

COMPSCI 514: Algorithms for Data Science

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University of Massachusetts Amherst. Fall 2023.

Lecture 17

- Problem Set 3 is due Friday 11/17, 11:59pm.

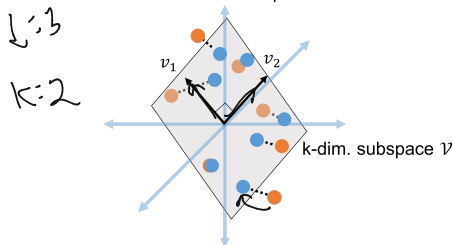
Questions about participation grade.

- Additional linear algebra review office hours – **Monday**
11/13 3:00-4:00pm.

2 3

Basic Set Up

Reminder of Set Up: Assume that $\vec{x}_1, \dots, \vec{x}_n$ 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 $\vec{v}_1, \dots, \vec{v}_k$ 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} .
 - $\mathbf{X}\mathbf{V}\mathbf{V}^T$ gives the closest approximation to \mathbf{X} with rows in \mathcal{V} .
 - The rows of $\mathbf{X}\mathbf{V}\mathbf{V}^T$ are approximations to our input points in \mathcal{V} .
- $n \times k$ The rows of $\mathbf{X}\mathbf{V}$ are compressions of these approximate points.

Last Class

$$\operatorname{argmin} \|X - XV\|_F^2 = 0$$

- V minimizing $\|X - XV\|_F^2$ is given by:

$$\operatorname{argmin}_{\text{orthonormal } V \in \mathbb{R}^{d \times k}} \|X - XV\|_F^2 = \operatorname{argmax}_{\text{orthonormal } V \in \mathbb{R}^{d \times k}} \|XV\|_F^2$$

- This optimal V can be found greedily. Equivalently, by computing the top k eigenvectors of $X^T X$.

$$\operatorname{argmax} F(x)$$

Last Class

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

$$\arg \min_{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}} \|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2 = \arg \max_{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}} \|\mathbf{X}\mathbf{V}\|_F^2$$

- This optimal \mathbf{V} can be found greedily. Equivalently, by computing the top k eigenvectors of $\mathbf{X}^T\mathbf{X}$.

This Class:

↳ k eigenvectors correspond to largest eigenvalues

- Finish up discussion of how optimal \mathbf{V} is computed via eigendecomposition.

↳ How do we assess the error of this optimal \mathbf{V} .

↳ Connection to the **singular value decomposition**.

Solution via Eigendecomposition

\mathbf{V} maximizing $\|\mathbf{XV}\|_F^2$ is given by: $\|\mathbf{XV}\|_F^2 = \|\mathbf{XV}\|_F^2$ $\mathbf{XV}^T \mathbf{XV}^T \mathbf{I}$

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

Can find the columns of \mathbf{V} , $\vec{v}_1, \dots, \vec{v}_k$ greedily.

$$\vec{v}_1^T \mathbf{X}^T \mathbf{X} \vec{v}_1 = \|\mathbf{X}\vec{v}_1\|_2^2 = \lambda_1 \quad \vec{v}_1 = \arg \max_{\vec{v} \text{ with } \|\vec{v}\|_2=1} \|\mathbf{X}\vec{v}\|_2^2 \quad \mathbf{V}^T \mathbf{X}^T \mathbf{X} \mathbf{V}$$

$$\|\mathbf{X}\vec{v}_i\|_2^2 = \lambda_i$$

$$\vec{v}_2 = \arg \max_{\vec{v} \text{ with } \|\vec{v}\|_2=1, \langle \vec{v}, \vec{v}_1 \rangle = 0} \vec{v}^T \mathbf{X}^T \mathbf{X} \vec{v}.$$

...

$$\vec{v}_k = \arg \max_{\vec{v} \text{ with } \|\vec{v}\|_2=1, \langle \vec{v}, \vec{v}_j \rangle = 0 \quad \forall j < k} \vec{v}^T \mathbf{X}^T \mathbf{X} \vec{v}.$$

$\vec{v}_1, \dots, \vec{v}_k$ are the top k eigenvectors of $\mathbf{X}^T \mathbf{X}$ by the Courant-Fischer Principle.

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

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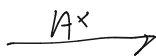
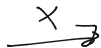
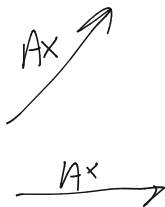
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Review of Eigenvectors and Eigendecomposition

Eigenvector: $\vec{x} \in \mathbb{R}^d$ is an eigenvector of a matrix $\mathbf{A} \in \mathbb{R}^{d \times d}$ if $\mathbf{A}\vec{x} = \lambda\vec{x}$ for some scalar λ (the eigenvalue corresponding to \vec{x}).

$\mathbf{A}\vec{x}$



Review of Eigenvectors and Eigendecomposition

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- That is, \mathbf{A} just 'stretches' x .

Review of Eigenvectors and Eigendecomposition

^{Symmetric}
 $A_{ij} = A_{ji} \quad \forall i, j$ $(X^T X)^T = X^T (X^T)^T = X^T X$

$\hat{A} = A$ **Eigenvector:** $\vec{x} \in \mathbb{R}^d$ is an eigenvector of a matrix $A \in \mathbb{R}^{d \times d}$ if $A\vec{x} = \lambda\vec{x}$ for some scalar λ (the eigenvalue corresponding to \vec{x}).

- That is, A just 'stretches' x . $\mathbb{I}x = x \cdot \lambda \quad x \neq 0$
 e_1, \dots, e_d
- If A is **symmetric**, can find d orthonormal eigenvectors $\vec{v}_1, \dots, \vec{v}_d$. Let $V \in \mathbb{R}^{d \times d}$ have these vectors as columns.
- $\lambda_1 \dots \lambda_d$ are always real.

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- If \mathbf{A} is **symmetric**, can find d orthonormal eigenvectors $\vec{v}_1, \dots, \vec{v}_d$. Let $\mathbf{V} \in \mathbb{R}^{d \times d}$ have these vectors as columns.

$$\mathbf{AV} = \begin{bmatrix} | & | & | & | \\ \mathbf{A}\vec{v}_1 & \mathbf{A}\vec{v}_2 & \cdots & \mathbf{A}\vec{v}_d \\ | & | & | & | \end{bmatrix}$$

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$$\begin{bmatrix} | & | & | & | \\ \vec{v}_1 & \cdots & \vec{v}_d & \\ | & | & | & | \end{bmatrix} \begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \vdots \\ \lambda_d \end{bmatrix} = \begin{bmatrix} | & | & | & | \\ \lambda_1\vec{v}_1 & \cdots & \lambda_d\vec{v}_d & \\ | & | & | & | \end{bmatrix}$$

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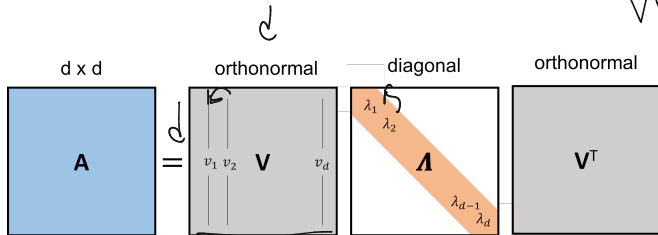
Yields eigendecomposition: $\underline{\mathbf{A}\mathbf{V}\mathbf{V}^T} = \underline{\mathbf{A}} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T$.

Review of Eigenvectors and Eigendecomposition

$$V^T V = V^{-1}$$

$$V^T V = I$$

$$V V^T = I \text{ if } k=d$$



Typically order the eigenvectors in decreasing order:

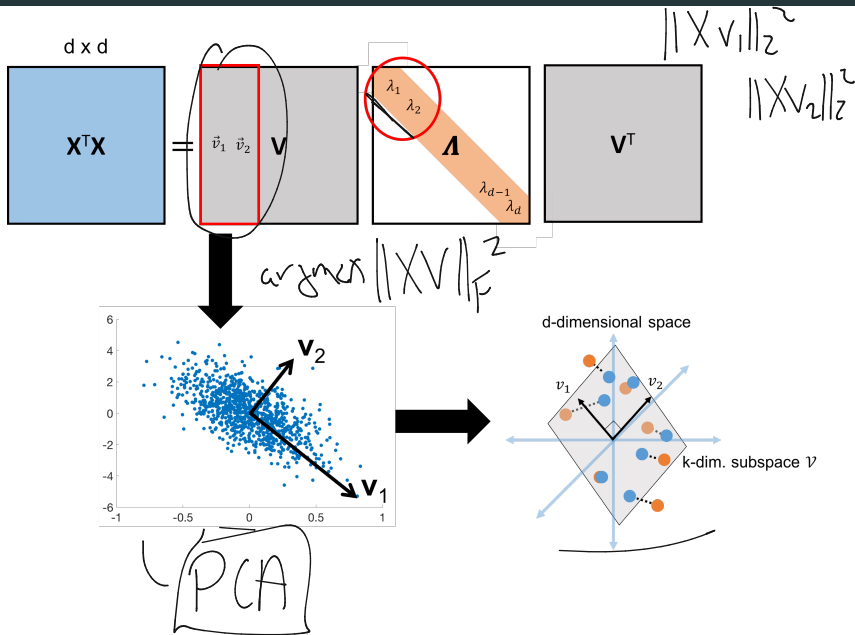
$$\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_d$$

$$v_1 \quad v_2 \quad \dots \quad v_d$$

$$A V V^T = A$$

projection onto column span V
 \downarrow
 \mathbb{R}^d
 -no-op

Low-Rank Approximation via Eigendecomposition



Low-Rank Approximation via Eigendecomposition

Upshot: Letting \mathbf{V}_k have columns $\vec{v}_1, \dots, \vec{v}_k$ corresponding to the top k eigenvectors of the covariance matrix $\mathbf{X}^T\mathbf{X}$, \mathbf{V}_k is the orthogonal basis minimizing

$$\|\mathbf{X} - \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T\|_F^2.$$

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

Low-Rank Approximation via Eigendecomposition

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This is principal component analysis (PCA).

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

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How accurate is this low-rank approximation?

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How accurate is this low-rank approximation? Can understand using eigenvalues of $\mathbf{X}^T\mathbf{X}$.

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Spectrum Analysis

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

$$\underbrace{\|\mathbf{X} - \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T\|_F^2}$$

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

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

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

$$[\mathbf{X}^T\mathbf{X}][\vec{v}_i] = \lambda_i \cdot \vec{v}_i$$

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

$$\begin{bmatrix} \vec{v}_1^T \\ \vdots \\ \vec{v}_k^T \end{bmatrix} \left(\mathbf{X}^T\mathbf{X} \right) \begin{bmatrix} \vec{v}_1 \\ \vdots \\ \vec{v}_k \end{bmatrix}$$

$\vec{v}_i^T \mathbf{X}^T\mathbf{X} \vec{v}_i$

$$\vec{v}_i^T \mathbf{X}^T\mathbf{X} \vec{v}_i = \lambda_i(\mathbf{X}^T\mathbf{X}) \cdot \vec{v}_i^T \vec{v}_i = \lambda_i(\mathbf{X}^T\mathbf{X})$$

$$\|\mathbf{X}\vec{v}_i\|_2^2 = \lambda_i(\mathbf{X}^T\mathbf{X})$$

$\vec{v}_i^T \lambda_i(\mathbf{X}^T\mathbf{X}) \cdot \vec{v}_i$ because \vec{v}_i is eigenvector of $\mathbf{X}^T\mathbf{X}$

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

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

$$\mathbf{X}^T\mathbf{X}\vec{v} = \lambda\vec{v} \quad \mathbf{X}^T\mathbf{X}(-\vec{v}) = -\lambda\vec{v} = \lambda(-\vec{v})$$

Spectrum Analysis

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

$$\begin{aligned}\| \mathbf{X} - \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T \|_F^2 &= \underbrace{\text{tr}(\mathbf{X}^T\mathbf{X})} - \underbrace{\text{tr}(\mathbf{V}_k^T\mathbf{X}^T\mathbf{X}\mathbf{V}_k)} \\ &= \sum_{i=1}^d \lambda_i(\mathbf{X}^T\mathbf{X}) - \sum_{i=1}^k \vec{v}_i^T \mathbf{X}^T\mathbf{X} \vec{v}_i \\ &= \sum_{i=1}^d \lambda_i(\mathbf{X}^T\mathbf{X}) - \sum_{i=1}^k \lambda_i(\mathbf{X}^T\mathbf{X})\end{aligned}$$

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

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

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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:

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

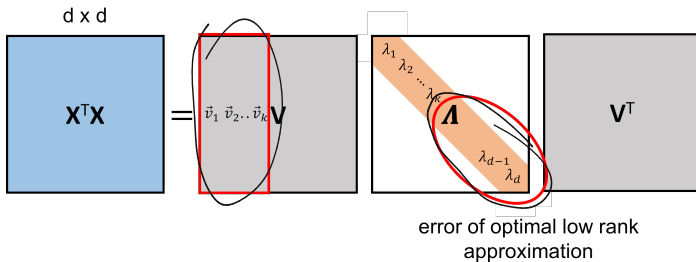
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Spectrum Analysis

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

non-zero eigenvalues
 $= \text{rank}(X) = \text{rank}(X^T X)$

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

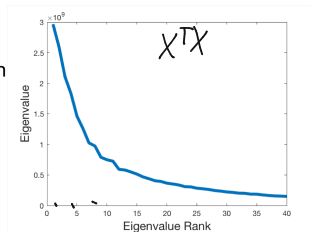
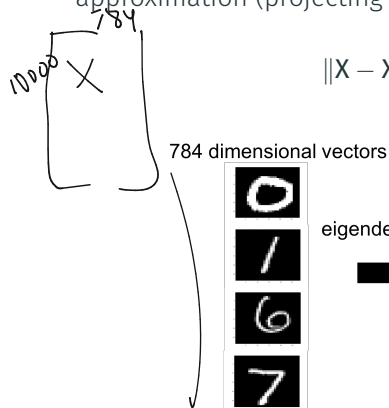


$\vec{x}_1, \dots, \vec{x}_n \in \mathbb{R}^d$: data points, $X \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \dots, \vec{v}_k \in \mathbb{R}^d$: top eigenvectors of $X^T X$, $V_k \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \dots, \vec{v}_k$.

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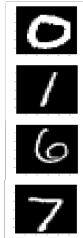
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Spectrum Analysis

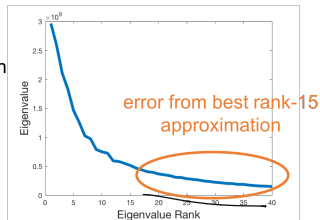
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$$\|X - X V_k V_k^T\|_F^2 = \sum_{i=k+1}^d \lambda_i(X^T X)$$

784 dimensional vectors



eigendecomposition



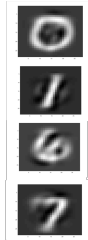
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Spectrum Analysis

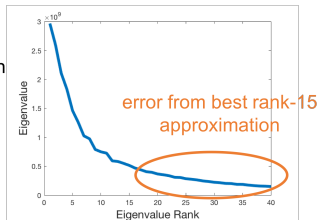
Claim: The error in approximating \mathbf{X} with the best rank k approximation (projecting onto the top k eigenvectors of $\mathbf{X}^T\mathbf{X}$) is:

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

784 dimensional vectors



eigendecomposition



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

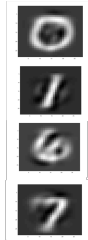
Spectrum Analysis

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

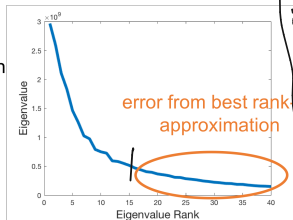
$$\|X - X V_k V_k^T\|_F^2 = \sum_{i=k+1}^d \lambda_i(X^T X)$$

Exercise
 $\|X - X V_k V_k^T\|_F^2$
 $\approx \sum_{i=k+1}^d \lambda_i(X^T X)$
 $\approx \sum_{i=1}^d \lambda_i(X^T X) - \sum_{i=1}^k \lambda_i(X^T X)$

784 dimensional vectors



eigendecomposition



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

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

Spectrum Analysis

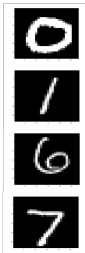
Plotting the **spectrum** of $X^T X$ (its eigenvalues) shows how compressible X is using low-rank approximation (i.e., how close $\vec{x}_1, \dots, \vec{x}_n$ are to a low-dimensional subspace).

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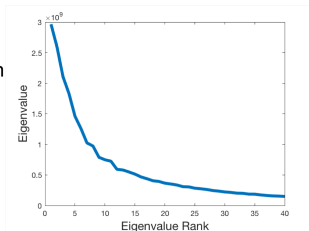
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eigendecomposition



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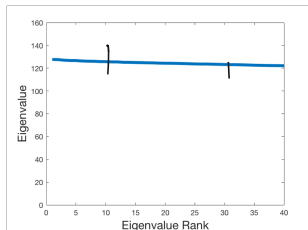
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784 dimensional vectors



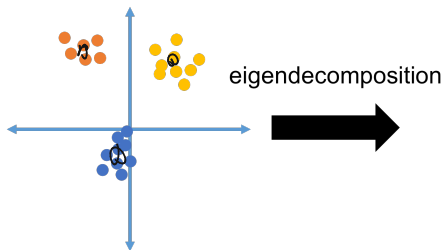
eigendecomposition



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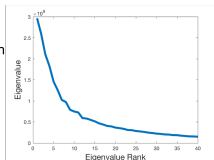
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Spectrum Analysis

784 dimensional vectors



eigendecomposition



Exercises:

non-negative

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

Summary

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

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

- 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.

$10000 * \text{bathrooms} + 10 * (\text{sq. ft.}) \approx \text{list price}$

	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

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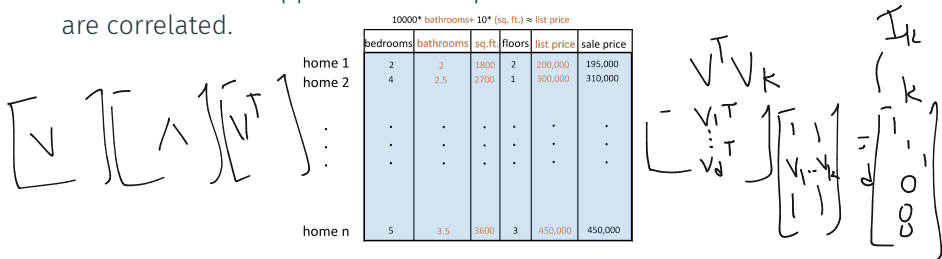
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Our compressed dataset is $\mathbf{C} = \mathbf{X}\mathbf{V}_k$ where the columns of \mathbf{V}_k are the top k eigenvectors of $\mathbf{X}^T\mathbf{X}$.

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Interpretation in Terms of Correlation

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



Our compressed dataset is $C = XV_k$ where the columns of V_k are the top k eigenvectors of $X^T X$.

Observe that $C^T C = V_k^T X^T X V_k = \begin{bmatrix} \lambda_1 & 0 \\ \vdots & \vdots \\ 0 & \lambda_k \end{bmatrix}$

$V_k^T V_k = I_k$ and $V_k V_k^T = \begin{bmatrix} I_k & 0 \\ 0 & 0 \end{bmatrix}$

Handwritten annotations: $\Lambda_k = \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_k \end{bmatrix}$, $\begin{bmatrix} I \\ 0 \end{bmatrix}$, $\begin{bmatrix} I \\ v \end{bmatrix}$.

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

$\mathbf{C}^T\mathbf{C}$ is diagonal. I.e., all columns are orthogonal to each other, and correlations have been removed. Maximal compression.

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Algorithmic Considerations

Runtime to compute an optimal low-rank approximation:

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Algorithmic Considerations

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- Computing $\mathbf{X}^T\mathbf{X}$ requires $O(nd^2)$ time.

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

Many faster iterative and randomized methods. Runtime is roughly

$\tilde{O}(ndk)$ to output just the top k eigenvectors $\vec{v}_1, \dots, \vec{v}_k$. *eigs eig*

• Will see in a few classes (power method, Krylov methods).

One of the most intensively studied problems in numerical computation.

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