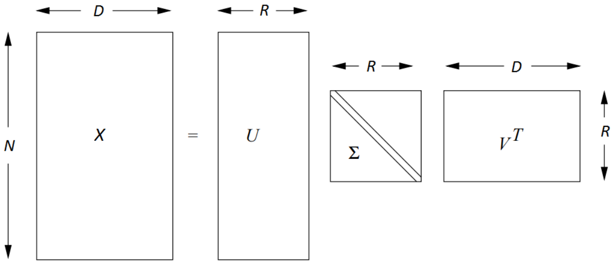
- $U \in \mathbb{R}^{NxR}$, $\Sigma \in \mathbb{R}^{RxR}$, $V^T \in \mathbb{R}^{RxD}$
- $\Sigma = diag\{\sigma_1, \sigma_2, ...\sigma_R\}$, $\sigma_1 \geq \sigma_2 \geq ... \geq \sigma_R \geq 0$
- $U^T U = I$, $V^T V = I$, where $I \in \mathbb{R}^{RxR}$ is identity matrix.

Equivalent:

$$X = \sum_{i=1}^{R} u_i \sigma_i v_i^T$$

where u_i - i-th column of U and v_i^T - i-th row of V^T.

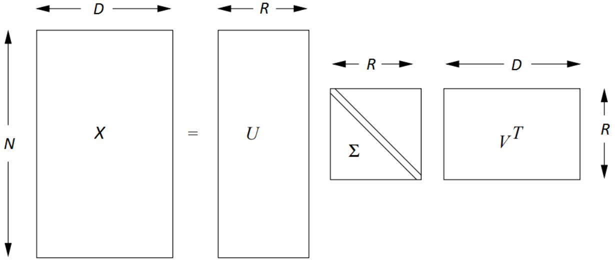
Interpretation of SVD



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 V

$$X^TX = \left(U\Sigma V^T\right)^T U\Sigma V^T = (V\Sigma U^T)U\Sigma V^T = V\Sigma^2 V^T$$

It follows that[1]

$$X^TXV = V\Sigma^2 V^T V = V\Sigma^2 \tag{1}$$

So V consists of eigenvectors of X^TX with corresponding eigenvalues $\sigma_1^2, \sigma_2^2, ...\sigma_R^2$ - **these are top R principal components!**

[1] Singular values for matrix X are square roots of eigenvalues of X^TX. From (1) it follows that $\sigma_1, ...\sigma_R$ are singular values of X.

Finding U

$$XX^T = U\Sigma V^T\left(U\Sigma V^T\right)^T = U\Sigma V^T V\Sigma U^T = U\Sigma^2 U^T$$

It follows that

$$XX^T U = U\Sigma^2 U^T U = U\Sigma^2.$$

So U consists of eigenvectors of XX^T with corresponding eigenvalues $\sigma_1^2, \sigma_2^2, ...\sigma_R^2$.

SVD: existence & uniqueness

Theorem 1

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

Theorem 2

SVD decomposition is unique up to sign <=> $X^T X \in \mathbb{R}^{DxD}$ has a set of D unique eigenvalues.

Unique up to sign means that we can always simultaneously change signs of u_i and v_i^T for $\forall i = 1, 2, ...R$.

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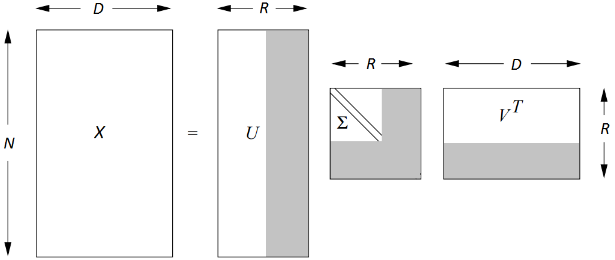
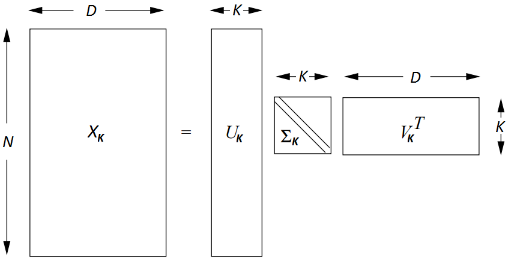
Truncated SVD decomposition



- Truncation: remove least important columns of U and rows of V^T.
- Importance measures by $\sigma_1, \sigma_2, ...\sigma_R$.
- So replace

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

Truncated SVD decomposition



Simplification to rank $K \le R$:

$$X_K = U_K \Sigma_K V_K \approx X$$

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

Properties of truncated 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 3

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

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

Which K to choose for approximation?

Theorem 4

For any matrix X and its SVD decomposition $X = U\Sigma V^T$, $\Sigma = diag\{\sigma_1, ...\sigma_R\}$:

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

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

$$\left\|X - \widehat{X}_K\right\|_F^2 = \sum_{i=K+1}^{R} \sigma_i^2$$

Which K to choose for approximation?

Using theorem 4, we can select K giving relative error below some threshold t:

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

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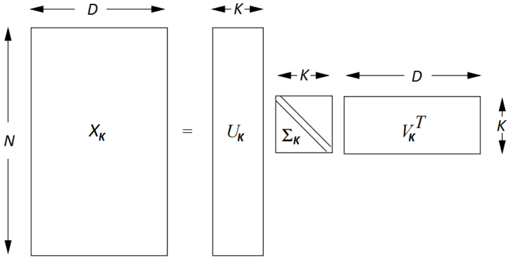
Dimensionality reduction



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

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	?
truncated SVD to rank K	?

Performance efficiency

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

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

Finding similar objects and similar features

- Similar objects have co-appearing features.
- Similar features co-appear in objects.
- Example: text analysis.
    - LSA gives compact representations, invariant to synonyms
    - can compare documents
    - can compare words

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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
Jessica	0	0	0	4	5	4

Example

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

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

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

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:

$$\widehat{x} = y V_2^T = \begin{pmatrix} 1.5 & 1.6 & 1.6 & 0 & 0 & 0 \end{pmatrix}$$

Summary

- SVD decomposition $X = U\Sigma V^T$, $U^T U = I$, $V^T V = I$, $\Sigma = \text{diag}\{\sigma_1, ...\sigma_R\}$ exists $\forall X$.
- Reduced SVD decomposition of order K solves:

$$X_K = \arg \min_{B:\text{rank}\, B \leq K} \|X - B\|_F^2$$

- SVD (reduced SVD) extracts structure of large matrices with small (close to small) rank
  - gives intuitive representation
  - efficient representations
  - fast matrix multiplications
- Helpful in recommendation engines
  - pitfall: treats 0 (no vote) as real vote.