COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

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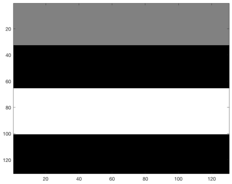
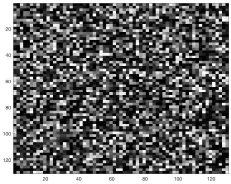
University of Massachusetts Amherst. Fall 2020.
Lecture 16

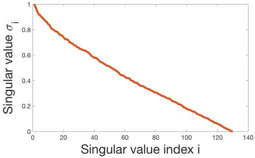
LOGISTICS

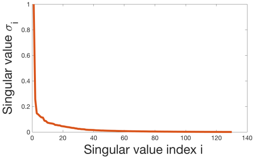
- Problem Set 3 is due **this Friday 10/23 at 8pm**.
- Midterm grades were released this weekend. Mean/median $\approx 35/40$. Higher than I was aiming for – so nice work!
- If you are concerned about your grade let me know and we can chat about how to pull it up going forward.
- The curve is not fixed, but if you need a B for core requirement, you should be shooting for a raw grade in around the mid 70s.
- Remember that your can get up to 5% extra credit for participation. Also attempting the EC problems on the problem sets can have a big effect. Often account for $> 20\%$ of the score.
- A number of people want more review problems, especially for linear algebra. I will plan to post a set of review problems probably early next week.

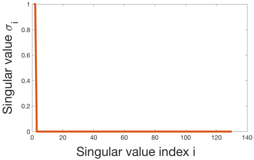
QUIZ PROBLEM











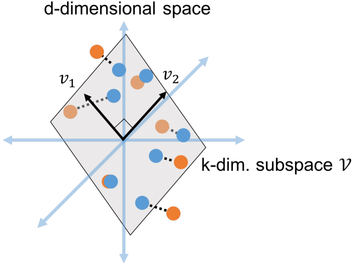
Last Class: Low-Rank Approximation, Eigendecomposition, and PCA

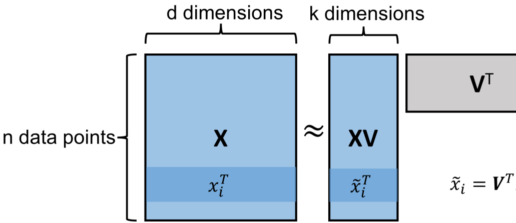
- Can approximate data lying close to in a k-dimensional subspace by projecting data points into that space.
- Can find the best k-dimensional subspace via eigendecomposition applied to $\mathbf{X}^T\mathbf{X}$ (PCA).
- Measuring error in terms of the eigenvalue spectrum.

This Class: Finish Low-Rank Approximation and Connection to the singular value decomposition (SVD)

- Finish up optimal low-rank approximation (PCA). Runtime considerations.
- View of optimal low-rank approximation using the SVD.
- Applications of low-rank approximation beyond compression.

Set Up: Assume that data points $\vec{x}_1, \ldots, \vec{x}_n$ 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:

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

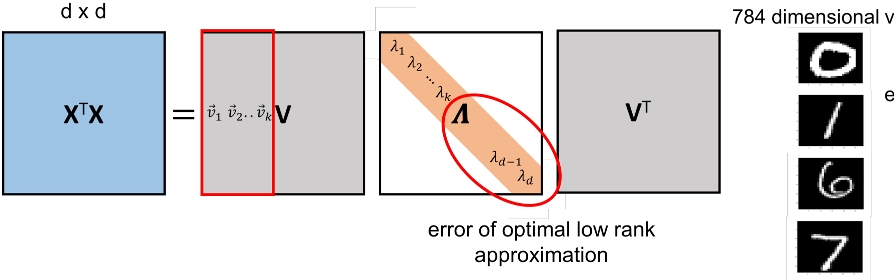
Solution via eigendecomposition: Letting $\mathbf{V}_k$ have columns $\vec{v}_1, \ldots, \vec{v}_k$ corresponding to the top k eigenvectors of the covariance matrix $\mathbf{X}^T\mathbf{X}$,

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

- Proof via Courant-Fischer and greedy maximization.
- Approximation error is $\|\mathbf{X}\|_F^2 - \|\mathbf{X}\mathbf{V}_k\|_F^2 = \sum_{i=k+1}^{d} \lambda_i(\mathbf{X}^T\mathbf{X})$.

$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: 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 $\vec{v}_1, \ldots, \vec{v}_k$.

Plotting the spectrum of the covariance matrix $\mathbf{X}^T\mathbf{X}$ (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).



- Choose k to balance accuracy and 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 $\vec{v}_1, \ldots, \vec{v}_k$.

Runtime to compute an optimal low-rank approximation:

- Computing the covariance matrix $\mathbf{X}^T\mathbf{X}$ 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 $(\mathbf{X}^T\mathbf{X})^{-1}$).

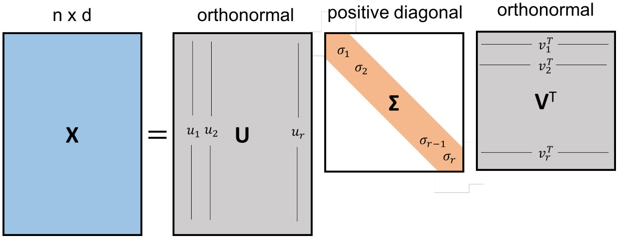
Many faster iterative and randomized methods. Runtime is roughly $\tilde{O}(ndk)$ to output just to top k eigenvectors $\vec{v}_1, \ldots, \vec{v}_k$.

- 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 $\vec{v}_1, \ldots, \vec{v}_k$.

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

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



The ‘swiss army knife’ of modern linear algebra.

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

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

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

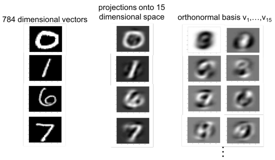
The best low-rank approximation to $\mathbf{X}$:

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

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

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

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 $\mathbf{X}$:

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

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

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

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

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