COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

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University of Massachusetts Amherst. Spring 2020.
Lecture 17

LOGISTICS

- Problem Set 2 was released this weekend. Due Monday 4/13.
- See Piazza (and email from college) for clarification on P/F policy.

SUMMARY

Last Few Classes: Low-Rank Approximation and PCA

- Compress data that lies close to a k-dimensional subspace.
- Equivalent to finding a low-rank approximation of the data matrix $\mathbf{X}$: $\underline{\mathbf{X}} \approx \underline{\mathbf{X}\mathbf{V}}\mathbf{V}^T$ for orthonormal $\mathbf{V} \in \mathbb{R}^{d \times k}$.
- Optimal solution via PCA (eigendecomposition of $\mathbf{X}^T\mathbf{X}$ or equivalently, SVD of $\mathbf{X}$).
- Singular vectors of $\mathbf{X}$ are the eigenvectors of $\mathbf{X}\mathbf{X}^T$ and $\mathbf{X}^T\mathbf{X}$. Singular values squared are the eigenvalues.

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This Class: Applications of low-rank approx. beyond compression.

- Matrix completion and collaborative filtering
- Entity embeddings (word embeddings, node embeddings, etc.)
- Low-rank approximation for non-linear dimensionality reduction.
- Spectral graph theory, spectral clustering.

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).

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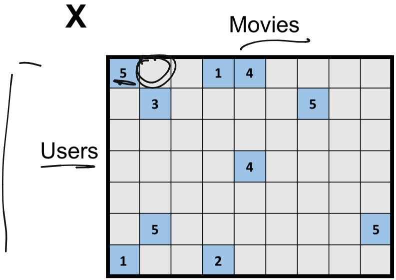

5			1	4				
	3					5		
				4				
	5							5
1			2					

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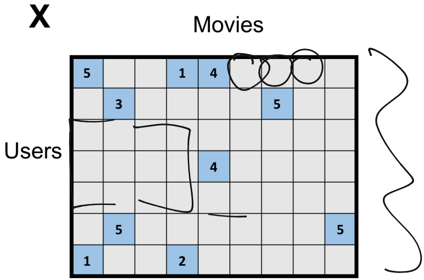
observed all of X

↓

eigen decomp

$X^T X$



5			1	4				
	3					5		
				4				
	5							5
1			2					

$\min \|X - B\|_F^2$

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

MATRIX COMPLETION

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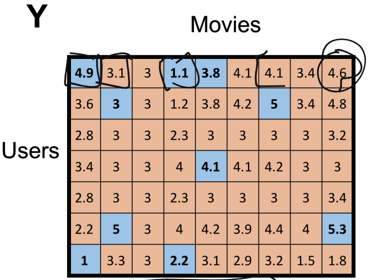
regression using low rank approx.



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

$B = [Z][W]$

Under certain assumptions, can show that **Y** well approximates **X** on both the observed and (most importantly) unobserved entries.

ENTITY EMBEDDINGS

Dimensionality reduction embeds d-dimensional vectors into $\underline{x} =$ d' dimensions. But what about when you want to embed objects other than vectors?

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

ENTITY EMBEDDINGS

$$X \in \mathbb{R}^{n\times d} \approx \underline{XVV^T} \in \mathbb{R}^{n\times d}$$

$$\underline{\|X - XVV^T\|_F^2}$$

compression $\underline{XV} \in \mathbb{R}^{n\times k}$

Dimensionality reduction embeds d-dimensional vectors into d' dimensions. But what about when you want to embed objects other than vectors?

- Documents (for topic-based search and classification)
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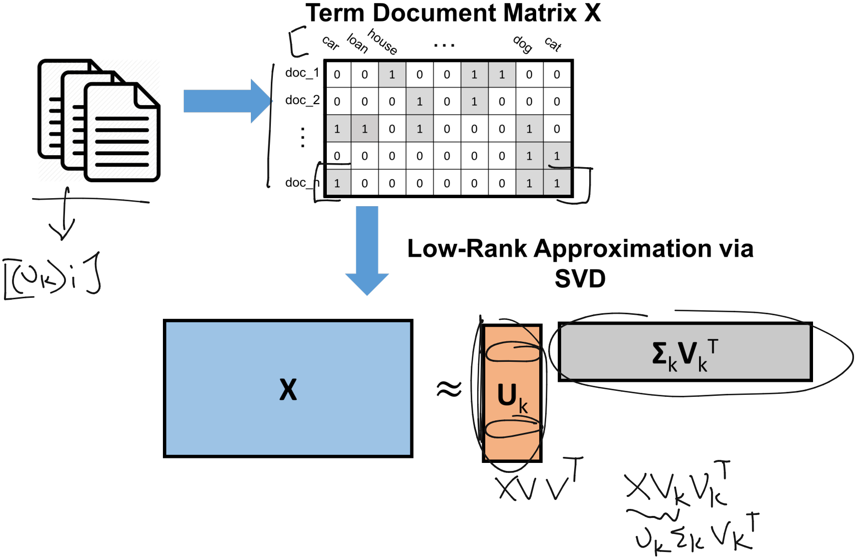
Usual Approach: Convert each item into a high-dimensional feature vector and then apply low-rank approximation.

entity embedding

word
node
document

$$\rightarrow \underset{d}{[\text{feature vector}]} \rightarrow \underset{k}{[\text{feature vector}]}$$

EXAMPLE: LATENT SEMANTIC ANALYSIS



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

$[(U_k)_i]$

Low-Rank Approximation via SVD

$$X \approx U_k \Sigma_k V_k^T$$

XVV^T

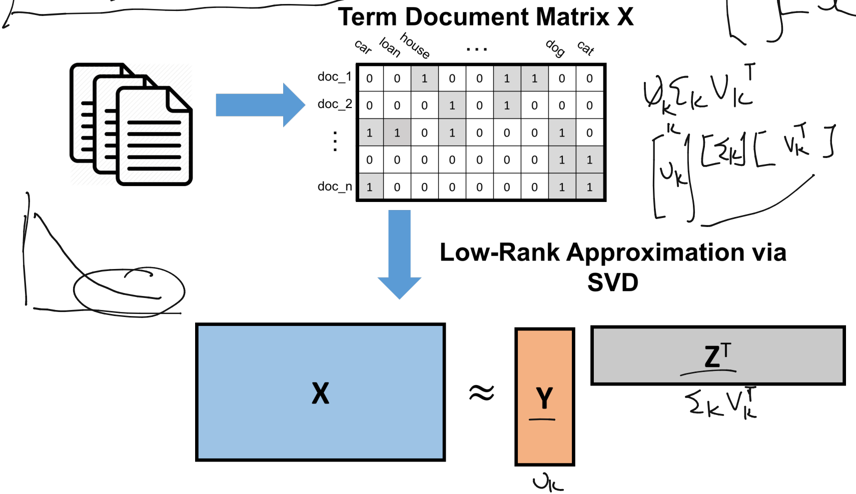
$\underbrace{XV_k}V_k^T$

$U_k \Sigma_k V_k^T$

EXAMPLE: LATENT SEMANTIC ANALYSIS

$$\boxed{\sigma_i(X)^2 = \lambda_i(X^TX) = \lambda_i(XX^T)}$$

$$X = \left[U\right]\left[\Sigma\right]\left[V^T\right]$$



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	0	0	0	0	0	0	0	1	1
doc_n	1	0	0	0	0	0	0	1	1

$U_k \Sigma_k V_k^T$

$$\overset{k}{\left[U_k\right]}\left[\Sigma_k\right]\left[V_k^T\right] = X_k$$

Low-Rank Approximation via SVD

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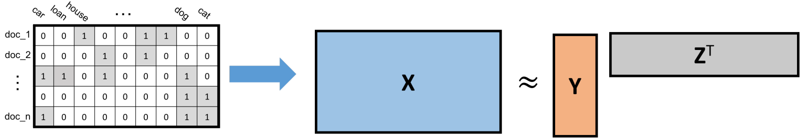

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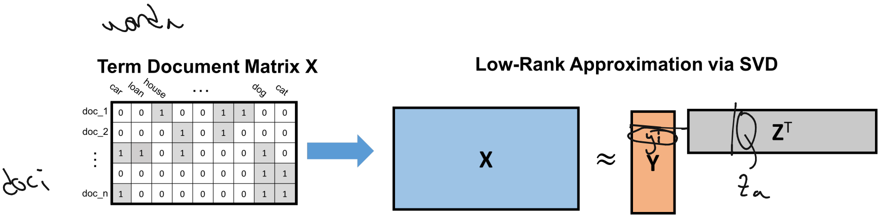

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	0	0	0	0	0	0	0	1	1
doc_n	1	0	0	0	0	0	0	1	1

- If the error $\underline{\|X - YZ^T\|_F}$ is small, then on average,

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

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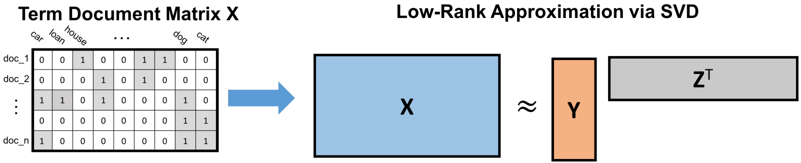

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doc_n	1	0	0	0	0	0	0	1	1

- If the error $\|X - YZ^T\|_F$ is small, then on average,

$$\underset{\overset{\|}{1}}{X_{i,a}} \approx (YZ^T)_{i,a} = \langle \vec{y}_i, \vec{z}_a \rangle.$$

- I.e., $\langle \vec{y}_i, \vec{z}_a \rangle \approx 1$ when doc_i contains $word_a$.

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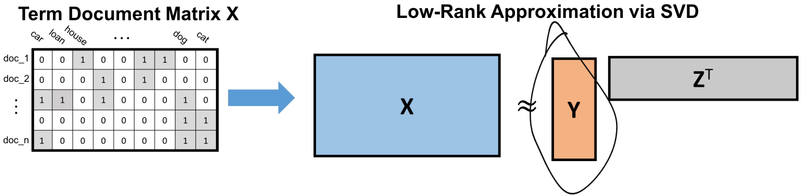

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⋮	1	1	0	1	0	0	0	1	0
	0	0	0	0	0	0	0	1	1
doc_n	1	0	0	0	0	0	0	1	1

- If the error $\|\mathbf{X} - \mathbf{Y}\mathbf{Z}^T\|_F$ is small, then on average,

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- I.e., $\langle \vec{y}_i, \vec{z}_a \rangle \approx 1$ 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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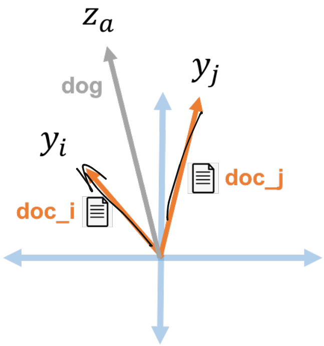
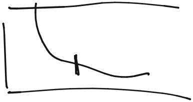


$$\|X - YZ^T\|_F^2$$



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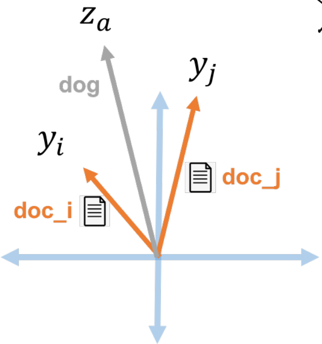
k

$n \begin{bmatrix} 1 & 1 & .5 & 0 \end{bmatrix}$ $\begin{bmatrix} z_a \end{bmatrix}$

Y

$X \approx_n \begin{bmatrix} Y \end{bmatrix} \begin{bmatrix} Z^T \end{bmatrix}_k$

k d



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

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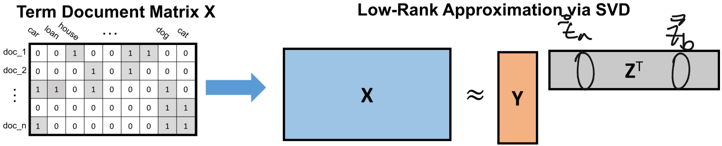

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- Just like with documents, $\vec{z}_a$ and $\vec{z}_b$ will tend to have high dot product if $word_a$ and $word_b$ appear in many of the same documents.

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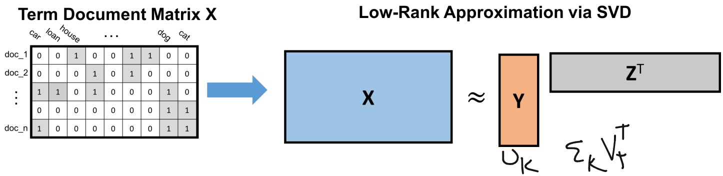

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- In an SVD decomposition we set $\mathbf{Z} = \mathbf{\Sigma}_k \mathbf{V}_K^T$.
- The columns of $\underline{\mathbf{V}_k}$ are equivalently: the top k eigenvectors of $\underline{\mathbf{X}^T\mathbf{X}}$.

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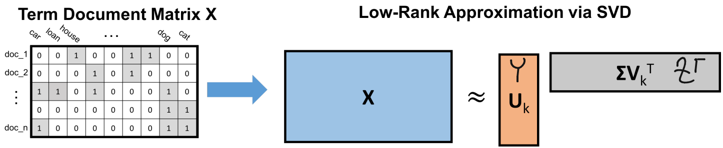

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$X = U\Sigma V^T \quad X^T X = V\Sigma U^T U \Sigma V^T = \underline{V\Sigma^2 V^T}$

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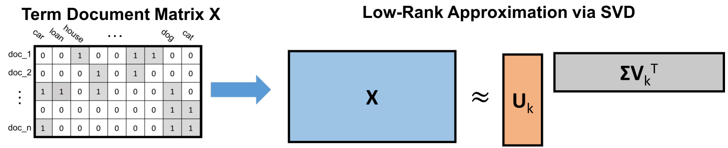

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Low-Rank Approximation via SVD

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- What is the best rank-k approximation of $\mathbf{X}^T\mathbf{X}$? I.e. $\arg\min_{\text{rank}-k\ \mathbf{B}} \|\mathbf{X}^T\mathbf{X} - \mathbf{B}\|_F$

$$d\overset{k}{\left[\, Z \,\right]}$$

ZZ^T is best LRA of X^TX

$$\overset{d}{\left[V_k\right]}\left[\Sigma_k^2\right]\left[V_k^T\right] = d\overset{d}{\left[ZZ^T\right]}$$

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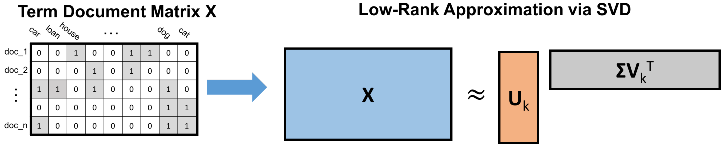

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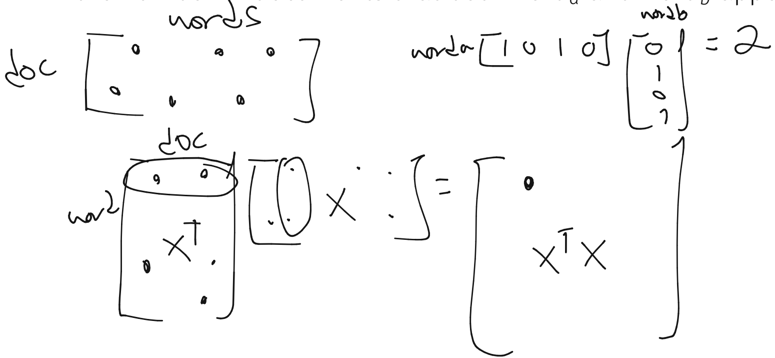
- What is the best rank-k approximation of $\mathbf{X}^T\mathbf{X}$? I.e. $\arg\min_{\text{rank}-k\ \mathbf{B}} \|\mathbf{X}^T\mathbf{X} - \mathbf{B}\|_F$
- $\mathbf{X}^T\mathbf{X} = \mathbf{V}_k\mathbf{\Sigma}_k^2\mathbf{V}_k^T = \mathbf{Z}\mathbf{Z}^T$.

EXAMPLE: WORD EMBEDDING

LSA gives a way of embedding words into k-dimensional space. $\left[z \right]$

- Embedding is via low-rank approximation of $\underline{X^T X}$: where $\underline{(X^T X)}_{a,b}$ is the number of documents that both $word_a$ and $word_b$ appear in.



EXAMPLE: WORD EMBEDDING

$X \approx [Y][Z^T]$

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$$ZZ^T = \arg\min \|X^T X - B\|_F^2$$

- Think about $X^T X$ as a similarity matrix (gram matrix, kernel matrix) with entry $\underline{(a, b)}$ being the similarity between *word*$_a$ and *word*$_b$.

EXAMPLE: WORD EMBEDDING

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- Embedding is via low-rank approximation of X^TX: where $(X^TX)_{a,b}$ is the number of documents that both $word_a$ and $word_b$ appear in.

- Think about $\underline{X^TX}$ as a similarity matrix (gram matrix, kernel matrix) with entry (a, b) being the similarity between $word_a$ and $word_b$.
- 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.

S d

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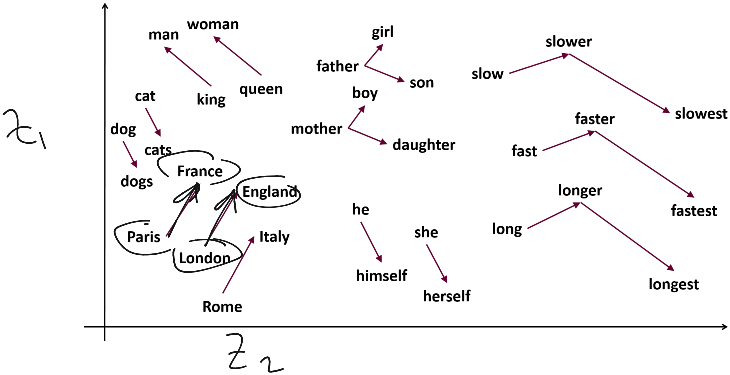
- Think about $\mathbf{X}^T\mathbf{X}$ as a similarity matrix (gram matrix, kernel matrix) with entry (a, b) being the similarity between $word_a$ and $word_b$.
- Many ways to measure similarity: number of sentences both occur in, number of times both appear in the same window of w words, in similar positions of documents in different languages, etc.
- Replacing $\mathbf{X}^T\mathbf{X}$ with these different metrics (sometimes appropriately transformed) leads to popular word embedding algorithms: word2vec, GloVe, fastText, etc.

EXAMPLE: WORD EMBEDDING

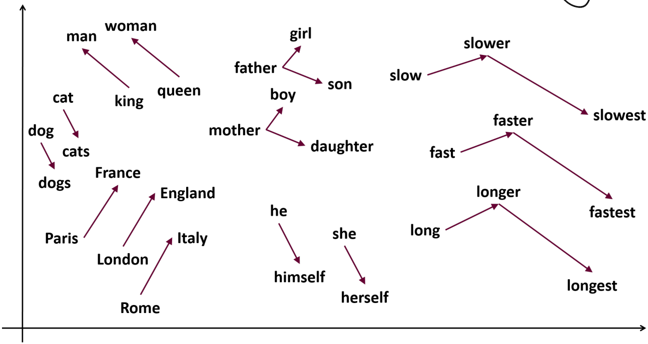


EXAMPLE: WORD EMBEDDING

entities → similarity mtx → LRA

↓

embedding



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.

SIMILARITY VIA GRAPHS

A common way of encoding similarity is via a graph. E.g., a k-nearest neighbor graph.

- Connect items to similar items, possibly with higher weight edges when they are more similar.

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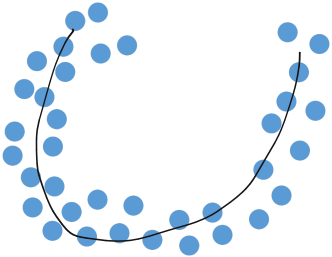

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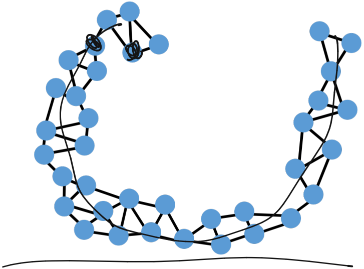
Non-linear compression



SIMILARITY VIA GRAPHS

A common way of encoding similarity is via a graph. E.g., a *k*-nearest neighbor graph.

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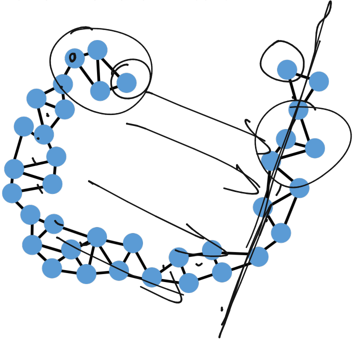

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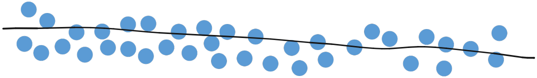

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LINEAR ALGEBRAIC REPRESENTATION OF A GRAPH

Once we have connected n data points $x_1, \ldots, x_n$ into a graph, we can represent that graph by its (weighted) adjacency matrix.

$$\mathbf{A} \in \mathbb{R}^{n \times n} \text{ with } \mathbf{A}_{i,j} = \text{ edge weight between nodes } i \text{ and } j$$

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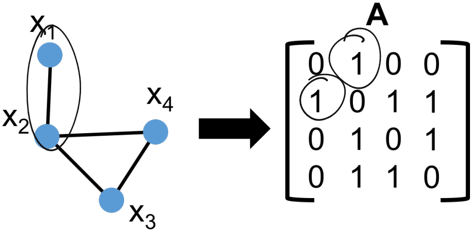

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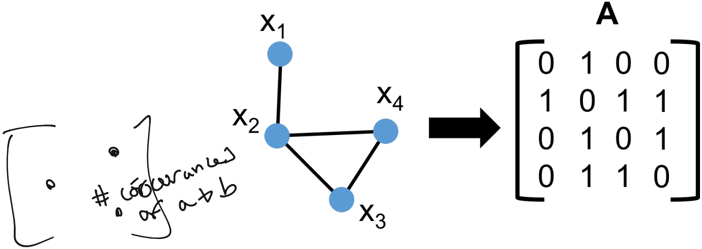

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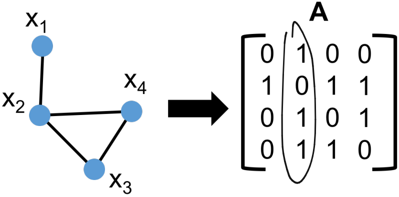
In LSA example, when $\mathbf{X}$ is the term-document matrix, $\mathbf{X}^T\mathbf{X}$ is like an adjacency matrix, where $word_a$ and $word_b$ are connected if they appear in at least 1 document together (edge weight is # documents they appear in together).

NORMALIZED ADJACENCY MATRIX



$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

What is the sum of entries in the i^{th} column of A?

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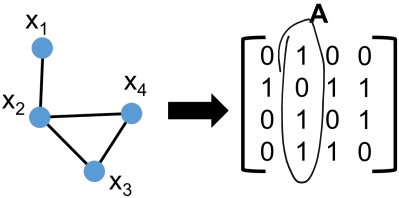

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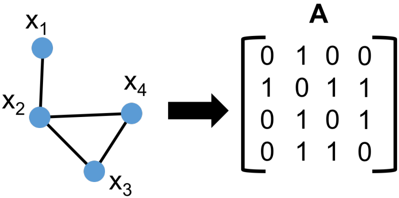

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Often, $\mathbf{A}$ is normalized as $\underline{\bar{\mathbf{A}}} = \underline{\mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}}^{-1/2}$ where $\mathbf{D}$ is the degree matrix.

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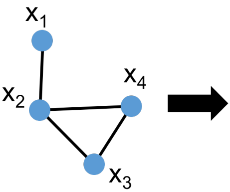

$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

$$\mathbf{D} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}$$

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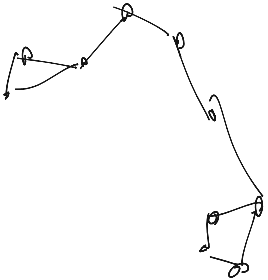
Spectral graph theory is the field of representing graphs as matrices and applying linear algebraic techniques.

ADJACENCY MATRIX EIGENVECTORS

How do we compute an optimal low-rank approximation of $\mathbf{A}$?



ADJACENCY MATRIX EIGENVECTORS

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- Project onto the top k eigenvectors of $\mathbf{A}^T\mathbf{A} = \mathbf{A}^2$.

ADJACENCY MATRIX EIGENVECTORS

How do we compute an optimal low-rank approximation of **A**?

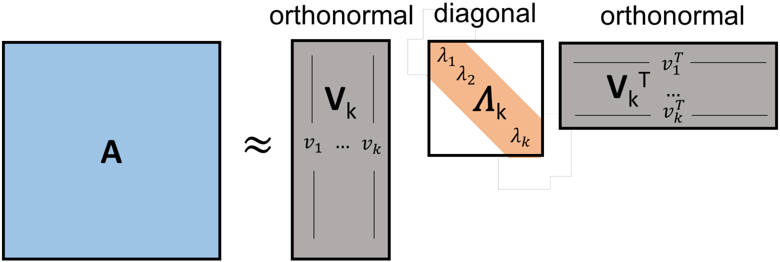
- Project onto the top k eigenvectors of $\mathbf{A}^T\mathbf{A} = \mathbf{A}^2$. These are just the eigenvectors of **A**.

$$A = V \Lambda V^T$$

$$A^T A = A^2 = V \Lambda V^T V \Lambda V^T$$

$$= \underline{V} \Lambda^2 V^T$$

ADJACENCY MATRIX EIGENVECTORS



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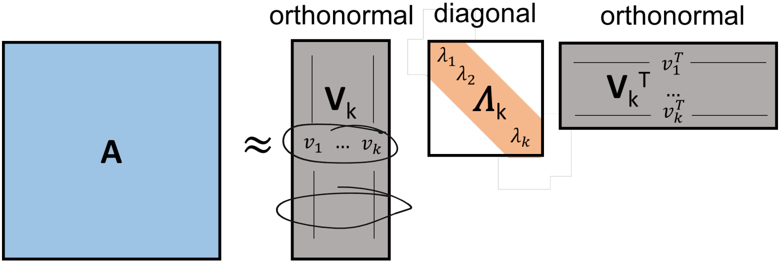


- Similar vertices (close with regards to graph proximity) should have similar embeddings. I.e., $V_k(i)$ should be similar to $V_k(j)$.

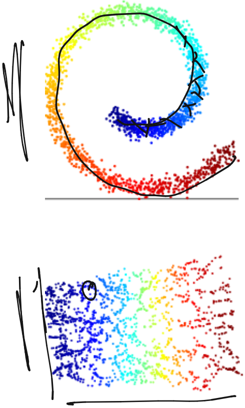
SPECTRAL EMBEDDING

"jelly roll"

$$\begin{bmatrix} A \end{bmatrix}$$

$$\downarrow$$

$$\begin{bmatrix} Z \end{bmatrix}_2 \begin{bmatrix} Z^T \end{bmatrix}^2$$



Summary:

LRA used beyond compression of vectors

- matrix completion
- entity embedding
- nonlinear dimension