COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

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University of Massachusetts Amherst. Spring 2020.
Lecture 16

SUMMARY

Last Class: Low-Rank Approximation, Eigendecomposition, and PCA

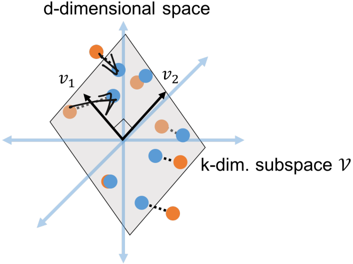
- Can approximate data lying close to in a *k*-dimensional subspace by projecting data points into that space.
- Finding the best *k*-dimensional subspace via eigendecomposition (PCA). $[X^T X]_{d \times d}$ $v_1 \ldots v_k$
- Measuring error in terms of the eigenvalue spectrum.

This Class: Finish Low-Rank Approximation and Connection to the singular value decomposition (SVD)

- Finish up PCA – runtime considerations and picking *k*.
- View of optimal low-rank approximation using the SVD.
- Applications of low-rank approximation beyond compression.

BASIC SET UP

Set Up: Assume that data points $\vec{x}_1, \ldots, \vec{x}_n$ lie close to any k-dimensional subspace $\mathcal{V}$ of $\mathbb{R}^d$. Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ be the data matrix.



Let $\vec{v}_1, \ldots, \vec{v}_k$ be an orthonormal basis for $\mathcal{V}$ and $\mathbf{V} \in \mathbb{R}^{d \times k}$ be the matrix with these vectors as its columns.

- $\mathbf{V}\mathbf{V}^T \in \mathbb{R}^{d \times d}$ is the projection matrix onto $\mathcal{V}$.
- $\mathbf{X} \approx \mathbf{X}(\mathbf{V}\mathbf{V}^T)$. Gives the closest approximation to $\mathbf{X}$ with rows in $\mathcal{V}$.

$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: orthogonal basis for subspace $\mathcal{V}$. $\mathbf{V} \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

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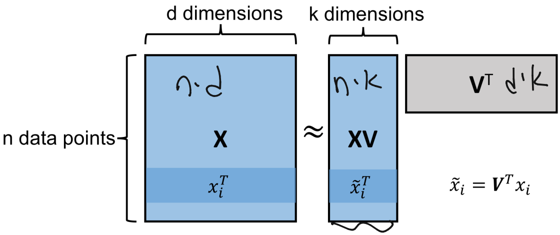

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LOW-RANK APPROXIMATION VIA EIGENDECOMPOSITION

$\mathbf{V}$ minimizing $\|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2$ is given by:

$$\underset{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}}{\arg\max} \|\mathbf{X}\mathbf{V}\|_F^2 = \sum_{j=1}^{k} \|\mathbf{X}\vec{v}_j\|_2^2$$

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LOW-RANK APPROXIMATION VIA EIGENDECOMPOSITION

V minimizing $\|X - XVV^T\|_F^2$ is given by:

$$\underset{\text{orthonormal } V \in \mathbb{R}^{d \times k}}{\arg\max} \|XV\|_F^2 = \sum_{j=1}^{k} \|X\vec{v}_j\|_2^2$$

Solution via eigendecomposition: Letting V_k have columns $\vec{v}_1, \ldots, \vec{v}_k$ corresponding to the top k eigenvectors of the covariance matrix $X^T X$,

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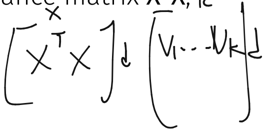

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$\mathbb{E}[yy^T]$ $\quad \sum_i x_i x_i^T = X^TX$ $\quad \sum x_i = 0$ $\quad \mathbb{E}(y - \mathbb{E}y)^2 = \mathbb{E}y^2$

- Proof via Courant-Fischer and greedy maximization.
- Approximation error is $\|X\|_F^2 - \|XV_k\|_F^2 = \sum_{i=k+1}^{d} \lambda_i(X^TX)$.

$tr(X^TX) =$ "total var" $\quad \|X - XVV^T\|_F^2$

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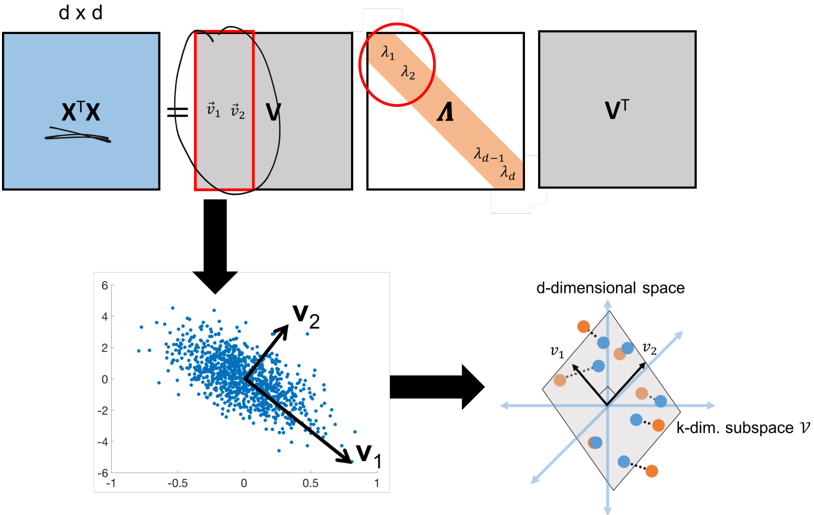
$\lambda_1 \geq \lambda_2 \geq \lambda_3 \cdots \geq \lambda_d$



Plotting the spectrum of the covariance matrix $\mathbf{X}^T\mathbf{X}$ (its eigenvalues) shows how compressible $\mathbf{X}$ is using low-rank approximation (i.e., how close $\vec{x}_1, \ldots, \vec{x}_n$ are to a low-dimensional subspace).

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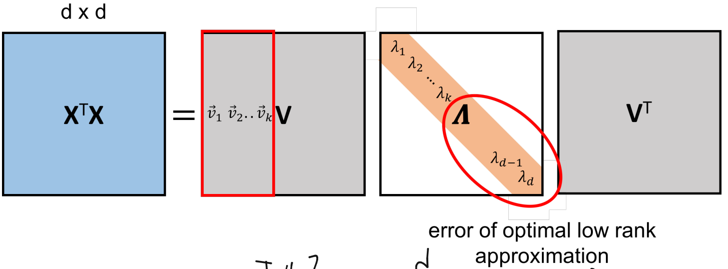

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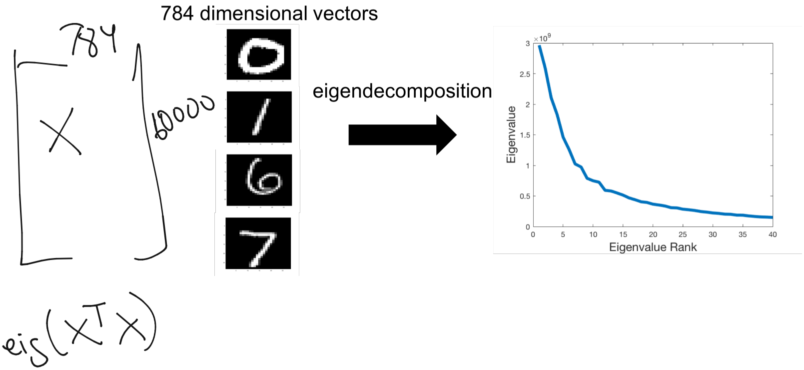

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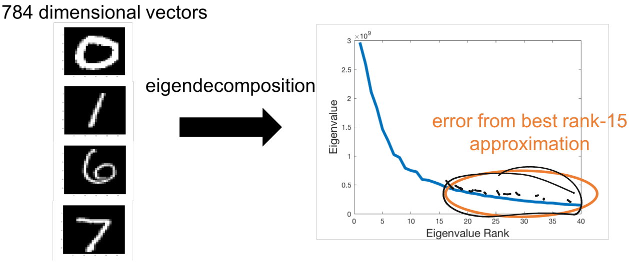

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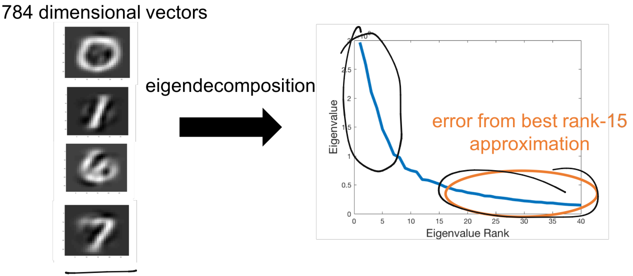

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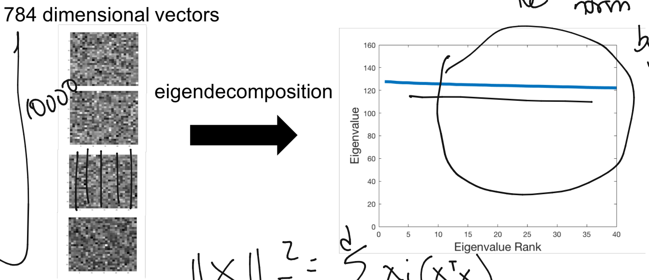

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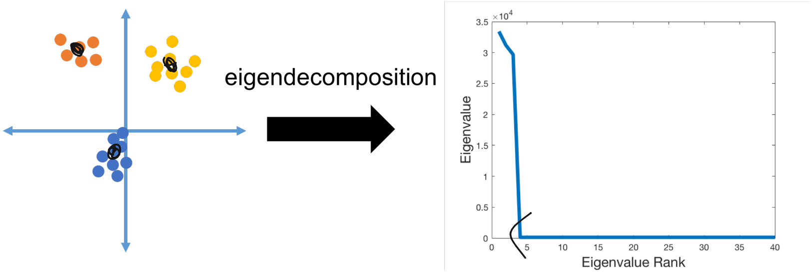

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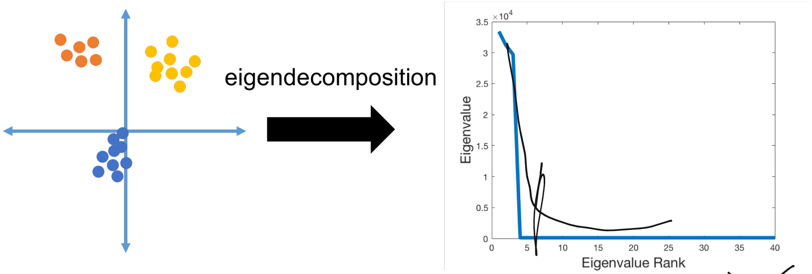

- Choose k to balance accuracy and compression.
- Often at an 'elbow'.

$tr(X^T X) = \sum \lambda_i (X^T X)$

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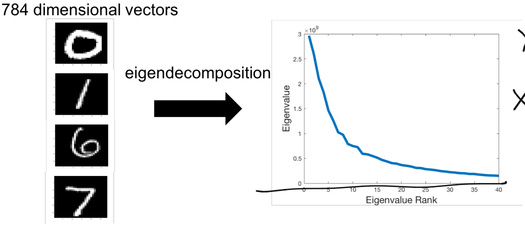

Exercise: Show that the eigenvalues of $X^T X$ are always positive.

Hint: Use that $\lambda_j = \vec{v}_j^T X^T X \vec{v}_j$.

Recall: Low-rank approximation is possible when our data features are correlated.

10000* bathrooms+ 10* (sq. ft.) ≈ list price

	bedrooms	bathrooms	sq.ft.	floors	list price	sale price
home 1	2	2	1800	2	200,000	195,000
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home n	5	3.5	3600	3	450,000	450,000

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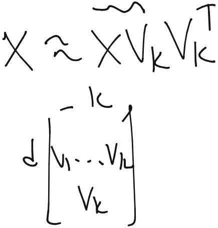

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What is the covariance of $\mathbf{C}$?

$$C^T C = V_k^T X^T X V_k$$

$$\downarrow$$

$$V_k^T V \Lambda V^T V_k^T$$

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$V_k^T V = [I \mid 0]$

$V_k^T V \Lambda V^T V_k = C^T C$

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$(V_k^T V)_{ij} = \langle v_i, v_j \rangle$

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INTERPRETATION IN TERMS OF CORRELATION

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Covariance becomes diagonal. I.e., all correlations have been removed. Maximal compression.

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What is the runtime to compute an optimal low-rank approximation?

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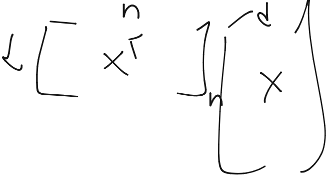
ALGORITHMIC CONSIDERATIONS

What is the runtime to compute an optimal low-rank approximation?

- Computing the covariance matrix X^TX requires $O(nd^2)$ time.



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What is the runtime to compute an optimal low-rank approximation?

- Computing the covariance matrix $\mathbf{X}^T\mathbf{X}$ requires $O(nd^2)$ time.
- Computing its full eigendecomposition to obtain $\vec{v}_1, \ldots, \vec{v}_k$ requires $O(d^3)$ time (similar to the inverse $(\mathbf{X}^T\mathbf{X})^{-1}$).

$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: top eigenvectors of $\mathbf{X}^T\mathbf{X}$, $\mathbf{V}_k \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

$d << n$

What is the runtime to compute an optimal low-rank approximation?

- Computing the covariance matrix $X^T X$ requires $O(nd^2)$ time.
- Computing its full eigendecomposition to obtain $\vec{v}_1, \ldots, \vec{v}_k$ requires $O(d^3)$ time (similar to the inverse $(X^T X)^{-1}$).

Many faster iterative and randomized methods. Runtime is roughly $\tilde{O}(ndk)$ to output just to top k eigenvectors $\vec{v}_1, \ldots, \vec{v}_k$.

- Will see in a few classes (power method, Krylov methods).

$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $X \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: top eigenvectors of $X^T X$, $V_k \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

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- $\mathbf{U}$ has orthonormal columns $\vec{u}_1, \ldots, \vec{u}_r \in \mathbb{R}^n$ (left singular vectors).
- $\mathbf{V}$ has orthonormal columns $\vec{v}_1, \ldots, \vec{v}_r \in \mathbb{R}^d$ (right singular vectors).
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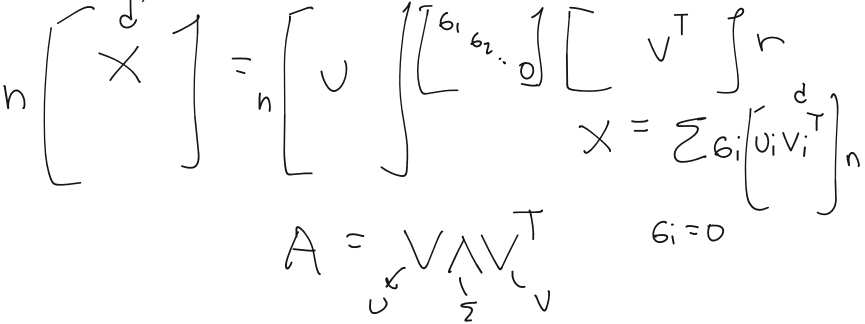

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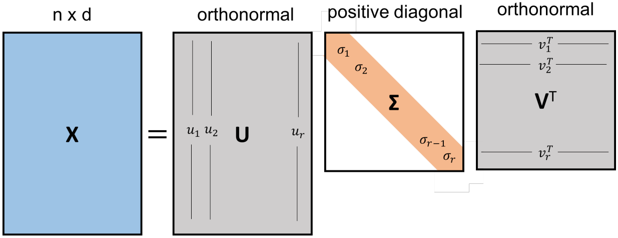

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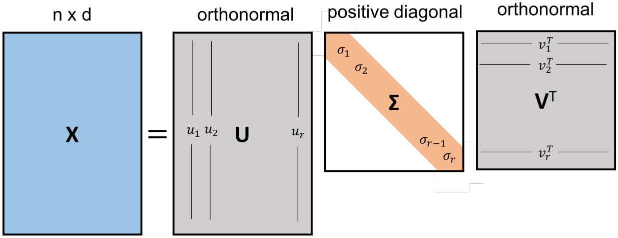

The 'swiss army knife' of modern linear algebra.

Writing $\mathbf{X} \in \mathbb{R}^{n \times d}$ in its singular value decomposition $\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$:

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CONNECTION OF THE SVD TO EIGENDECOMPOSITION

Writing $\mathbf{X} \in \mathbb{R}^{n \times d}$ in its singular value decomposition $\mathbf{X} = \mathbf{U\Sigma V}^T$:

$$\mathbf{X}^T\mathbf{X} = \mathbf{V\Sigma}\underbrace{\mathbf{U}^T\mathbf{U}}_{I}\mathbf{\Sigma V}^T$$

U, V orthonormal

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orthonormal diagonal)

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The left and right singular vectors are the eigenvectors of the covariance matrix $\mathbf{X}^T\mathbf{X}$ and the gram matrix $\mathbf{X}\mathbf{X}^T$ respectively.

Singular values squared are the eigenvalues.

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So, letting $\mathbf{V}_k \in \mathbb{R}^{d \times k}$ have columns equal to $\vec{v}_1, \ldots, \vec{v}_k$, we know that $\mathbf{X}\mathbf{V}_k\mathbf{V}_k^T$ is the best rank-k approximation to $\mathbf{X}$ (given by PCA).

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What about $\mathbf{U}_k\mathbf{U}_k^T\mathbf{X}$ where $\mathbf{U}_k \in \mathbb{R}^{n \times k}$ has columns equal to $\vec{u}_1, \ldots, \vec{u}_k$?

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What about $\mathbf{U}_k\mathbf{U}_k^T\mathbf{X}$ where $\mathbf{U}_k \in \mathbb{R}^{n \times k}$ has columns equal to $\vec{u}_1, \ldots, \vec{u}_k$?

Gives exactly the same approximation!

$XV_kV_k^T = U_kU_k^TX$

> $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\mathbf{U} \in \mathbb{R}^{n \times \text{rank}(\mathbf{X})}$: matrix with orthonormal columns $\vec{u}_1, \vec{u}_2, \ldots$ (left singular vectors), $\mathbf{V} \in \mathbb{R}^{d \times \text{rank}(\mathbf{X})}$: matrix with orthonormal columns $\vec{v}_1, \vec{v}_2, \ldots$ (right singular vectors), $\boldsymbol{\Sigma} \in \mathbb{R}^{\text{rank}(\mathbf{X}) \times \text{rank}(\mathbf{X})}$: positive diagonal matrix containing singular values of $\mathbf{X}$.

$X = U\Sigma V^T$

The best low-rank approximation to $\mathbf{X}$:

$\mathbf{X}_k = \arg\min_{\text{rank}-k\ \mathbf{B} \in \mathbb{R}^{n\times d}} \|\mathbf{X} - \mathbf{B}\|_F$ is given by:

$$\mathbf{X}_k = \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T = U_k \Sigma_k V_k^T = U_k U_k^T X$$

$$U_k U_k^T X = U_k U_k^T U \Sigma V^T = U_k [I : 0] \Sigma V^T$$

$$= U_k \Sigma_k V_k^T$$

$$\begin{bmatrix} u_1 \\ \vdots \\ u_k \end{bmatrix} \begin{bmatrix} u_1 \cdots u_d \end{bmatrix}$$

$X = U\Sigma V^T \quad X^TX = V\Sigma^2V^T \quad XX^T = U\Sigma^2U^T$

V right sing vect.

U left sing. vect.

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$XV_kV_k^T = U\Sigma V^TV_kV_k^T = U\Sigma \begin{bmatrix} I \\ 0 \end{bmatrix} V_k^T = U_k\Sigma_kV_k^T$

rest of proof ←

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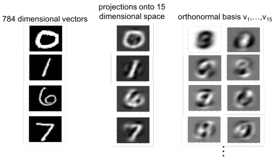
Correspond to projecting the rows (data points) onto the span of $\mathbf{V}_k$ or the columns (features) onto the span of $\mathbf{U}_k$

Row (data point) compression



Column (feature) compression

10000* bathrooms+ 10* (sq. ft.) ≈ list price

	bedrooms	bathrooms	sq.ft.	floors	list price	sale price
home 1	2	2	1800	2	200,000	195,000
home 2	4	2.5	2700	1	300,000	310,000
⋮	⋮	⋮	⋮	⋮	⋮	⋮
home n	5	3.5	3600	3	450,000	450,000

THE SVD AND OPTIMAL LOW-RANK APPROXIMATION

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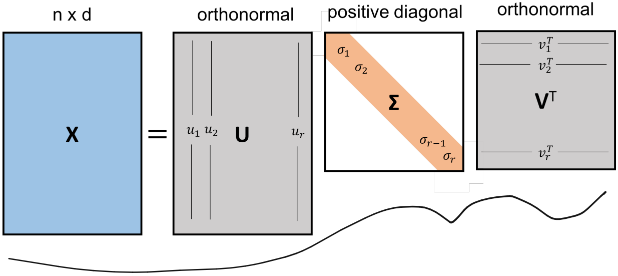

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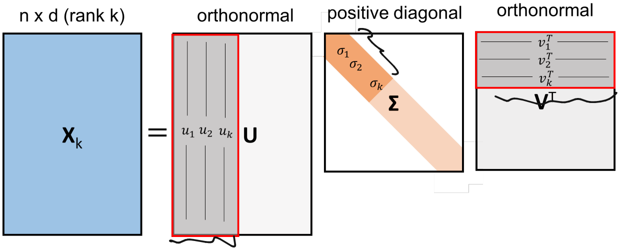

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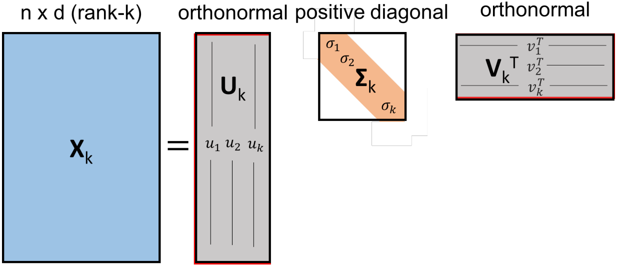

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Rest of Class: Examples of how low-rank approximation is applied in a variety of data science applications.

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- Used for many reasons other than dimensionality reduction/data compression.

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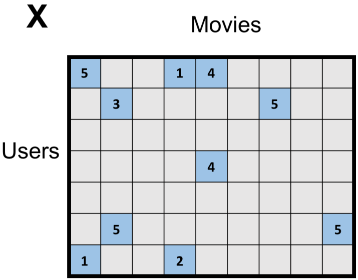

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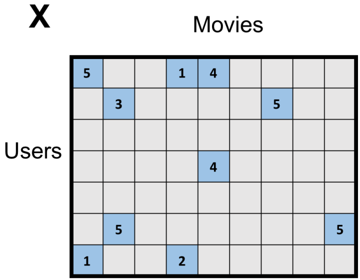

Solve: $Y = \arg\min_{\text{rank}-k\ \mathbf{B}} \sum_{\text{observed } (j,k)} \left[\mathbf{X}_{j,k} - \mathbf{B}_{j,k}\right]^2$

MATRIX COMPLETION

Consider a matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ which we cannot fully observe but believe is close to rank-k (i.e., well approximated by a rank k matrix). Classic example: the Netflix prize problem.

Y

Movies

Users

4.9	3.1	3	**1.1**	**3.8**	4.1	4.1	3.4	4.6
3.6	**3**	3	1.2	3.8	4.2	**5**	3.4	4.8
2.8	3	3	2.3	3	3	3	3	3.2
3.4	3	3	4	**4.1**	4.1	4.2	3	3
2.8	3	3	2.3	3	3	3	3	3.4
2.2	**5**	3	4	4.2	3.9	4.4	4	**5.3**
1	3.3	3	**2.2**	3.1	2.9	3.2	1.5	1.8

Solve: $$Y = \arg\min_{\text{rank}-k\ \mathbf{B}} \sum_{\text{observed } (j,k)} \left[\mathbf{X}_{j,k} - \mathbf{B}_{j,k}\right]^2$$

Under certain assumptions, can show that $\mathbf{Y}$ well approximates $\mathbf{X}$ on both the observed and (most importantly) unobserved entries.

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- Documents (for topic-based search and classification)
- Words (to identify synonyms, translations, etc.)
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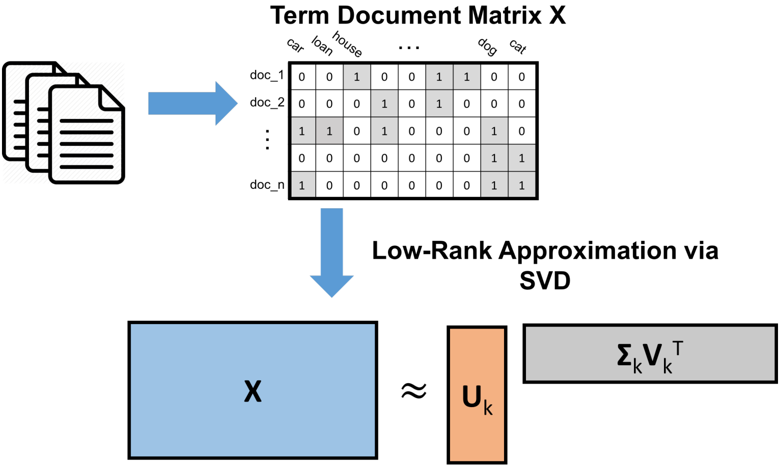
- Nodes in a social network

Usual Approach: Convert each item into a high-dimensional feature vector and then apply low-rank approximation.

EXAMPLE: LATENT SEMANTIC ANALYSIS



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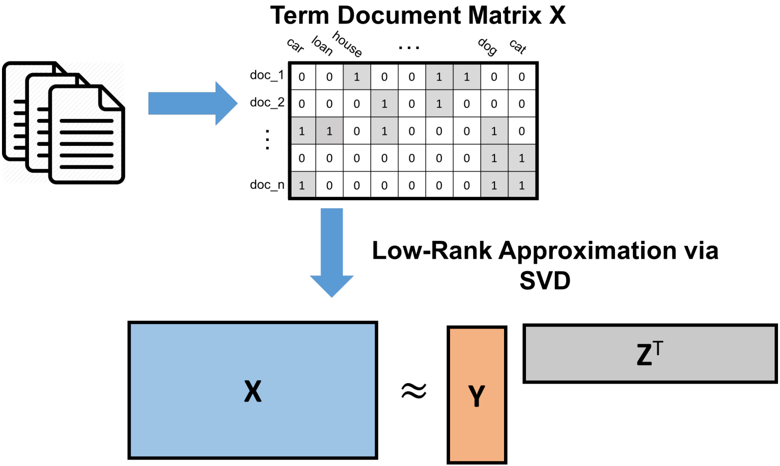

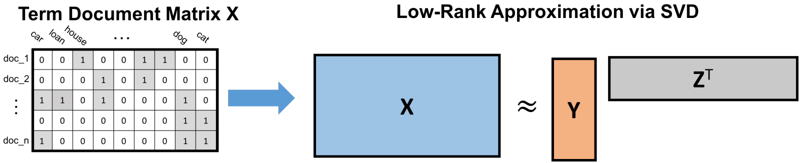
Term Document Matrix X
car loan house ... dog cat
doc_1 0 0 1 0 0 1 1 0 0
doc_2 0 0 0 1 0 1 0 0 0
1 1 0 1 0 0 0 1 0
0 0 0 0 0 0 0 1 1
doc_n 1 0 0 0 0 0 0 1 1
Low-Rank Approximation via SVD
X
≈
Y
Z^T

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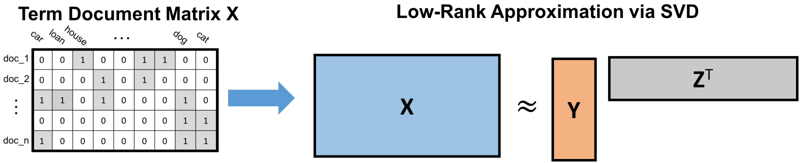

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$$X_{i,a} \approx (YZ^T)_{i,a} = \langle \vec{y}_i, \vec{z}_a \rangle.$$

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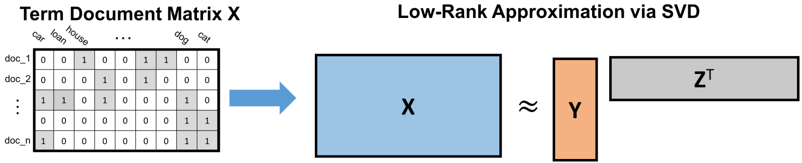

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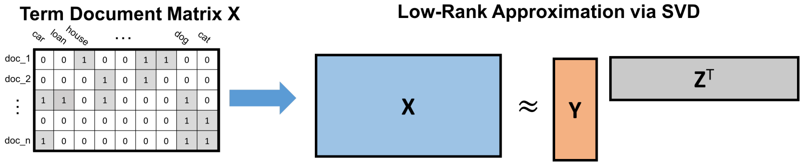

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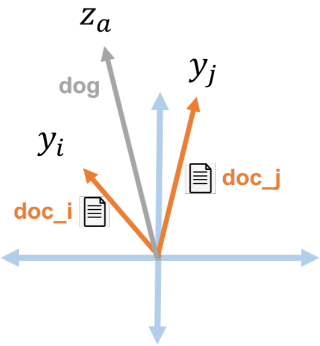

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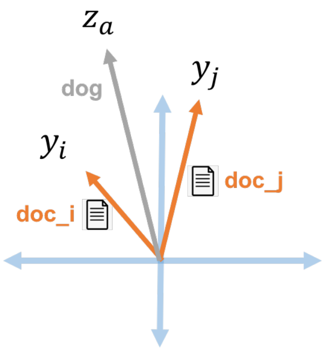

Another View: Each column of **Y** represents a 'topic'. $\vec{y}_i(j)$ indicates how much doc_i belongs to topic j. $\vec{z}_a(j)$ indicates how much $word_a$ associates with that topic.

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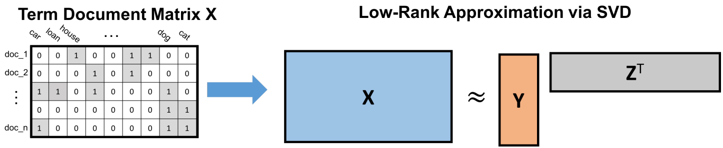

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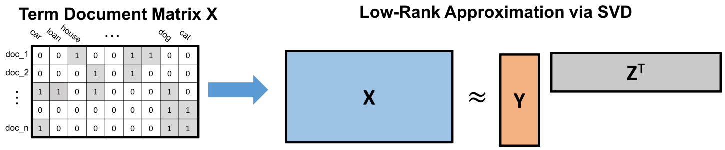

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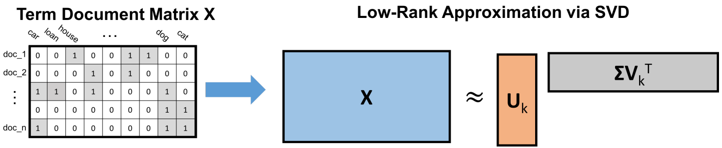

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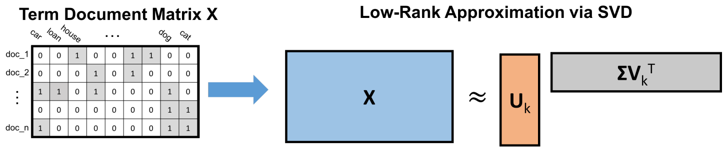

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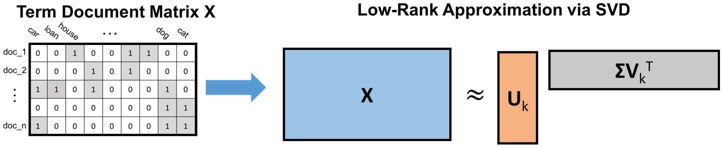

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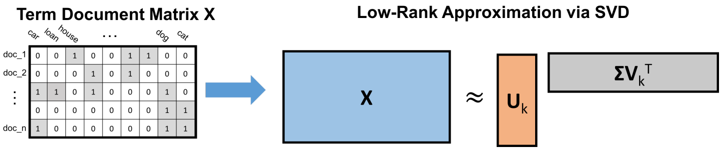

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- $\mathbf{X}^T\mathbf{X} = \mathbf{V}_k\mathbf{\Sigma}_k^2\mathbf{V}_k^T = \mathbf{Z}\mathbf{Z}^T$.

EXAMPLE: WORD EMBEDDING

LSA gives a way of embedding words into k-dimensional space.

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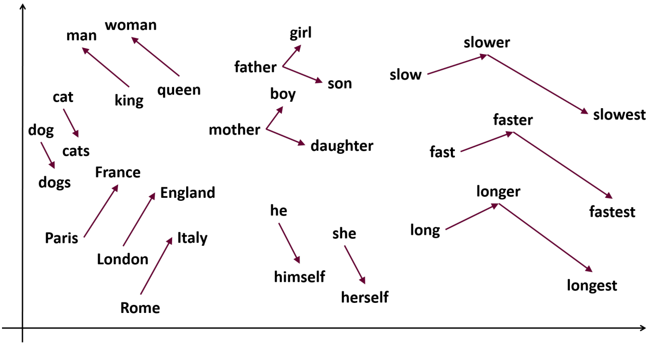
- Many ways to measure similarity: number of sentences both occur in, number of times both appear in the same window of w words, in similar positions of documents in different languages, etc.
- Replacing $X^T X$ with these different metrics (sometimes appropriately transformed) leads to popular word embedding algorithms: word2vec, GloVe, fastTest, etc.


man
woman
king
queen
cat
cats
dog
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France
Paris
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girl
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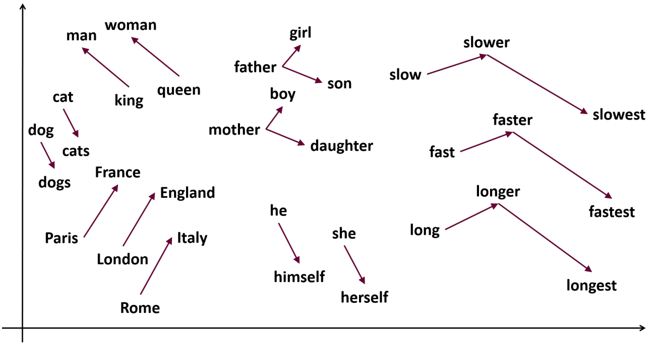

Note: word2vec is typically described as a neural-network method, but it is really just low-rank approximation of a specific similarity matrix. *Neural word embedding as implicit matrix factorization*, Levy and Goldberg.

Summary:

- Can use the SVD to understand optimal low-rank approximation in terms of the dual row/column projection view: $\mathbf{X}\mathbf{V}_k\mathbf{V}_k^T = \mathbf{U}_k\mathbf{U}_k^T\mathbf{X} = \mathbf{U}_k\mathbf{\Sigma}_k\mathbf{V}_k^T$.
- A generalization of eigendecomposition: singular vectors are eigenvectors of $\mathbf{X}\mathbf{X}^T$ and $\mathbf{X}^T\mathbf{X}$.
- Applications to low-rank approximation to matrix completion and entity embeddings.

Next Time: Low-rank representations of graphs and networks. Beginning of spectral graph theory.