# COMPSCI 514: ALGORITHMS FOR DATA SCIENCE 

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Lecture 16

## SUMMARY

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

- For any symmetric square matrix $A$, we can write $\mathbf{A}=\mathbf{V} \boldsymbol{\wedge} \mathbf{V}^{T}$ where columns of $\mathbf{V}$ 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 $\mathbf{X}^{T} \mathbf{X}$ (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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- 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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The 'swiss army knife' of modern linear algebra.

## CONNECTION OF THE SVD TO EIGENDECOMPOSITION

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

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$\mathbf{X} \in \mathbb{R}^{n \times d}$ : data matrix, $\mathbf{U} \in \mathbb{R}^{n \times \operatorname{rank}(\mathbf{X})}$ : matrix with orthonormal columns $\vec{u}_{1}, \vec{u}_{2}, \ldots$ (left singular vectors), $\mathbf{V} \in \mathbb{R}^{d \times \operatorname{rank}(\mathbf{X})}$ : matrix with orthonormal columns $\vec{v}_{1}, \vec{v}_{2}, \ldots$ (right singular vectors), $\boldsymbol{\Sigma} \in \mathbb{R}^{\operatorname{rank}(\mathbf{X}) \times \operatorname{rank}(\mathbf{X})}$ : positive diagonal matrix containing singular values of $\mathbf{X}$.

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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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Corresponds 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
projections onto 15
784 dimensional vectors


Column (feature) compression

|  | 10000* bathrooms $+10^{*}$ (sq. ft.) $\approx$ 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 | 3500 | 3 | 450,000 | 450,000 |

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$\mathrm{n} \times \mathrm{d}$ (rank k)

orthonormal positive diagonal

orthonormal


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- To see rest of the details, see https:
//math.mit.edu/classes/18.095/2016IAP/lec2/SVD_Notes.pdf


## APPLICATIONS OF LOW-RANK APPROXIMATION

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.


## 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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Movies


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

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Movies

Users | 4.9 | 3.1 | 3 | 1.1 | 3.8 | 4.1 | 4.1 | 3.4 | 4.6 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 3.6 | $\mathbf{3}$ | 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 | $\mathbf{5}$ | 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: $\boldsymbol{Y}=\underset{\text { rank }-k \mathbf{B}}{\arg \min } \sum_{\text {observed }(j, k)}\left[\mathbf{X}_{j, k}-\mathbf{B}_{j, k}\right]^{2}$
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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- Nodes in a social network


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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



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Term Document Matrix X


Low-Rank Approximation via SVD



## EXAMPLE: LATENT SEMANTIC ANALYSIS

Term Document Matrix $\mathbf{X}$

| 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


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

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

## EXAMPLE: LATENT SEMANTIC ANALYSIS

Term Document Matrix $\mathbf{X}$

|  | $c_{q,} o_{q_{\eta}} h_{o_{s}}$ |  |  | . |  |  | $\%_{9} \%_{t}$ |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 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


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

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

- I.e., $\left\langle\vec{y}_{i}, \vec{z}_{a}\right\rangle \approx 1$ when doc $_{i}$ contains word ${ }_{a}$.


## EXAMPLE: LATENT SEMANTIC ANALYSIS

If doc $i_{i}$ and doc $_{j}$ both contain word $_{a},\left\langle\vec{y}_{i}, \vec{z}_{a}\right\rangle \approx\left\langle\vec{y}_{j}, \vec{z}_{a}\right\rangle \approx 1$ If doc $c_{i}$ and doc $c_{j}$ both don't contain word ${ }_{a},\left\langle\vec{y}_{i}, \vec{z}_{a}\right\rangle \approx\left\langle\vec{y}_{j}, \vec{z}_{a}\right\rangle \approx 0$


Since this applies for all words, documents with that involve a similar set of words tend to have high dot product with each other.

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Since this applies for all words, documents with that involve a similar set of words tend to have high dot product with each other.

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 that topic.

## EXAMPLE: LATENT SEMANTIC ANALYSIS

Term Document Matrix X


Low-Rank Approximation via SVD

$\mathbf{Z}^{\top}$

- Just like with documents, $\vec{z}_{a}$ and $\vec{z}_{b}$ will tend to have high dot product if $\operatorname{word}_{a}$ and word ${ }_{b}$ appear in many of the same documents.


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- In an SVD decomposition we set $\mathbf{Z}^{T}=\boldsymbol{\Sigma}_{k} \mathbf{V}_{K}^{T}$ where columns of $\mathbf{V}_{k}$ are the top $k$ eigenvectors of $\mathbf{X}^{\top} \mathbf{X}$.


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## EXAMPLE: WORD EMBEDDING

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

- Embedding is via low-rank approximation of $\mathbf{X}^{T} \mathbf{X}$ : where $\left(\mathbf{X}^{T} \mathbf{X}\right)_{a, b}$ 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.


## EXAMPLE: WORD EMBEDDING



## EXAMPLE: WORD 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.

## GRAPH EMBEDDINGS

## NON-LINEAR DIMENSIONALITY REDUCTION



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

## NON-LINEAR DIMENSIONALITY REDUCTION

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## NON-LINEAR DIMENSIONALITY REDUCTION



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

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

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- Similar vertices (close with regards to graph proximity) should have similar embeddings since

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where we showed the equality in Lecture 14.

## SPECTRAL EMBEDDING



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Step 1: Produce a nearest neighbor graph based on your input data in $\mathbb{R}^{d}$.
Step 2: Apply low-rank approximation to the graph adjacency matrix to produce embeddings in $\mathbb{R}^{k}$.
Step 3: Work with the data in the embedded space. Where distances approximate distances in your original 'non-linear space.'

