COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

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University of Massachusetts Amherst. Fall 2019.

Lecture 13

- Pass/Fail Deadline is 10/29 for undergraduates and 10/31 for graduates. We will have your Problem Set 2 and midterm grades back before then.
- Will release Problem Set 3 next week due $\sim$ 11/11.

LOGISTICS

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- Will release Problem Set 3 next week due $\sim$ 11/11.
- MAP Feedback:
  - Going to adjust a bit how I take questions in class.
  - Will try to more clearly identify important information (what will appear on exams or problem sets) v.s. motivating examples.
  - Will try to use iPad more to write out proofs in class.

Last Few Classes: Low-Rank Approximation and PCA

SUMMARY

Last Few Classes: Low-Rank Approximation and PCA

- Discussed how to compress a dataset that lies close to a k-dimensional subspace.
- Optimal compression by projecting onto the top k eigenvectors of the covariance matrix $X^T X$ (PCA).
- Saw how to calculate the error of the approximation – interpret the spectrum of $X^T X$.

$X : \overset{d}{\left[\;\;\right]} n$

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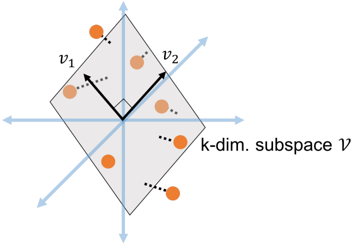
This Class: Low-rank approximation and connection to singular value decomposition.

- Show how PCA can be interpreted in terms of the singular value decomposition (SVD) of $\mathbf{X}$.
- Applications to word embeddings, graph embeddings, document classification, recommendation systems.

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.



$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: 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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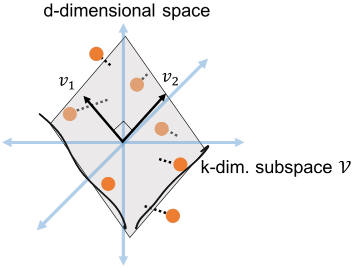

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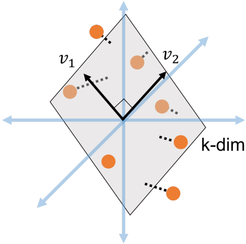

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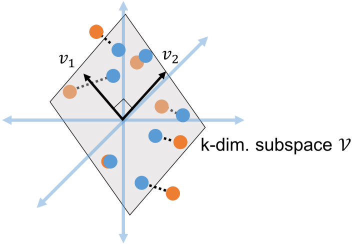

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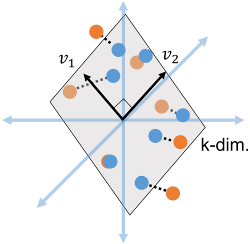

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- $\mathbf{V}\mathbf{V}^T \in \mathbb{R}^{d \times d}$ is the projection matrix onto $\mathcal{V}$.
- $\mathbf{X} \approx \mathbf{X}(\mathbf{V}\mathbf{V}^T)$ rank-k Gives the closest approximation to $\mathbf{X}$ with rows in $\mathcal{V}$.

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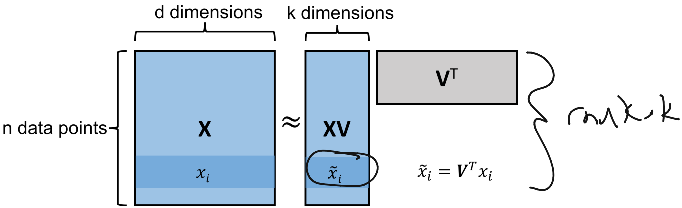
REVIEW OF LAST TIME

Low-Rank Approximation: Approximate $\mathbf{X} \approx \mathbf{X}\mathbf{V}\mathbf{V}^T$.



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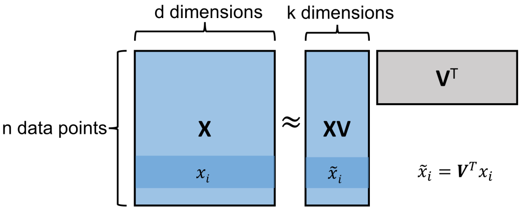

- $\mathbf{X}\mathbf{V}\mathbf{V}^T$ is a rank-k matrix – all its rows fall in $\mathcal{V}$.

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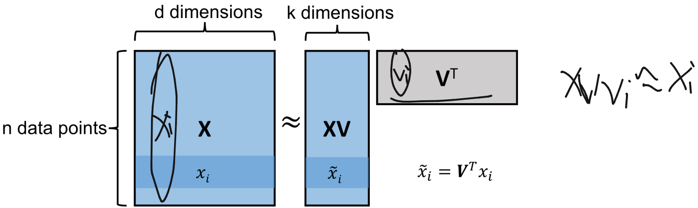

- $\mathbf{X}\mathbf{V}\mathbf{V}^T$ is a rank-k matrix – all its rows fall in $\mathcal{V}$.
- $\mathbf{X}$'s rows are approximately spanned by the columns of $\mathbf{V}$.
- $\mathbf{X}$'s columns are approximately spanned by the columns of $\mathbf{X}\mathbf{V}$.

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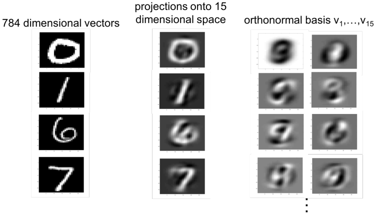
DUAL VIEW OF LOW-RANK APPROXIMATION



Row (data point) compression

Column (feature) compression

$10000 \cdot \text{bathrooms} + 10 \cdot (\text{sq. ft.}) \approx \text{list price}$

	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

Given $\vec{x}_1, \ldots, \vec{x}_n$ (the rows of $\mathbf{X}$) we want to find an orthonormal span $\mathbf{V} \in \mathbb{R}^{d \times k}$ (spanning a k-dimensional subspace $\mathcal{V}$).

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$$\underset{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}}{\arg\min} \|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2$$

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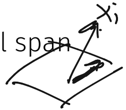

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$\|XVV^T\|_F^2 = \|XV\|_F^2$

$\|A\|_F^2 = tr(A^TA)$

$a_1 \ldots a_d$

$\|A\|_F^2 = \sum \|a_i\|_2^2$

$tr(\underbrace{XVV^T}_{A} \underbrace{V V^T X^T}_{A^T})$, $V^TV = I$

$(A^TA)_{ij} = \langle a_i, a_j \rangle$

$tr(XVV^TX^T) = \|XV\|_F^2$

$(A^TA)_{ii} = \langle a_i, a_i \rangle = \|a_i\|_2^2$

$$XV = \begin{bmatrix} X \end{bmatrix} \begin{bmatrix} v_1 & v_2 & \cdots & v_k \end{bmatrix} = \begin{bmatrix} | & & | \\ Xv_1 & Xv_2 \cdots & Xv_k \\ | & & | \end{bmatrix}$$

$\|XV\|_F^2 = \sum \|Xv_i\|_2^2$

$= \boxed{\sum_{i=1}^{k} v_i^T X^T X v_i}$

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OPTIMAL LOW-RANK APPROXIMATION

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SOLUTION VIA EIGENDECOMPOSITION

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

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

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

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Surprisingly, can find the columns of $\mathbf{V}$, $\vec{v}_1, \ldots, \vec{v}_k$ greedily.

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$V_2 \perp V_1$

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$$\cdots$$

$$\vec{v}_k = \underset{\vec{v} \text{ with } \|v\|_2 = 1,\ \langle \vec{v}, \vec{v}_j \rangle = 0\ \forall j < k}{\arg\max} \vec{v}^T \mathbf{X}^T \mathbf{X} \vec{v}.$$

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The top k eigenvectors of $\mathbf{X}^T\mathbf{X}$ by the Courant-Fischer Principal.

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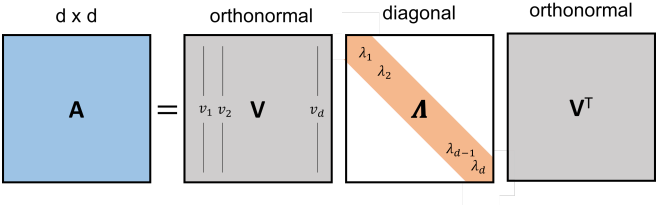
Any symmetric matrix $\mathbf{A}$ can be decomposed as $\mathbf{A} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^T$, where the columns $\mathbf{V}$ are d orthonormal eigenvectors $\vec{v}_1, \ldots, \vec{v}_d$.



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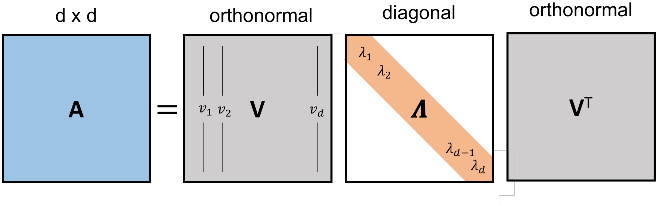

Typically order the eigenvalues in decreasing order: $\lambda_1 \geq \lambda_2 \geq \ldots \lambda_d$.

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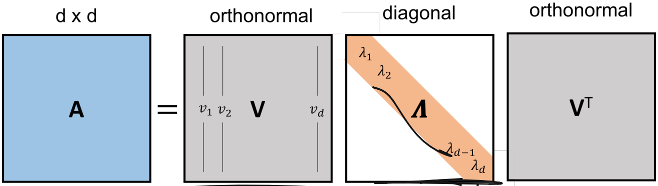
$tr(X^T X) = \|X\|_F^2 = tr(\Lambda) = \sum \lambda_i$



Typically order the eigenvalues in decreasing order: $\lambda_1 \geq \lambda_2 \geq \ldots \lambda_d \geq 0$

When $\mathbf{A} = \mathbf{X}^T\mathbf{X}$ all eigenvalues are ≥ 0. Why?

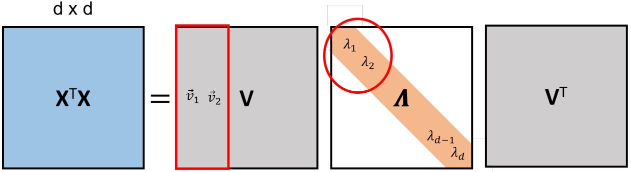
positive semidefinite

λ negative

$X^T X v = \lambda v$

$v^T X^T X v = \lambda v^T v = \lambda \|v\|_2^2$ — negative

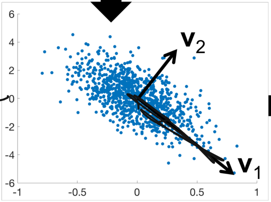
$v^T X^T X v = \|Xv\|_2^2 \geq 0$

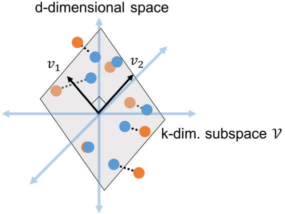


$\|XVV^T\|$

$= \sum v_i^T X^T X v_i$

$= \sum_{j=1} \langle x_j, v_i \rangle^2$





$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: 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^TX, $V_k \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

Upshot: Letting $\mathbf{V}_k$ have columns $\vec{v}_1, \ldots, \vec{v}_k$ corresponding to the top k eigenvectors of the covariance matrix $\mathbf{X}^T\mathbf{X}$, $\mathbf{V}_k$ is the orthogonal basis minimizing

$$\|\mathbf{X} - \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T\|_F^2,$$

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This is principal component analysis (PCA).

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Last Time: Saw how to determine accuracy by looking at the eigenvalues (the 'spectrum') of $\mathbf{X}^T\mathbf{X}$.

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The Singular Value Decomposition (SVD) generalizes the eigendecomposition to asymmetric (even rectangular) matrices.

The Singular Value Decomposition (SVD) generalizes the eigendecomposition to asymmetric (even rectangular) matrices. Any matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ with $\text{rank}(\mathbf{X}) = r$ can be written as $\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$.

- $\mathbf{U}$ 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).
- $\mathbf{\Sigma}$ is diagonal with elements $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_r > 0$ (singular values).

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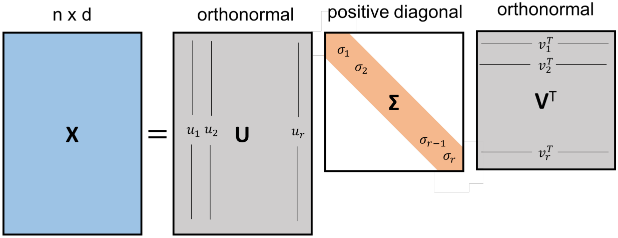

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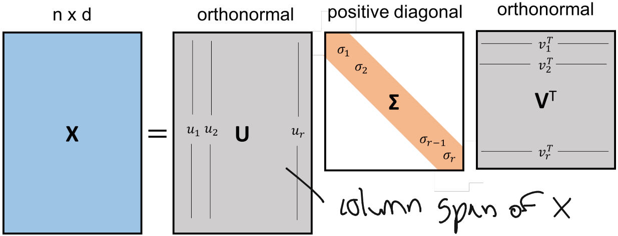

row span of X.

column span of X

The 'swiss army knife' of linear algebra.

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

$$\mathbf{X}^T\mathbf{X} =$$

$\mathbf{X} \in \mathbb{R}^{n \times d}$: 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 $\mathbf{X}$.

CONNECTION OF THE SVD TO EIGENDECOMPOSITION

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

$$\mathbf{X}^T\mathbf{X} = \mathbf{V}\mathbf{\Sigma}\overset{I}{\cancel{\mathbf{U}^T\mathbf{U}}}\mathbf{\Sigma}\mathbf{V}^T$$

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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 have that $\mathbf{X}\mathbf{V}_k\mathbf{V}_k^T$ is the best rank-k approximation to $\mathbf{X}$ (given by PCA approximation).

top k right singular vectors = eigenvectors of X^TX.

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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!

> $\mathbf{X} \in \mathbb{R}^{n \times d}$: 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), $\mathbf{\Sigma} \in \mathbb{R}^{\text{rank}(\mathbf{X}) \times \text{rank}(\mathbf{X})}$: positive diagonal matrix containing singular values of $\mathbf{X}$.

The best ~~low~~ k-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:

$$\mathbf{X}_k = \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T$$

$U \in \mathbb{R}^{n \times r} \quad V \in \mathbb{R}^{d \times r}$

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

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$X_k = U_k U_k^T U \Sigma V^T$

$= U_k \Sigma_k V_k^T$

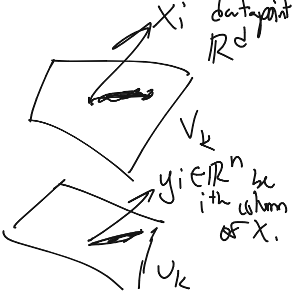
$n \times d \quad n \times k \quad k \times k \quad k \times d$

$X_k = U \Sigma V^T V_k V_k^T = U_k \Sigma_k V_k^T$

$$\underbrace{\begin{bmatrix} - & v_1^T & - \\ - & v_2^T & - \\ & \vdots & \\ - & v_d^T & - \end{bmatrix}}_{V^T} \begin{bmatrix} | & | & & | \\ v_1 & v_2 & \cdots & v_k \\ | & | & & | \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & & 1 & & 1 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{bmatrix} \Big\} k$$

$v_i^T V_k$

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



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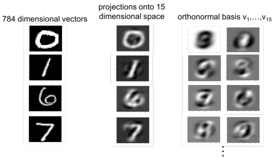
Correspond to projecting the rows (data points) onto the span of $\mathbf{V}_k$ or the columns (features) onto the span of $\mathbf{U}_k$

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 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:

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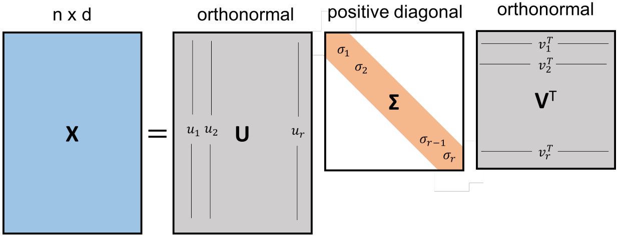

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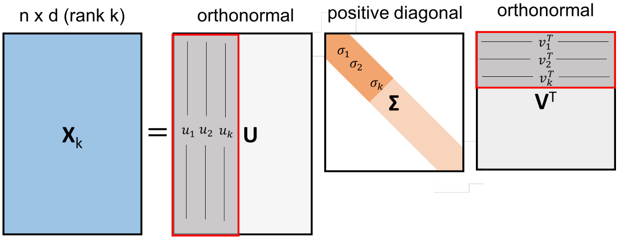
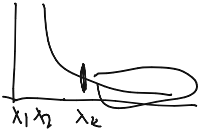


THE SVD AND OPTIMAL LOW-RANK APPROXIMATION

v_i X^TX u_i XX^T

eigenvalues of X^TX



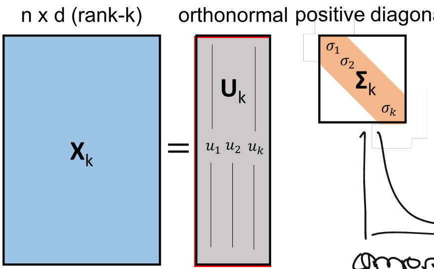
The best low-rank approximation to $\mathbf{X}$:
$\mathbf{X}_k = \arg\min_{\text{rank}-k\ \mathbf{B}\in\mathbb{R}^{n\times d}} \|\mathbf{X}-\mathbf{B}\|_F$ is given by:

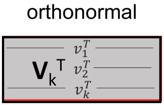
$$\mathbf{X}_k = \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T = \mathbf{U}_k\mathbf{U}_k^T\mathbf{X} = \mathbf{U}_k\boldsymbol{\Sigma}_k\mathbf{V}_k^T$$

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

$\lambda_i(X^TX) = \sigma_i^2(X)$

best rank-k approx to X

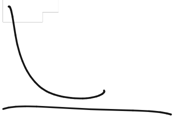




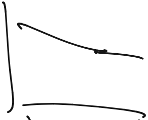
$X = U\Sigma V^T$

$Xc = U\Sigma V^Tc$

$= Uz$



compressible (near low rank)



not compressible

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:

$$\mathbf{X}_k = \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T = \mathbf{U}_k\mathbf{U}_k^T\mathbf{X} = \mathbf{U}_k\boldsymbol{\Sigma}_k\mathbf{V}_k^T$$

$\mathbf{X} \in \mathbb{R}^{n \times d}$: 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 $\mathbf{X}$.

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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.

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).

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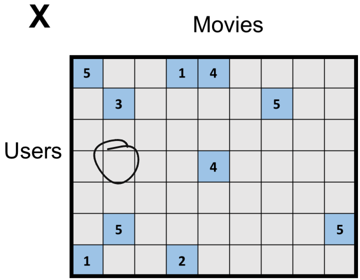

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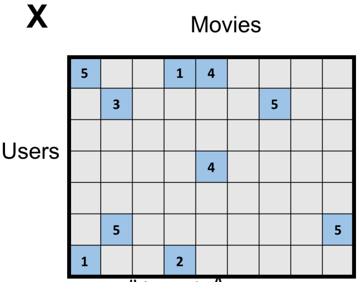

$\|X - B\|_F$

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

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Y ≈ X

rank-k

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

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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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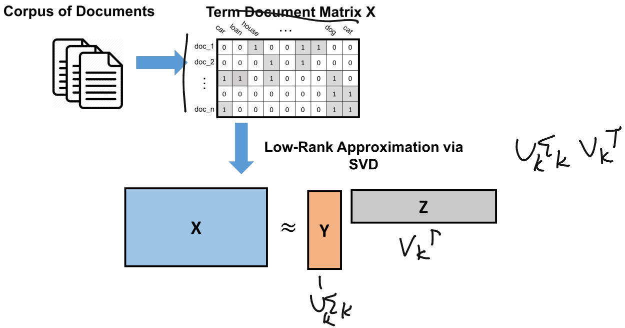
Classical approach is to convert each item into a high-dimensional feature vector and then apply low-rank approximation

EXAMPLE: LATENT SEMANTIC ANALYSIS



	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

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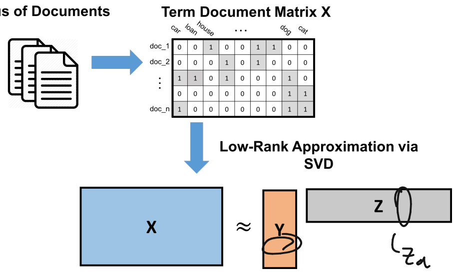

- $\langle \vec{y}_i, \vec{z}_a \rangle \approx 1$ when doc_i contains $word_a$.
- If doc_i and doc_j both contain $word_a$, $\langle \vec{y}_i, \vec{z}_a \rangle \approx \langle \vec{y}_j, \vec{z}_a \rangle \approx 1$.

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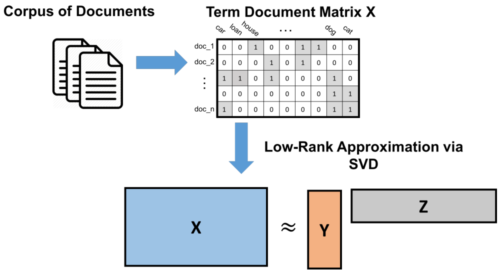

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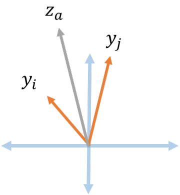
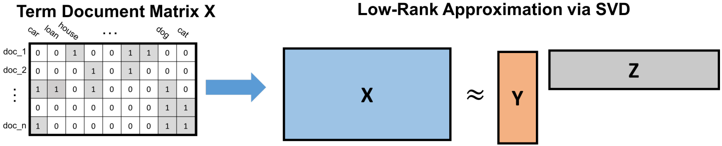
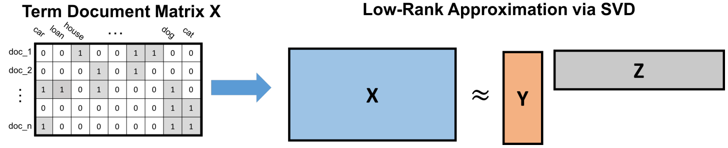



Term Document Matrix X
car
loan
house
...
dog
cat
doc_1
doc_2
doc_n
0 0 1 0 0 1 1 0 0
0 0 0 1 0 1 0 0 0
1 1 0 1 0 0 0 1 0
0 0 0 0 0 0 0 1 1
1 0 0 0 0 0 0 1 1
Low-Rank Approximation via SVD
X
≈
Y
Z



- The columns $\vec{z}_1, \vec{z}_2, \ldots$ give representations of words, with $\vec{z}_i$ and $\vec{z}_j$ tending to have high dot product if $word_i$ and $word_j$ appear in many of the same documents. z_i, z_j
- $\mathbf{Z}$ corresponds to the top k right singular vectors: the eigenvectors of $\mathbf{X}\mathbf{X}^T$.

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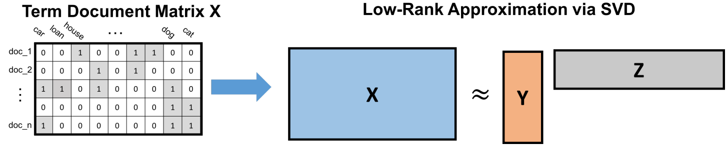

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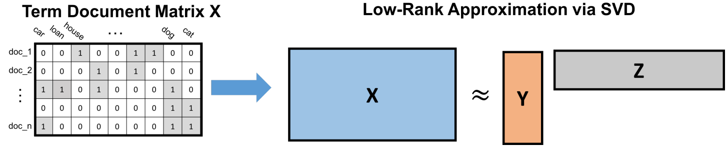

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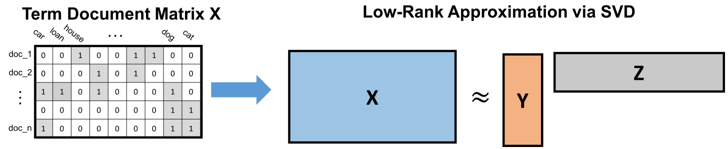

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- A document based similarity matrix.

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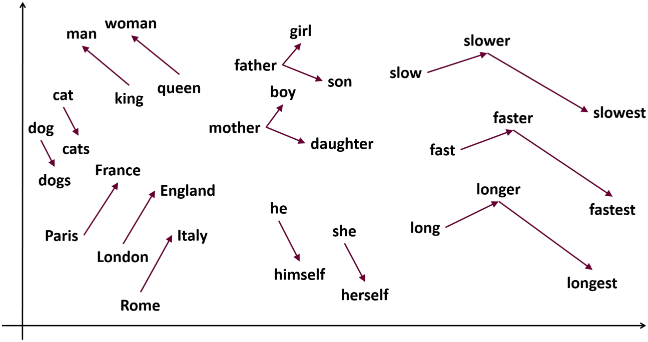
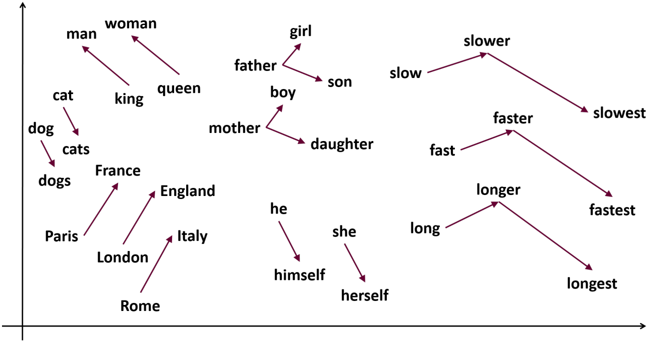
- Perform low-rank approximation of similarity matrix directly.


man
woman
king
queen
girl
father
son
boy
mother
daughter
slow
slower
slowest
fast
faster
fastest
long
longer
longest
cat
cats
dog
dogs
France
Paris
England
London
Italy
Rome
he
himself
she
herself

EXAMPLE: WORD EMBEDDING



word2vec was originally described as a neural-network method, but Levy and Goldberg show that it is simply low-rank approximation of a specific similarity matrix. *Neural word embedding as implicit matrix factorization.*

Next Time: Build on the idea of low-rank approximation of similarity matrix low-rank approximation to perform non-linear dimensionality reduction for data that is not close to a low-dimensional linear subspace.

Questions?