COMPSCI 514: Algorithms for Data Science

Cameron Musco

University of Massachusetts Amherst. Fall 2022.

Lecture 17

Logistics

- Problem Set 3 is posted. Due Monday 11/14, 11:59pm.
- Quiz this week due Monday at 8pm.

Summary

Last Class: Optimal Low-Rank Approximation

- When data lies close to $\mathcal{V}$, the optimal embedding in that space is given by projecting onto that space.

$$XVV^T = \underset{B \text{ with rows in } \mathcal{V}}{\arg\min} \|X - B\|_F^2.$$

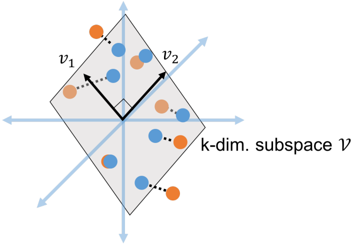
- Optimal V maximizes $\|XVV^T\|_F$ and can be found greedily. Equivalently by computing the top k eigenvectors of X^TX.

This Class:

- How do we assess the error of this optimal V.
- Connection to the singular value decomposition.

Basic Set Up

Reminder of Set Up: Assume that $\vec{x}_1, \ldots, \vec{x}_n$ lie close to any k-dimensional subspace $\mathcal{V}$ of $\mathbb{R}^d$. Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ be the data matrix.



Let $\vec{v}_1, \ldots, \vec{v}_k$ be an orthonormal basis for $\mathcal{V}$ and $\mathbf{V} \in \mathbb{R}^{d \times k}$ be the matrix with these vectors as its columns.

- $\mathbf{V}\mathbf{V}^T \in \mathbb{R}^{d \times d}$ is the projection matrix onto $\mathcal{V}$.
- $\mathbf{X} \approx \mathbf{X}(\mathbf{V}\mathbf{V}^T)$. Gives the closest approximation to $\mathbf{X}$ with rows in $\mathcal{V}$.

$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: orthogonal basis for subspace $\mathcal{V}$. $\mathbf{V} \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

Low-Rank Approximation via Eigendecomposition

$\mathbf{V}$ minimizing $\|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2$ is given by:

$$\underset{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}}{\arg\min} \|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2 = \underset{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}}{\arg\max} \|\mathbf{X}\mathbf{V}\|_F^2 = \sum_{j=1}^{k} \|\mathbf{X}\vec{v}_j\|_2^2$$

Solution via eigendecomposition: Letting $\mathbf{V}_k$ have columns $\vec{v}_1, \ldots, \vec{v}_k$ corresponding to the top k eigenvectors of $\mathbf{X}^T\mathbf{X}$,

$$\mathbf{V}_k = \underset{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}}{\arg\max} \|\mathbf{X}\mathbf{V}\|_F^2$$

- Proof via Courant-Fischer and greedy maximization.
- How accurate is this low-rank approximation? Can understand using eigenvalues of $\mathbf{X}^T\mathbf{X}$.

$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: orthogonal basis for subspace $\mathcal{V}$. $\mathbf{V} \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

Spectrum Analysis

Let $\vec{v}_1, \ldots, \vec{v}_k$ be the top k eigenvectors of $\mathbf{X}^T\mathbf{X}$ (the top k principal components). Approximation error is:

$$\|\mathbf{X} - \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T\|_F^2 = \|\mathbf{X}\|_F^2 \operatorname{tr}(\mathbf{X}^T\mathbf{X}) - \|\mathbf{X}\mathbf{V}_k\mathbf{V}_k^T\|_F^2 \operatorname{tr}(\mathbf{V}_k^T\mathbf{X}^T\mathbf{X}\mathbf{V}_k)$$

$$= \sum_{i=1}^{d} \lambda_i(\mathbf{X}^T\mathbf{X}) - \sum_{i=1}^{k} \vec{v}_i^T\mathbf{X}^T\mathbf{X}\vec{v}_i$$

$$= \sum_{i=1}^{d} \lambda_i(\mathbf{X}^T\mathbf{X}) - \sum_{i=1}^{k} \lambda_i(\mathbf{X}^T\mathbf{X}) = \sum_{i=k+1}^{d} \lambda_i(\mathbf{X}^T\mathbf{X})$$

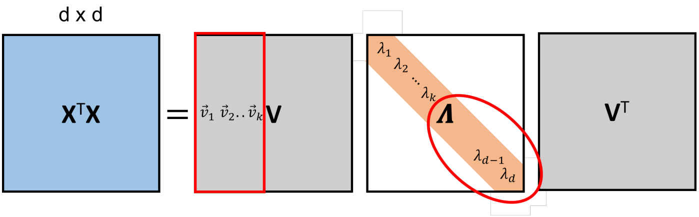
- **Exercise:** For any matrix $\mathbf{A}$, $\|\mathbf{A}\|_F^2 = \sum_{i=1}^{d} \|\vec{a}_i\|_2^2 = \operatorname{tr}(\mathbf{A}^T\mathbf{A})$ (sum of diagonal entries = sum eigenvalues).

$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: top eigenvectors of $\mathbf{X}^T\mathbf{X}$, $\mathbf{V}_k \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

Spectrum Analysis

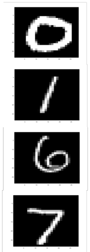
Claim: The error in approximating $\mathbf{X}$ with the best rank k approximation (projecting onto the top k eigenvectors of $\mathbf{X}^T\mathbf{X}$ is:

$$\|\mathbf{X} - \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T\|_F^2 = \sum_{i=k+1}^{d} \lambda_i(\mathbf{X}^T\mathbf{X})$$



error of optimal low rank approximation

784 dimensional vect



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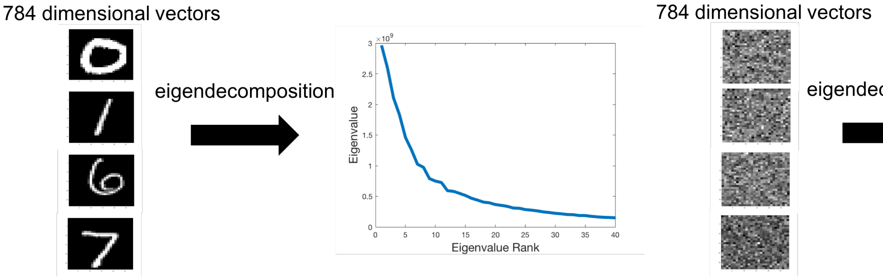
- Choose k to balance accuracy/compression – often at an 'elbow'.

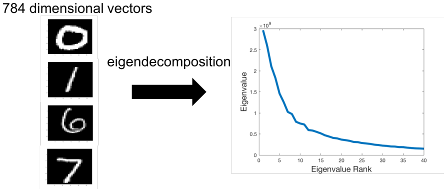
$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: top eigenvectors of $\mathbf{X}^T\mathbf{X}$, $\mathbf{V}_k \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

Plotting the spectrum of $\mathbf{X}^T\mathbf{X}$ (its eigenvalues) shows how compressible $\mathbf{X}$ is using low-rank approximation (i.e., how close $\vec{x}_1, \ldots, \vec{x}_n$ are to a low-dimensional subspace).



$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: top eigenvectors of $\mathbf{X}^T\mathbf{X}$, $\mathbf{V}_k \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

Spectrum Analysis



Exercises:

1. Show that the eigenvalues of $\mathbf{X}^T\mathbf{X}$ are always positive. **Hint:** Use that $\lambda_j = \vec{v}_j^T \mathbf{X}^T \mathbf{X} \vec{v}_j$.
2. Show that for symmetric $\mathbf{A}$, the trace is the sum of eigenvalues: $\mathbf{tr}(\mathbf{A}) = \sum_{i=1}^{n} \lambda_i(\mathbf{A})$. **Hint:** First prove the cyclic property of trace, that for any $\mathbf{MN}$, $\mathbf{tr}(\mathbf{MN}) = \mathbf{tr}(\mathbf{NM})$ and then apply this to $\mathbf{A}$'s eigendecomposition

Summary

- Many (most) datasets can be approximated via projection onto a low-dimensional subspace.
- Find this subspace via a maximization problem:

$$\max_{\text{orthonormal } \mathbf{V}} \|\mathbf{X}\mathbf{V}\|_F^2.$$

- Greedy solution via eigendecomposition of $\mathbf{X}^T\mathbf{X}$.
- Columns of $\mathbf{V}$ are the top eigenvectors of $\mathbf{X}^T\mathbf{X}$.
- Error of best low-rank approximation (compressibility of data) is determined by the tail of $\mathbf{X}^T\mathbf{X}$'s eigenvalue spectrum.

Interpretation in Terms of Correlation

Recall: Low-rank approximation is possible when our data features are correlated.

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

Our compressed dataset is $\mathbf{C} = \mathbf{X}\mathbf{V}_k$ where the columns of $\mathbf{V}_k$ are the top k eigenvectors of $\mathbf{X}^T\mathbf{X}$.

Observe that $\mathbf{C}^T\mathbf{C} = \mathbf{\Lambda}_k$

C^TC is diagonal. I.e., all columns are orthogonal to each other, and correlations have been removed. Maximal compression.

$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: top eigenvectors of $\mathbf{X}^T\mathbf{X}$, $\mathbf{V}_k \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

Algorithmic Considerations

Runtime to compute an optimal low-rank approximation:

- Computing $\mathbf{X}^T\mathbf{X}$ requires $O(nd^2)$ time.
- Computing its full eigendecomposition to obtain $\vec{v}_1, \ldots, \vec{v}_k$ requires $O(d^3)$ time (similar to the inverse $(\mathbf{X}^T\mathbf{X})^{-1}$).

Many faster iterative and randomized methods. Runtime is roughly $\tilde{O}(ndk)$ to output just to top k eigenvectors $\vec{v}_1, \ldots, \vec{v}_k$.

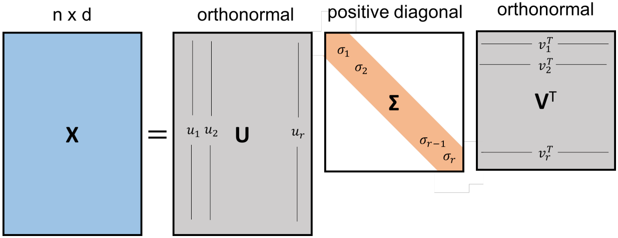
- Will see in a few classes (power method, Krylov methods).
- One of the most intensively studied problems in numerical computation.

$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: top eigenvectors of $\mathbf{X}^T\mathbf{X}$, $\mathbf{V}_k \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

Singular Value Decomposition

The Singular Value Decomposition (SVD) generalizes the eigendecomposition to asymmetric (even rectangular) matrices. Any matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ with $\text{rank}(\mathbf{X}) = r$ can be written as $\mathbf{X} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T$.

- $\mathbf{U}$ 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).
- $\boldsymbol{\Sigma}$ is diagonal with elements $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_r > 0$ (singular values).



Connection of the SVD to Eigendecomposition

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

$$\mathbf{X}^T\mathbf{X} = \mathbf{V}\boldsymbol{\Sigma}\mathbf{U}^T\mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T = \mathbf{V}\boldsymbol{\Sigma}^2\mathbf{V}^T \text{ (the eigendecomposition)}$$

Similarly: $\mathbf{X}\mathbf{X}^T = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T\mathbf{V}\boldsymbol{\Sigma}\mathbf{U}^T = \mathbf{U}\boldsymbol{\Sigma}^2\mathbf{U}^T$.

The left and right singular vectors are the eigenvectors of the covariance matrix $\mathbf{X}^T\mathbf{X}$ and the gram matrix $\mathbf{X}\mathbf{X}^T$ respectively.

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).

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 $\vec{u}_1, \ldots, \vec{u}_k$?
Gives exactly the same approximation!

$\mathbf{X} \in \mathbb{R}^{n \times d}$: 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), $\boldsymbol{\Sigma} \in \mathbb{R}^{\text{rank}(\mathbf{X}) \times \text{rank}(\mathbf{X})}$: positive diagonal matrix containing singular values of $\mathbf{X}$.

The SVD and Optimal Low-Rank Approximation

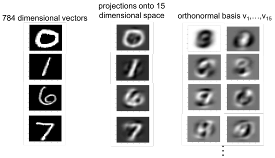
The best low-rank approximation to $\mathbf{X}$:

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

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

Correspond 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



Column (feature) compression

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⋮	⋮	⋮	⋮	⋮	⋮	⋮
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n x d orthonormal positive diagonal orthonormal n x d (rank k) orthonorma

The SVD and Optimal Low-Rank Approximation

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