COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

Andrew McGregor

Lecture 17

Last Class:

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- SVD: Can write any matrix $\mathbf{X}$ with rank r as $\mathbf{U\Sigma V}^T$ where $\mathbf{\Sigma} \in \mathbb{R}^{r \times r}$ is diagonal and columns of $\mathbf{U}$ and $\mathbf{V}$ are orthonormal.

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Today: Spectral Graph Theory & Spectral Clustering.

- Low-rank approximation on graph adjacency matrix for non-linear dimensionality reduction.
- Eigendecomposition to partition graphs into clusters.

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ENTITY EMBEDDINGS

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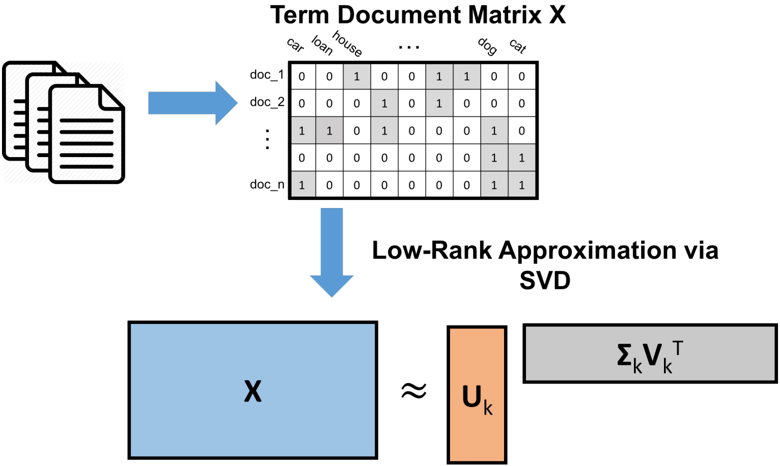
Usual Approach: Convert each item into a high-dimensional feature vector and then apply low-rank approximation.



	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
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Term Document Matrix X

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Low-Rank Approximation via SVD

$$\mathbf{X} \approx \mathbf{Y}\,\mathbf{Z}^T$$

EXAMPLE: LATENT SEMANTIC ANALYSIS

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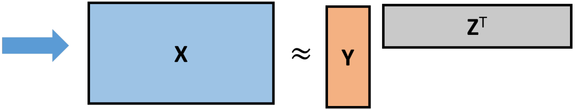

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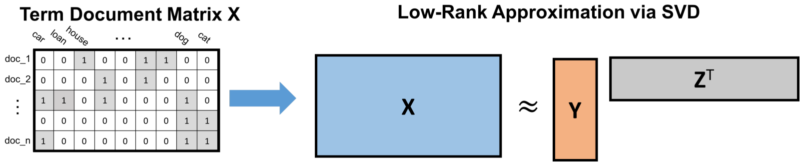

- If the error $\|\mathbf{X} - \mathbf{Y}\mathbf{Z}^T\|_F$ is small, then on average,

$$\mathbf{X}_{i,a} \approx (\mathbf{Y}\mathbf{Z}^T)_{i,a} = \langle \vec{y}_i, \vec{z}_a \rangle.$$

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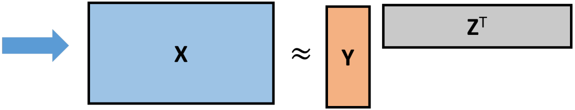

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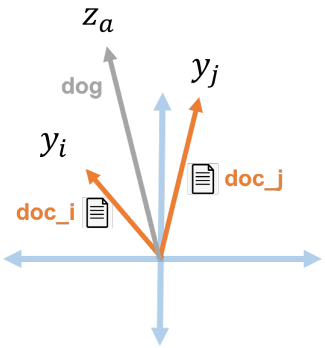
$$\mathbf{X}_{i,a} \approx (\mathbf{YZ}^T)_{i,a} = \langle \vec{y}_i, \vec{z}_a \rangle.$$

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

EXAMPLE: LATENT SEMANTIC ANALYSIS

If doc_i and doc_j both contain $word_a$, $\langle \vec{y}_i, \vec{z}_a \rangle \approx 1$ and $\langle \vec{y}_j, \vec{z}_a \rangle \approx 1$ and so $\langle \vec{y}_i, \vec{z}_a \rangle \approx \langle \vec{y}_j, \vec{z}_a \rangle$. Similarly if both don't contain $word_a$, $\langle \vec{y}_i, \vec{z}_a \rangle \approx \langle \vec{y}_j, \vec{z}_a \rangle$



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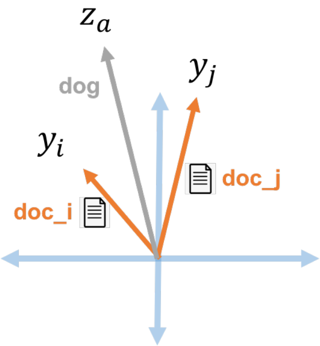

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Another View: Column of $\mathbf{Y}$ represent 'topics'. $\vec{y}_i(j)$ indicates how much doc_i belongs to topic j. $\vec{z}_a(j)$ indicates how much $word_a$ associates with topic j.

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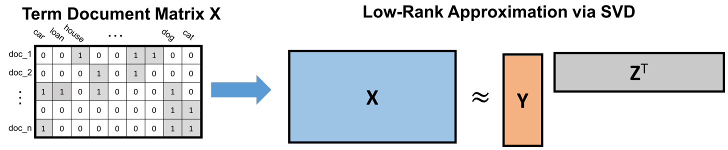

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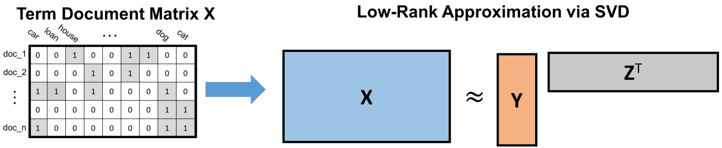

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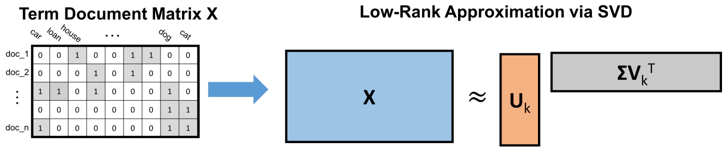

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LSA gives a way of embedding words into k-dimensional space.

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

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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 $\mathbf{X}^T\mathbf{X}$ with these different metrics (sometimes appropriately transformed) leads to popular word embedding algorithms: word2vec, GloVe, fastText, etc.

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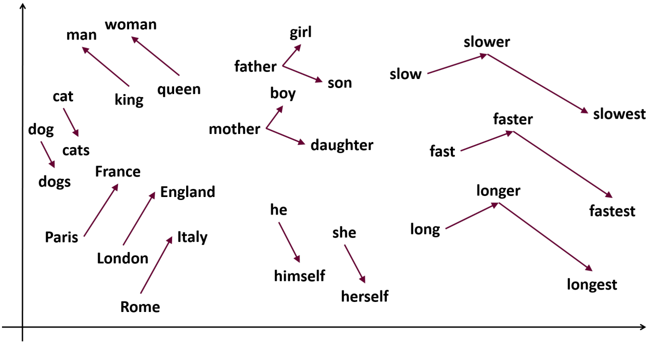

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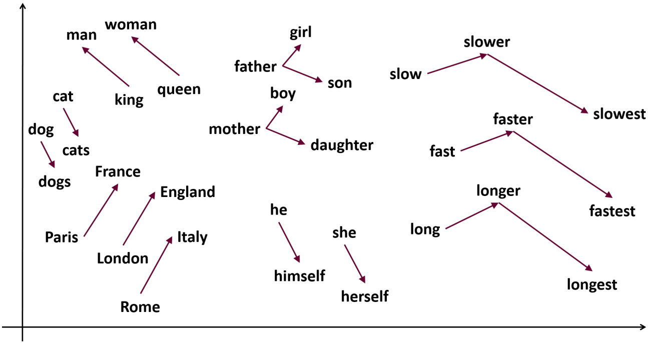
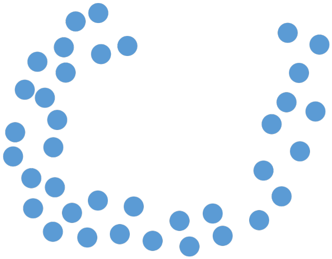
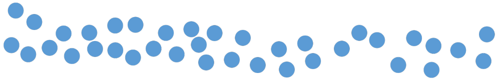


Note: word2vec is typically described as a neural-network method, but it is really just low-rank approximation of a specific similarity matrix. *Neural word embedding as implicit matrix factorization*, Levy and Goldberg.

GRAPH EMBEDDINGS



Is this set of points compressible? Does it lie close to a low-dimensional subspace? (A 1-dimensional subspace of $\mathbb{R}^d$.)



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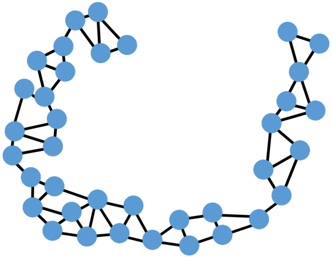

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A common way of automatically identifying this non-linear structure is to connect data points in a graph. E.g., a k-nearest neighbor graph.

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

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.

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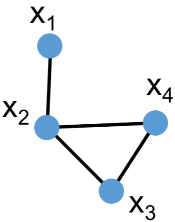
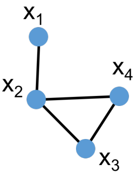


$$\mathbf{A} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

THE LAPLACIAN VIEW

For a graph with adjacency matrix **A** and degree matrix **D**, $\mathbf{L} = \mathbf{D} - \mathbf{A}$ is the graph Laplacian.



$$\overset{\mathbf{D}}{\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 2 \end{bmatrix}} - \overset{\mathbf{A}}{\begin{bmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 \\ 0 & 1 & 1 & 0 \end{bmatrix}} = \overset{\mathbf{L}}{\begin{bmatrix} 1 & -1 & 0 & 0 \\ -1 & 3 & -1 & -1 \\ 0 & -1 & 2 & -1 \\ 0 & -1 & -1 & 2 \end{bmatrix}}$$

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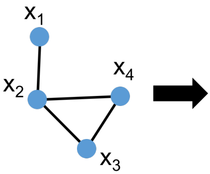

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For any vector $\vec{v}$, its 'smoothness' over the graph is given by:

$$\sum_{(i,j)\in E} (\vec{v}(i) - \vec{v}(j))^2 = \vec{v}^T \mathbf{L} \vec{v}.$$

REWRITING LAPLACIAN

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- If $e = (i, j)$, then $\vec{v}^T \mathbf{L}_e \vec{v} = (v(i) - v(j))^2$

ADJACENCY MATRIX EIGENVECTORS

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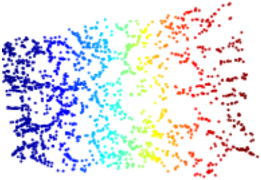
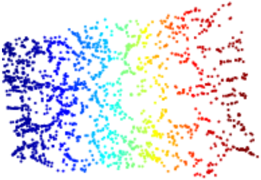
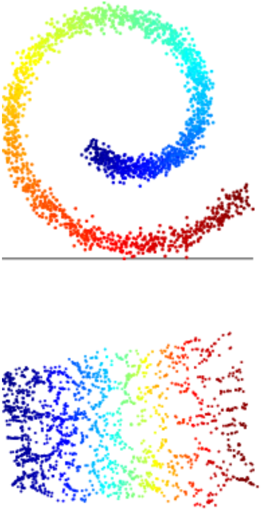
  where we showed the equality in Lecture 14.





Step 1: Produce a nearest neighbor graph based on your input data in $\mathbb{R}^d$.



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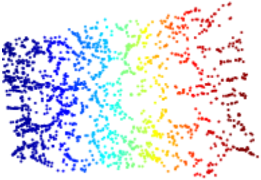
SPECTRAL EMBEDDING



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Step 3: Work with the data in the embedded space. Where distances approximate distances in your original ‘non-linear space.’