# COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

Andrew McGregor Lecture 16

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

- For any symmetric square matrix A, we can write A = VΛV<sup>T</sup> 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<sup>T</sup>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).
- V has orthonormal columns  $\vec{v_1}, \ldots, \vec{v_r} \in \mathbb{R}^d$  (right singular vectors).
- Σ is diagonal with elements σ<sub>1</sub> ≥ σ<sub>2</sub> ≥ ... ≥ σ<sub>r</sub> > 0 (singular values).

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The 'swiss army knife' of modern linear algebra.

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

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

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

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

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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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**Exercise:** 
$$\mathbf{U}_k \mathbf{U}_k^T \mathbf{X} = \mathbf{X} \mathbf{V}_k \mathbf{V}_k^T = \mathbf{U}_k \mathbf{\Sigma}_k \mathbf{V}_k^T$$

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### THE SVD AND OPTIMAL LOW-RANK APPROXIMATION

The best low-rank approximation to  $\mathbf{X}$ , i.e.,

$$\begin{split} \mathbf{X}_k &= \mathop{\arg\min}_{\operatorname{rank}-k} \|\mathbf{X} - \mathbf{B}\|_F\\ \text{is given by } \mathbf{X}_k &= \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T = \mathbf{U}_k\mathbf{U}_k^T\mathbf{X} = \mathbf{U}_k\mathbf{\Sigma}_k\mathbf{V}_k^T \end{split}$$

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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 X, i.e.,

$$\mathbf{X}_{k} = \arg\min_{\mathsf{rank} - k} \min_{\mathbf{B} \in \mathbb{R}^{n \times d}} \|\mathbf{X} - \mathbf{B}\|_{F}$$

is given by  $\mathbf{X}_k = \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T = \mathbf{U}_k\mathbf{U}_k^T\mathbf{X} = \mathbf{U}_k\mathbf{\Sigma}_k\mathbf{V}_k^T$ 

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# BASIC IDEA TO PROVE EXISTENCE OF SVD

• Let  $\vec{v_1}, \vec{v_2}, \ldots, \in \mathbb{R}^d$  be orthonormal eigenvectors of  $\mathbf{X}^T \mathbf{X}$ .

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- This establishes that  $XV=U\Sigma$  and that V and U have the required properties.
- To see rest of the details, see https: //math.mit.edu/classes/18.095/2016IAP/lec2/SVD\_Notes.pdf

**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.

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

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Ŷ	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		

**Solve:** 
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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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**Usual Approach:** Convert each item into a high-dimensional feature vector and then apply low-rank approximation.









• 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<sub>i</sub> and doc<sub>j</sub> both contain word<sub>a</sub>,  $\langle \vec{y_i}, \vec{z_a} \rangle \approx \langle \vec{y_j}, \vec{z_a} \rangle \approx 1$  If doc<sub>i</sub> and doc<sub>j</sub> both don't contain word<sub>a</sub>,  $\langle \vec{y_i}, \vec{z_a} \rangle \approx \langle \vec{y_j}, \vec{z_a} \rangle \approx 0$ 



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**Another View:** Column of **Y** represent 'topics'.  $\vec{y_i}(j)$  indicates how much  $doc_i$  belongs to topic j.  $\vec{z_a}(j)$  indicates how much *word<sub>a</sub>* associates with that topic.

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- In an SVD decomposition we set Z<sup>T</sup> = Σ<sub>k</sub>V<sub>k</sub><sup>T</sup> where columns of V<sub>k</sub> are the top k eigenvectors of X<sup>T</sup>X.



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- In an SVD decomposition we set Z<sup>T</sup> = Σ<sub>k</sub>V<sub>k</sub><sup>T</sup> where columns of V<sub>k</sub> are the top k eigenvectors of X<sup>T</sup>X.

 Embedding is via low-rank approximation of X<sup>T</sup>X: where (X<sup>T</sup>X)<sub>a,b</sub> is the number of documents that both word<sub>a</sub> and word<sub>b</sub> 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 X<sup>T</sup>X with these different metrics (sometimes appropriately transformed) leads to popular word embedding algorithms: word2vec, GloVe, fastText, etc.

# EXAMPLE: WORD EMBEDDING



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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

# NON-LINEAR DIMENSIONALITY REDUCTION



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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.

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

$$\|(\mathbf{A})_i - (\mathbf{A})_j\|_2 \approx \|(\mathbf{A}\mathbf{V}_k\mathbf{V}_k^{\mathsf{T}})_i - (\mathbf{A}\mathbf{V}_k\mathbf{V}_k^{\mathsf{T}})_j\|_2 = \|(\mathbf{A}\mathbf{V}_k)_i - (\mathbf{A}\mathbf{V}_k)_j\|_2$$

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where we showed the equality in Lecture 14.







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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.'