COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

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Lecture 17
Last Class: Low-Rank Approximation, Eigendecomposition, PCA

- For any symmetric square matrix $A$, we can write $A = V \Lambda V^T$ where columns of $V$ are orthonormal eigenvectors.

- Can approximate data lying close to in a $k$-dimensional subspace by projecting data points into that space.

- Can find the best $k$-dimensional subspace via eigendecomposition applied to $X^T X$ (PCA).

- Measuring error in terms of the eigenvalue spectrum.

This Class: SVD and Applications

- SVD and connection to eigenvalue value decomposition.

- Applications of low-rank approximation beyond compression.
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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).
- $\Sigma$ is diagonal with elements $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_r > 0$ (singular values).
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The ‘swiss army knife’ of modern linear algebra.
Writing $X \in \mathbb{R}^{n \times d}$ in its singular value decomposition $X = U \Sigma V^T$:

$$X^T X =$$

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

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Writing \( X \in \mathbb{R}^{n \times d} \) in its singular value decomposition \( X = UV^T \):

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X^T X = V\Sigma U^T U\Sigma V^T = V\Sigma^2 V^T
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Writing $X ∈ \mathbb{R}^{n×d}$ in its singular value decomposition $X = UΣV^T$:

$$X^TX = VΣU^T UΣV^T = VΣ^2V^T$$ (the eigendecomposition)

Similarly: $XX^T = UΣV^TVΣU^T = UΣ^2U^T$.

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

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

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

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

**Exercise:** $U_k U_k^T X = X V_k V_k^T = U_k \Sigma_k V_k^T$

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

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

$$X_k = XV_k V_k^T = U_k U_k^T X = U_k \Sigma_k V_k^T$$
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Correspond to projecting the rows (data points) onto the span of $V_k$ or the columns (features) onto the span of $U_k$
The best low-rank approximation to $\mathbf{X}$:

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

is given by:

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

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**Diagram Description:**

- The diagram represents the SVD of a matrix $\mathbf{X}$, where $\mathbf{X}$ is an $n \times d$ matrix (rank $k$).
- $\mathbf{U}$ is the matrix of left singular vectors.
- $\mathbf{\Sigma}$ is the diagonal matrix of singular values.
- $\mathbf{V}$ is the matrix of right singular vectors.

The diagram illustrates how $\mathbf{X}$ can be approximated by $\mathbf{X}_k = \mathbf{U}_k \mathbf{\Sigma}_k \mathbf{V}_k^T$. The best low-rank approximation is achieved by projecting the data onto the span of the top $k$ singular vectors.
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Correspond to projecting the rows (data points) onto the span of $V_k$ or the columns (features) onto the span of $U_k$.
• Let \( \vec{v}_1, \vec{v}_2, \ldots, \in \mathbb{R}^d \) be orthonormal eigenvectors of \( X^T X \).

• Exercise: Show \( \vec{u}_1, \vec{u}_2, \ldots \) are orthonormal.

• This establishes that \( XV = U\Sigma \) and that \( V \) and \( U \) have the required properties to show \( X = U\Sigma V^T \).

• To see rest of the details, see https://math.mit.edu/classes/18.095/2016IAP/lec2/SVD_Notes.pdf
Basic Idea to Prove Existence of SVD

- Let \( \vec{v}_1, \vec{v}_2, \ldots, \in \mathbb{R}^d \) be orthonormal eigenvectors of \( \mathbf{X}^T \mathbf{X} \).
- Let \( \sigma_i = \| \mathbf{X} \vec{v}_i \|_2 \) and define unit vector \( \vec{u}_i = \frac{\mathbf{X} \vec{v}_i}{\sigma_i} \).
BASIC IDEA TO PROVE EXISTENCE OF SVD

• Let $\vec{v}_1, \vec{v}_2, \ldots, \in \mathbb{R}^d$ be orthonormal eigenvectors of $X^TX$.

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- Exercise: Show \( \vec{u}_1, \vec{u}_2, \ldots \) are orthonormal.
- This establishes that \( XV = U\Sigma \) and that \( V \) and \( U \) have the required properties to show \( X = U\Sigma V^T \).
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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 $X \in \mathbb{R}^{n \times d}$ 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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Solve: $Y = \arg \min_{rank-k \ B \ \text{observed}} \sum_{(j,k)} [X_{j,k} - B_{j,k}]^2$
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.

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

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.)
- Nodes in a social network
Dimensionality reduction embeds $d$-dimensional vectors into $k \ll d$ dimensions. But what about when you want to embed objects other than vectors?

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**Usual Approach:** Convert each item into a high-dimensional feature vector and then apply low-rank approximation.
### EXAMPLE: LATENT SEMANTIC ANALYSIS

#### Term Document Matrix X

<table>
<thead>
<tr>
<th></th>
<th>car</th>
<th>loan</th>
<th>house</th>
<th>...</th>
<th>dog</th>
<th>cat</th>
</tr>
</thead>
<tbody>
<tr>
<td>doc_1</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>doc_2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>1</td>
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<td>0</td>
</tr>
<tr>
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<td>0</td>
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<td>0</td>
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<td></td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

#### Low-Rank Approximation via SVD

$$X \approx \Sigma_k V_k^T$$
EXAMPLE: LATENT SEMANTIC ANALYSIS

Term Document Matrix $X$

<table>
<thead>
<tr>
<th></th>
<th>car</th>
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<th>...</th>
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<th>cat</th>
</tr>
</thead>
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<tr>
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<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>doc_2</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>...</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>doc_n</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td></td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>

Low-Rank Approximation via SVD

$X \approx YZ^T$
If the error $\|X - YZ^T\|_F$ is small, then on average, $X_i, a \approx (YZ^T)_i, a = \langle \vec{y}_i, \vec{z}_a \rangle$.

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

If $doc_i$ and $doc_j$ both contain word $a$, $\langle \vec{y}_i, \vec{z}_a \rangle \approx \langle \vec{y}_j, \vec{z}_a \rangle \approx 1$. 

**Example: Latent Semantic Analysis**

Term Document Matrix $X$

<table>
<thead>
<tr>
<th></th>
<th>Cat</th>
<th>loan</th>
<th>house</th>
<th>...</th>
<th>doc</th>
<th>cat</th>
</tr>
</thead>
<tbody>
<tr>
<td>doc_1</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>doc_2</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>...</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
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<td>0</td>
<td>0</td>
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<td>0</td>
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</tr>
</tbody>
</table>

Low-Rank Approximation via SVD

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

$$X_{i,a} \approx (YZ^T)_{i,a} = \langle \bar{y}_i, \bar{z}_a \rangle.$$
### Example: Latent Semantic Analysis

#### Term Document Matrix $X$

<table>
<thead>
<tr>
<th>Doc_1</th>
<th>Doc_2</th>
<th>...</th>
<th>Doc_n</th>
</tr>
</thead>
<tbody>
<tr>
<td>Car</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>sofa</td>
<td>0</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>...</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>Car</td>
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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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Example: Latent Semantic Analysis

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

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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• The best rank-\( k \) approximation of \( \mathbf{X}^T \mathbf{X} \) is

\[
\arg \min_{\mathbf{B}} \| \mathbf{X}^T \mathbf{X} - \mathbf{B} \|_F = \mathbf{V}_k \Sigma_k^2 \mathbf{V}_k^T = \mathbf{Z} \mathbf{Z}^T
\]
EXAMPLE: WORD EMBEDDING

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

- Embedding is via low-rank approximation of $X^T X$: where $(X^T X)_{a,b}$ 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.
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- Replacing $X^TX$ with these different metrics (sometimes appropriately transformed) leads to popular word embedding algorithms: word2vec, GloVe, fastText, etc.
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