COMPSCI 514: Algorithms for Data Science

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University of Massachusetts Amherst. Fall 2026.

Lecture 17

Logistics

- Midterm 2 is **Wednesday in class**.
- Study guide and practice exams have been posted.
- Next week, we will have class on Monday, no class on Tuesday.
- No quizzes until after Thanksgiving break.

Summary

Last Class:

- Start on data dependent dimensionality reduction.
- Approximation via projection onto a low-dimensional subspace.

$x \in \mathbb{R}^d \quad V \in \mathbb{R}^{d \times k} \quad V^T x \in \mathbb{R}^k$

$$\|V^T x_i - V^T x_j\|_2 \approx \|x_i - x_j\|_2$$

Summary

Last Class:

- Start on data dependent dimensionality reduction.
- Approximation via projection onto a low-dimensional subspace.

This Class:

- Connection to low-rank approximation.
- Finding an optimal subspace via eigendecomposition. (PCA)
- Possibly some midterm review.

↳ only appear on EC question of midterm

Low-Rank Factorization

Claim: $\vec{x}_1, \ldots, \vec{x}_n$ lie in a k-dimensional subspace $\mathcal{V} \Leftrightarrow$ the data matrix $\mathbf{X} \in \mathbb{R}^{n \times d}$ has rank $\leq k$.

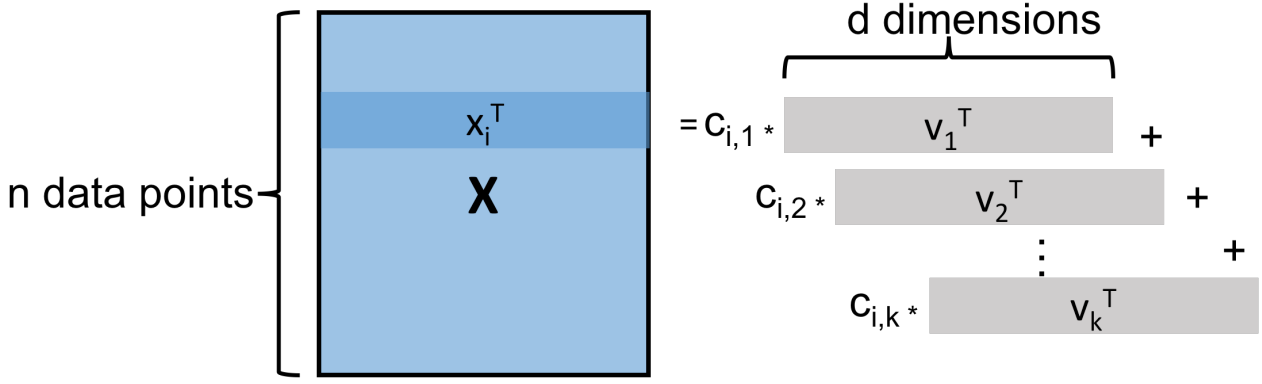
$$\mathbf{X} = \begin{bmatrix} \vec{x}_1^T \\ \vec{x}_2^T \\ \vdots \\ \vec{x}_n^T \end{bmatrix}$$

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- Letting $\vec{v}_1, \ldots, \vec{v}_k$ be an orthonormal basis for $\mathcal{V}$: $\vec{x}_i = \mathbf{V}\vec{c}_i = c_{i,1}\vec{v}_1 + \ldots + c_{i,k}\vec{v}_k$.

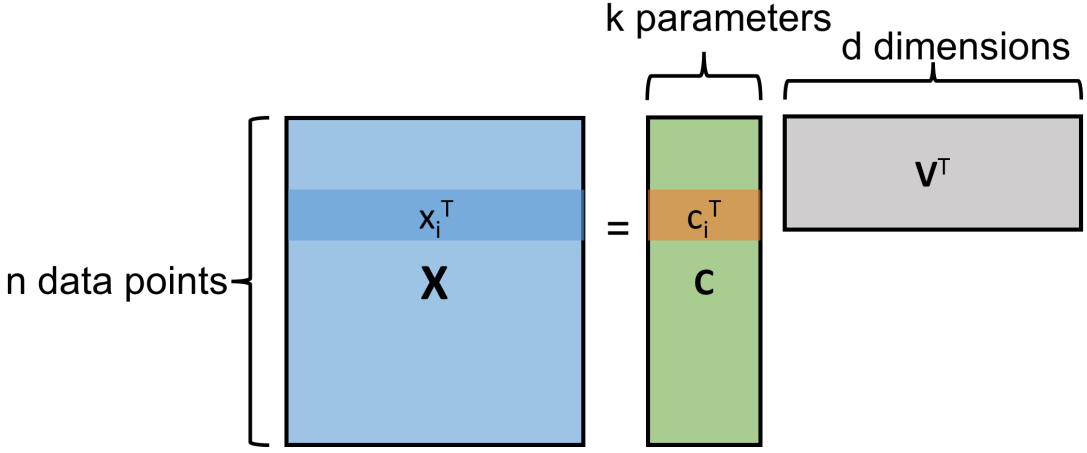
$$x_i^T = c_i^T V^T$$



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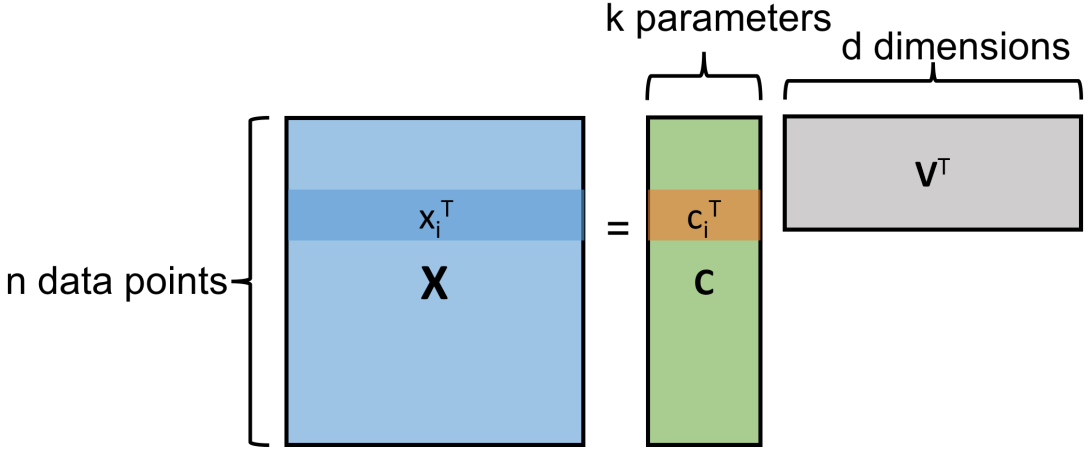
- Letting $\vec{v}_1, \ldots, \vec{v}_k$ be an orthonormal basis for $\mathcal{V}$: $\vec{x}_i = \mathbf{V}\vec{c}_i = c_{i,1}\vec{v}_1 + \ldots + c_{i,k}\vec{v}_k$.
- So $\mathbf{X} = \mathbf{C}\mathbf{V}^T$: rows of $\mathbf{X}$ spanned by $\vec{v}_1, \ldots, \vec{v}_k \implies \text{rank}(\mathbf{X}) \leq k$.



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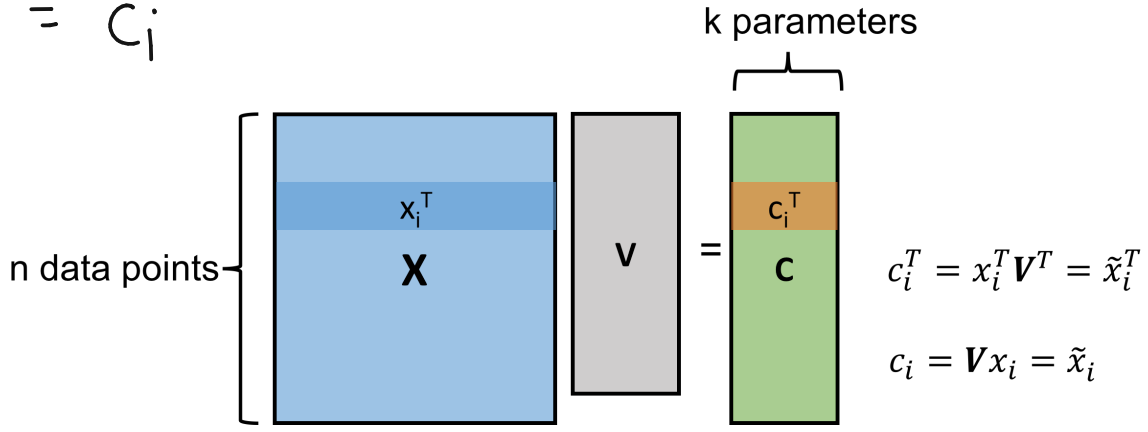


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- What is $\mathbf{C}$?

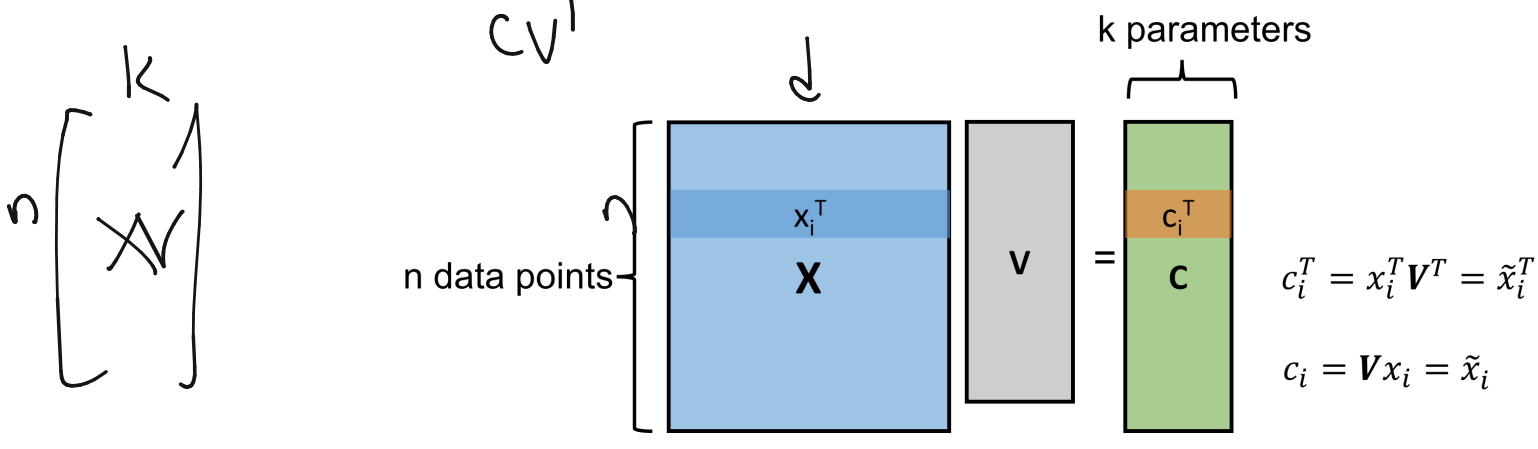
$V^T x_i = c_i$



Low-Rank Factorization

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- $\mathbf{X}$ can be represented by $(n + d) \cdot k$ parameters vs. $n \cdot d$.
- What is $\mathbf{C}$? $\mathbf{X}\mathbf{V} = \mathbf{C}\mathbf{V}^T\mathbf{V} = \mathbf{C}$.



Projection View and Low-Rank Approximation

Since $\mathbf{C} = \mathbf{XV}$, if $\vec{x}_1, \ldots, \vec{x}_n$ lie in $\mathcal{V}$, the data matrix can be written as

$$\mathbf{X} = \mathbf{C}\mathbf{V}^T = \mathbf{X}\mathbf{V}\mathbf{V}^T.$$

projection matrix onto subspace

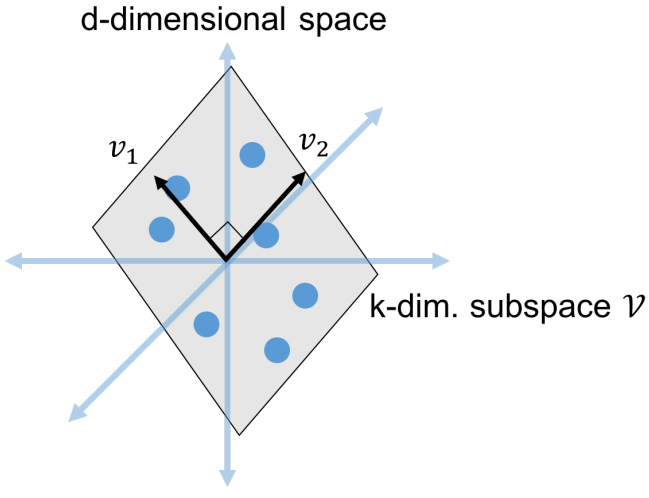
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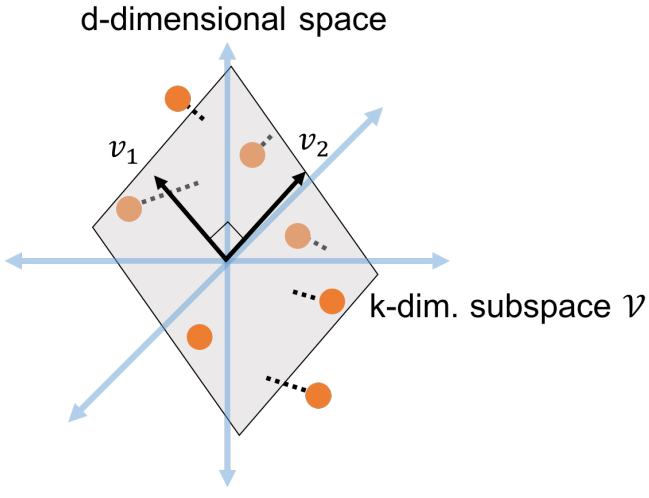
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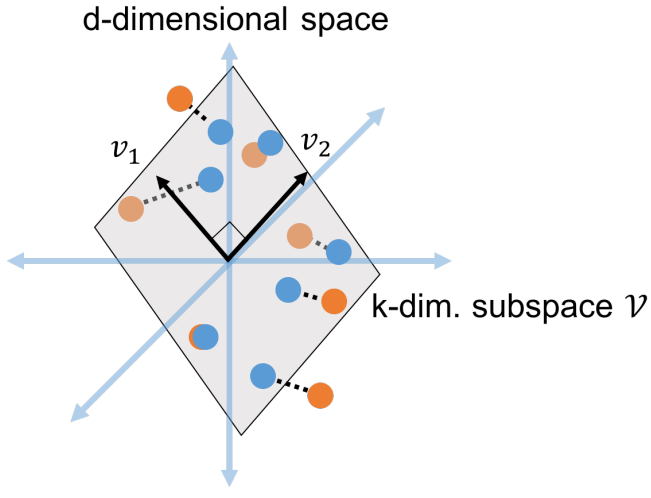
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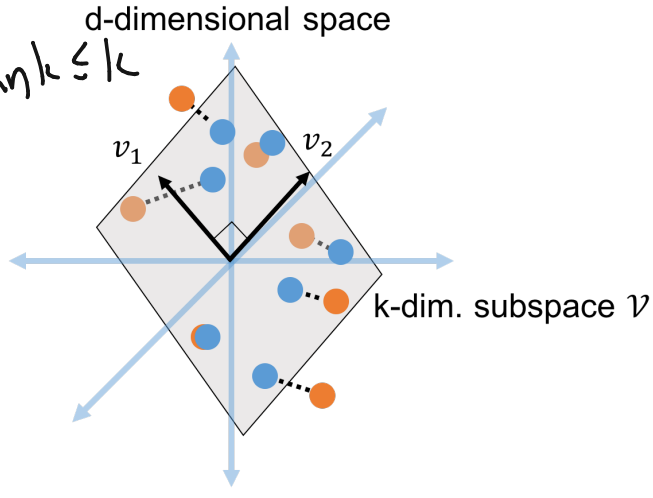
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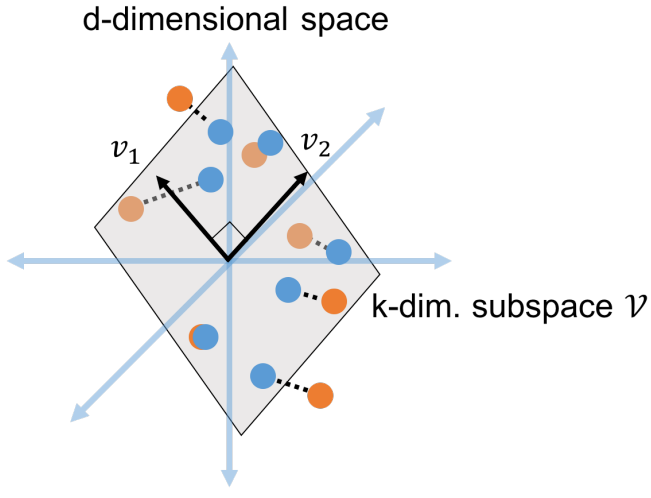
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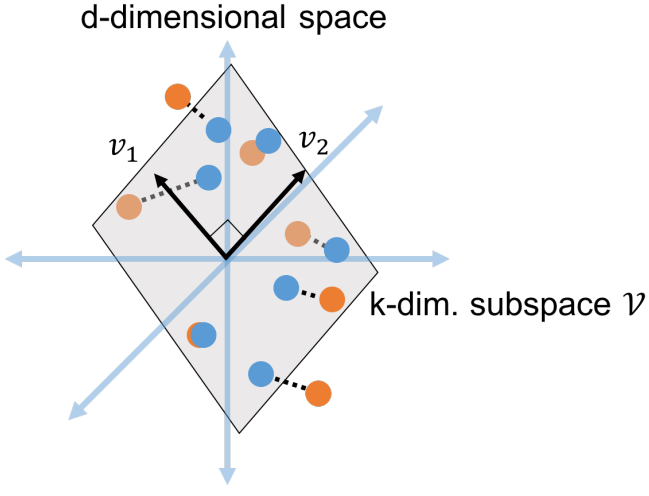
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- $\mathbf{VV}^T$ is a projection matrix, which projects vectors onto $\mathcal{V}$.
- If $\vec{x}_1, \ldots, \vec{x}_n$ lie close to $\mathcal{V}$, $\mathbf{X} \approx \mathbf{XVV}^T$: a low-rank approximation of $\mathbf{X}$.
- Can use $\mathbf{XV} \in \mathbb{R}^{n \times k}$ as a compressed approximate dataset.

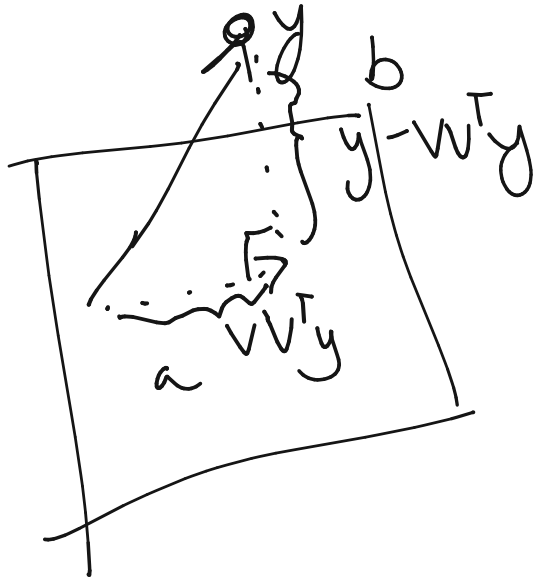


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Properties of Projection Matrices

$V^T V = I$



Exercise 1: Show that $\mathbf{V}\mathbf{V}^T$ is idempotent. I.e., $(\mathbf{V}\mathbf{V}^T)(\mathbf{V}\mathbf{V}^T)\vec{y} = (\mathbf{V}\mathbf{V}^T)\vec{y}$ for any $\vec{y} \in \mathbb{R}^d$.

$V(V^T V)V^T y = VV^T y$

Why does this make sense intuitively?

Exercise 2: (Pythagorean Theorem) Show that:

$(I - VV^T)y$

$$\|\vec{y}\|_2^2 = \|(\mathbf{V}\mathbf{V}^T)\vec{y}\|_2^2 + \|\vec{y} - (\mathbf{V}\mathbf{V}^T)\vec{y}\|_2^2.$$

$\|y\|_2^2 = \| \underbrace{V^T y}_{a} + \underbrace{(I - VV^T)y}_{b} \|_2^2$

$\|a+b\|_2^2 = (a+b)^T(a+b)$

$= a^T a + b^T b + 2a^T b$

$= \|V^T y\|_2^2 + \|y - VV^T y\|_2^2 + 0$

$(V^T y)^T (I - V^T)y$

$y^T VV^T (I - VV^T) y$

$y^T (VV^T - VV^T VV^T) y$

$y^T 0 y = 0$

Best Fit Subspaces

Best Fit Subspace

How do we find $\mathcal{V}$ (equivalently $\mathbf{V}$)?

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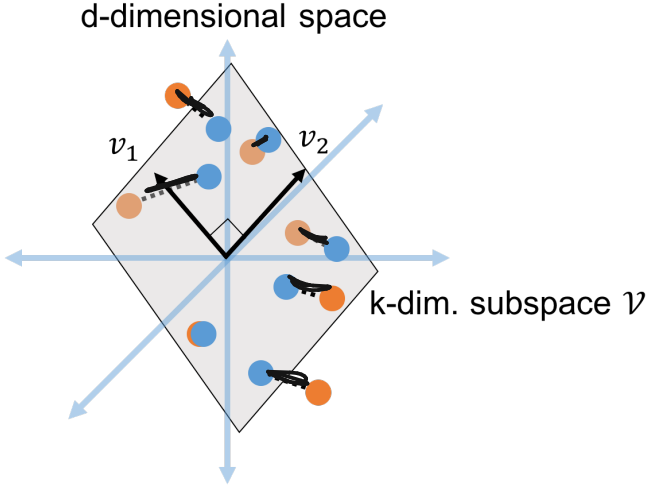
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$$\arg\min_{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}} \|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2 = \sum_{i,j} (\mathbf{X}_{i,j} - (\mathbf{X}\mathbf{V}\mathbf{V}^T)_{i,j})^2 = \sum_{i=1}^{n} \|\vec{x}_i - \mathbf{V}\mathbf{V}^T\vec{x}_i\|_2^2$$

$\|(\mathbf{I} - \mathbf{V}\mathbf{V}^T)x_i\|_2^2 + \|\mathbf{V}\mathbf{V}^T x_i\|_2^2 = \|x_i\|_2^2$

$$\sum_{i=1}^{n} \|x_i\|_2^2 - \|\mathbf{V}^T x_i\|_2^2$$

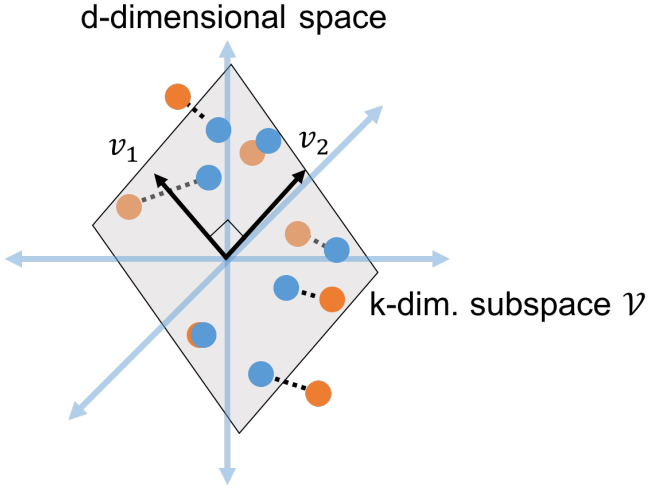


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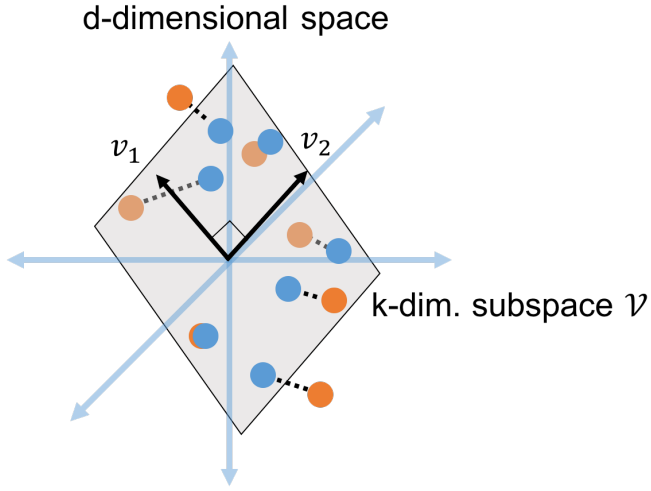


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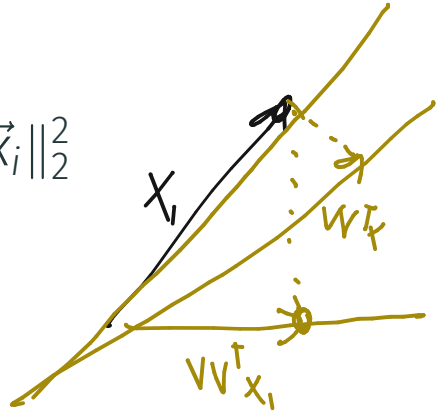


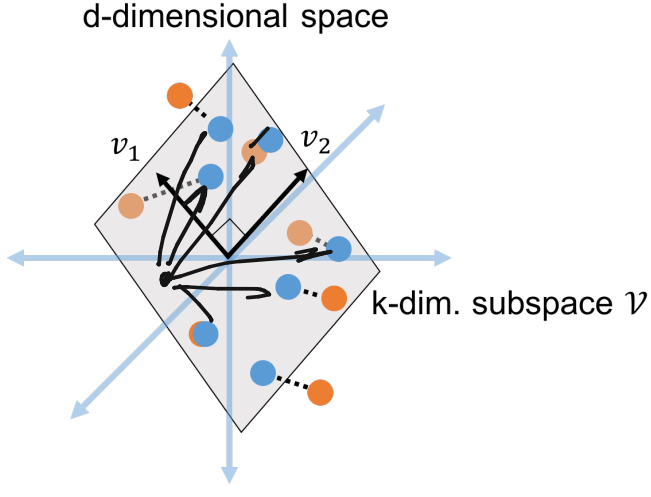
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$$\underset{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}}{\arg\max} \|\mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2 = \sum_{i=1}^{n} \|\mathbf{V}\mathbf{V}^T \vec{x}_i\|_2^2$$





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Solution via Eigendecomposition

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

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

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Surprisingly, can find the columns of $\mathbf{V}$, $\vec{v}_1, \ldots, \vec{v}_k$ greedily.

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$$\vec{v}_1 = \underset{\vec{v} \text{ with } \|v\|_2 = 1}{\arg\max} \|\mathbf{X}\vec{v}\|_2^2$$

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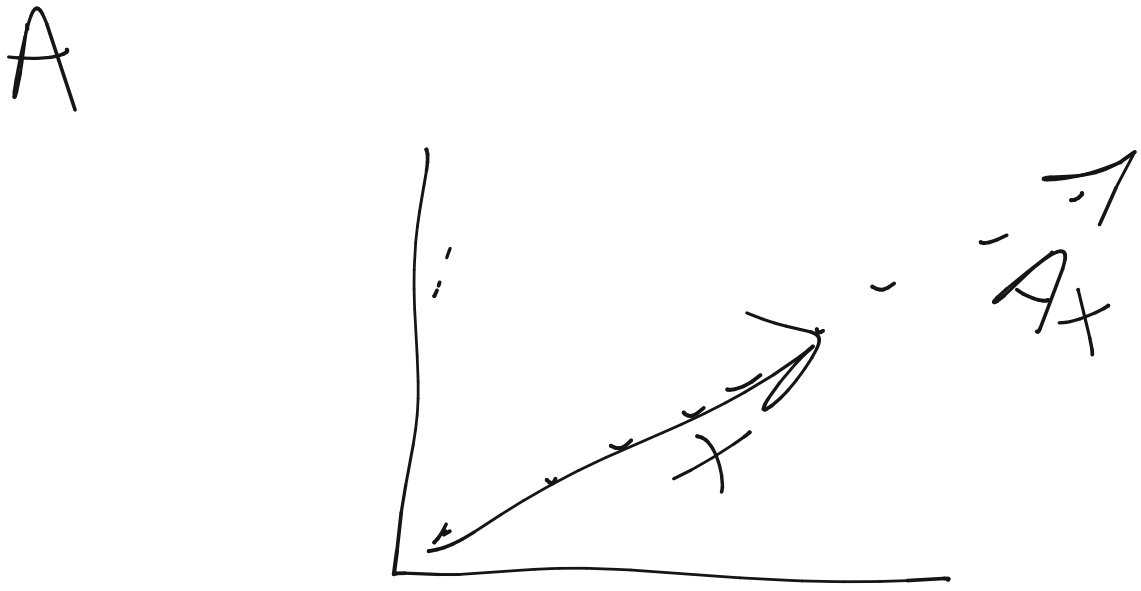
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$\vec{v}_1, \ldots, \vec{v}_k$ are the top k eigenvectors of $\mathbf{X}^T\mathbf{X}$ by the *Courant-Fischer Principle.*

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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 $\vec{x}$).



Review of Eigenvectors and Eigendecomposition

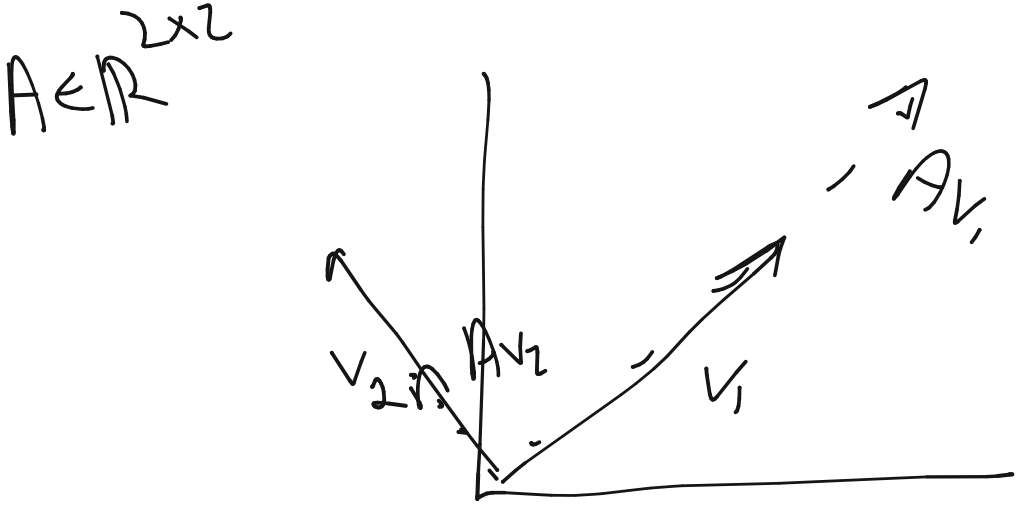
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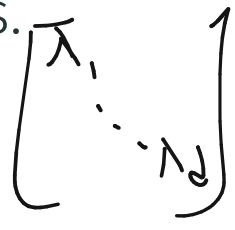
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Review of Eigenvectors and Eigendecomposition

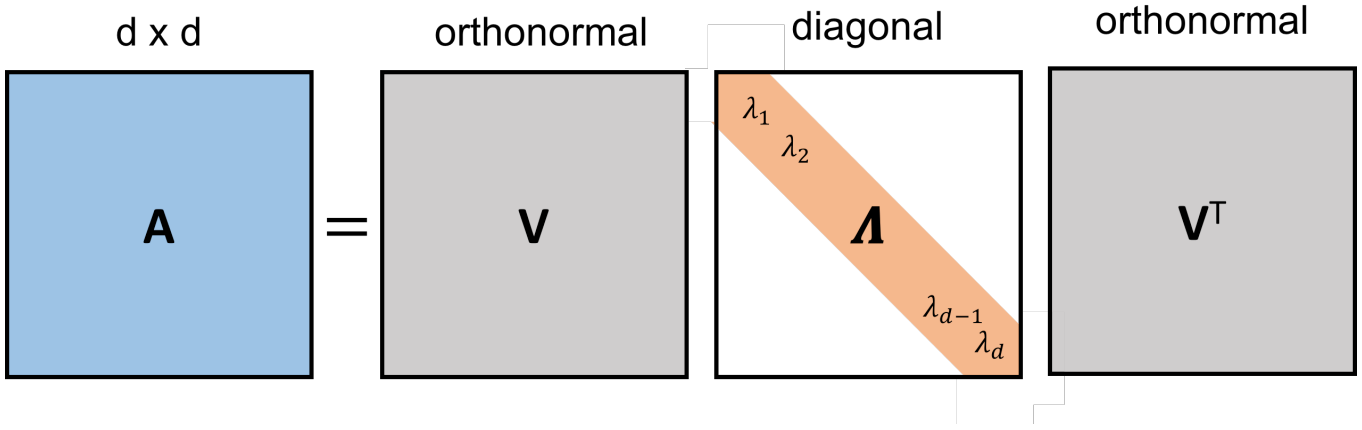
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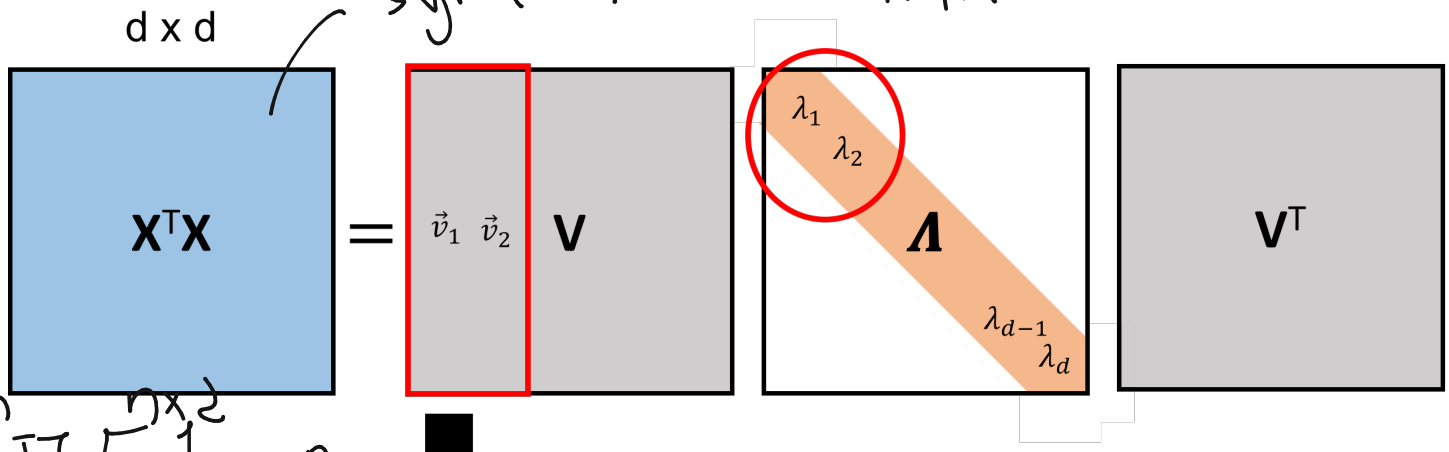
Yields eigendecomposition: $\mathbf{AVV}^T = \mathbf{A} = \mathbf{V\Lambda V}^T$.

Review of Eigenvectors and Eigendecomposition



Typically order the eigenvectors in decreasing order:
$\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_d$.

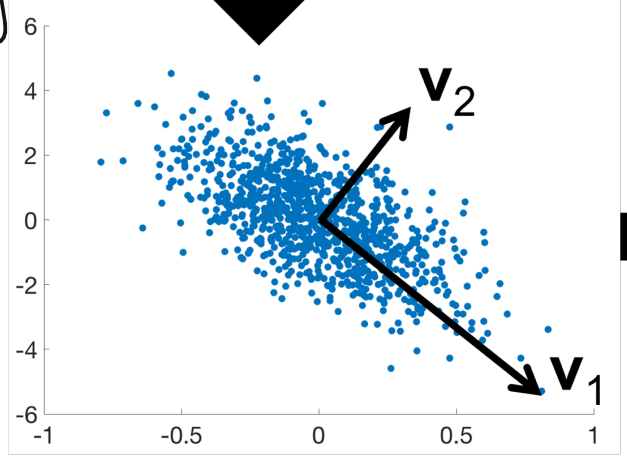
Low-Rank Approximation via Eigendecomposition

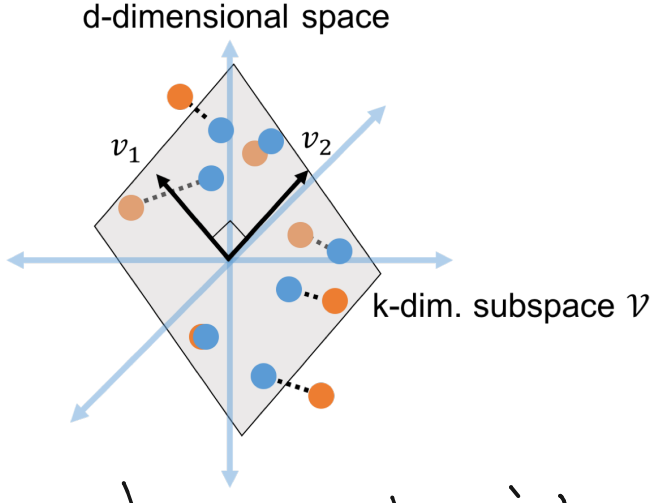


$n \times 2$

$2[X^T]\begin{bmatrix} X \end{bmatrix} = A$

$d \times 2$





"PCA" principal component analysis

Low-Rank Approximation via Eigendecomposition

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

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

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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:

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

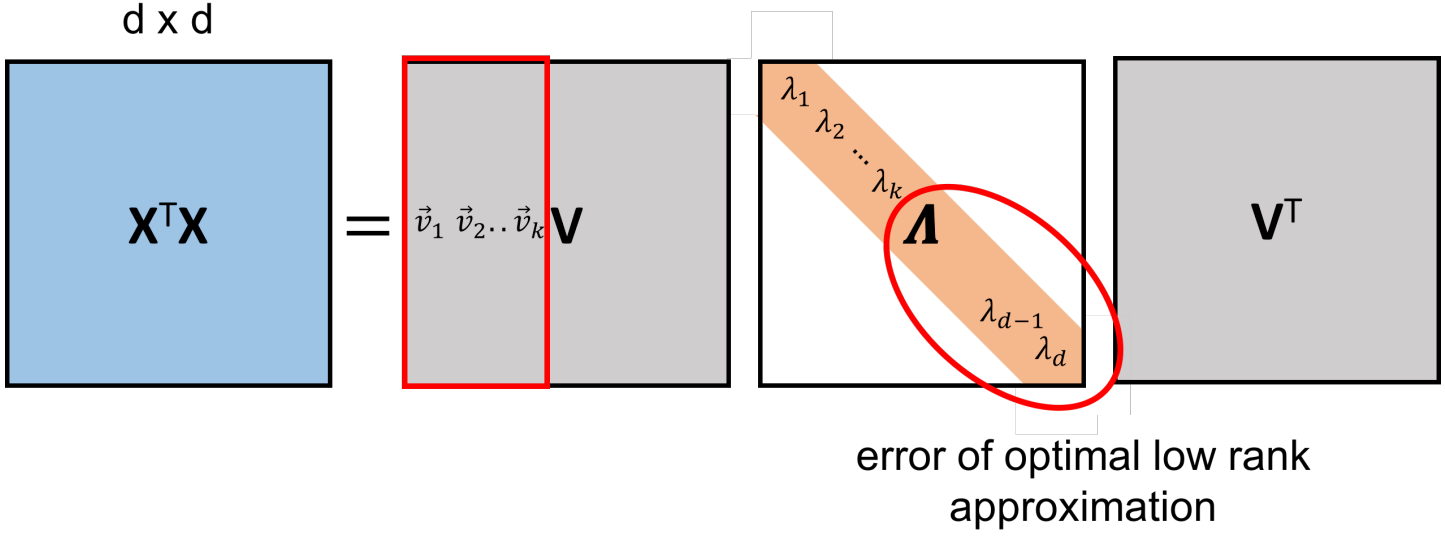
prove for fun over Thanksgiving
- Pythagorean theorem
- def. of eigenvectors

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

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



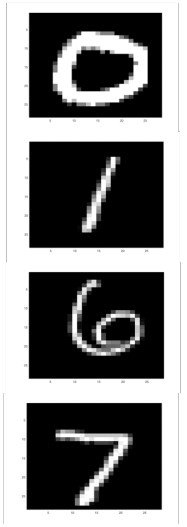
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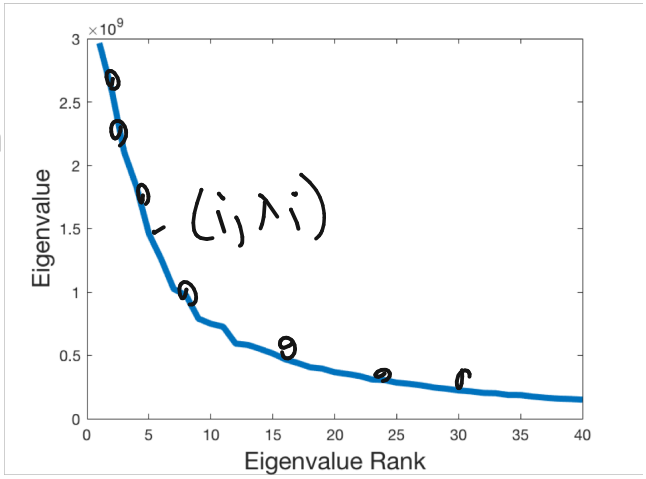
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784 dimensional vectors



eigendecomposition



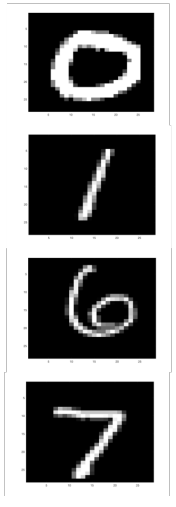
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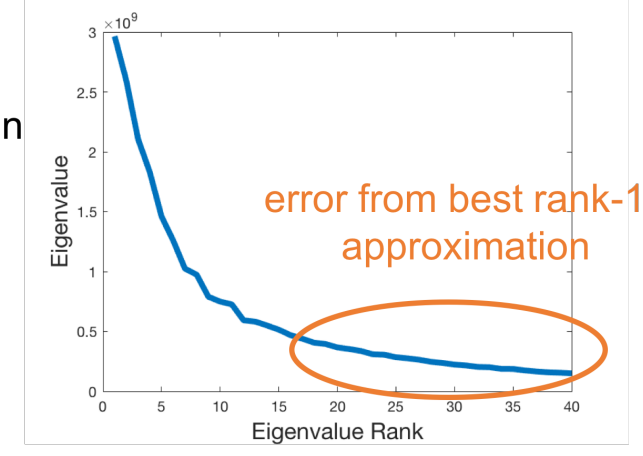
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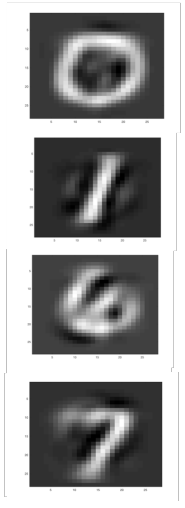
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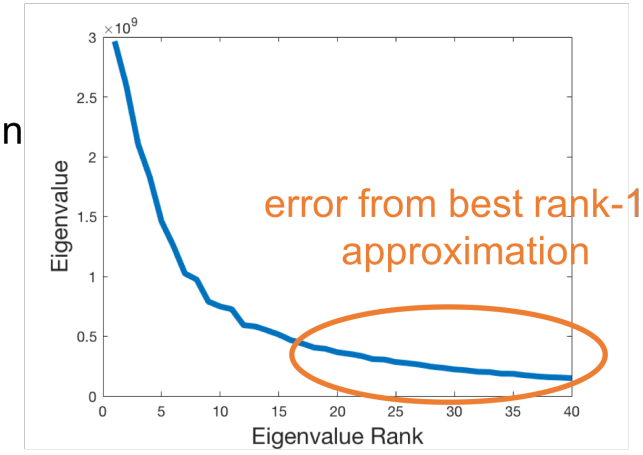
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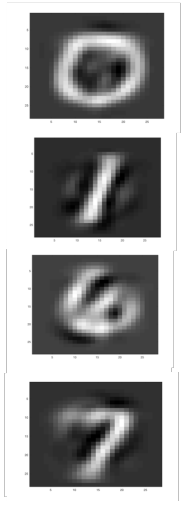
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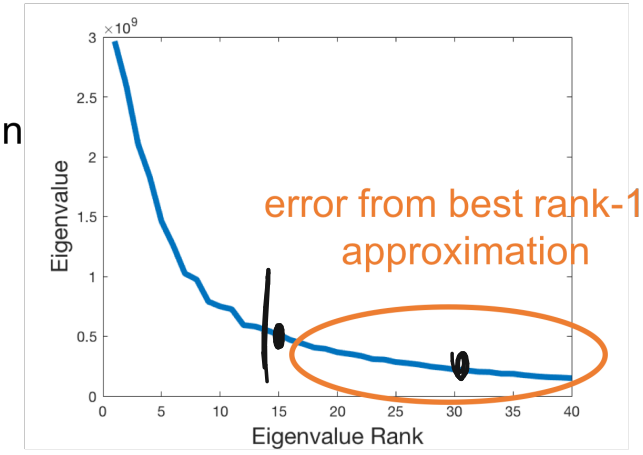
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eigendecomposition



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

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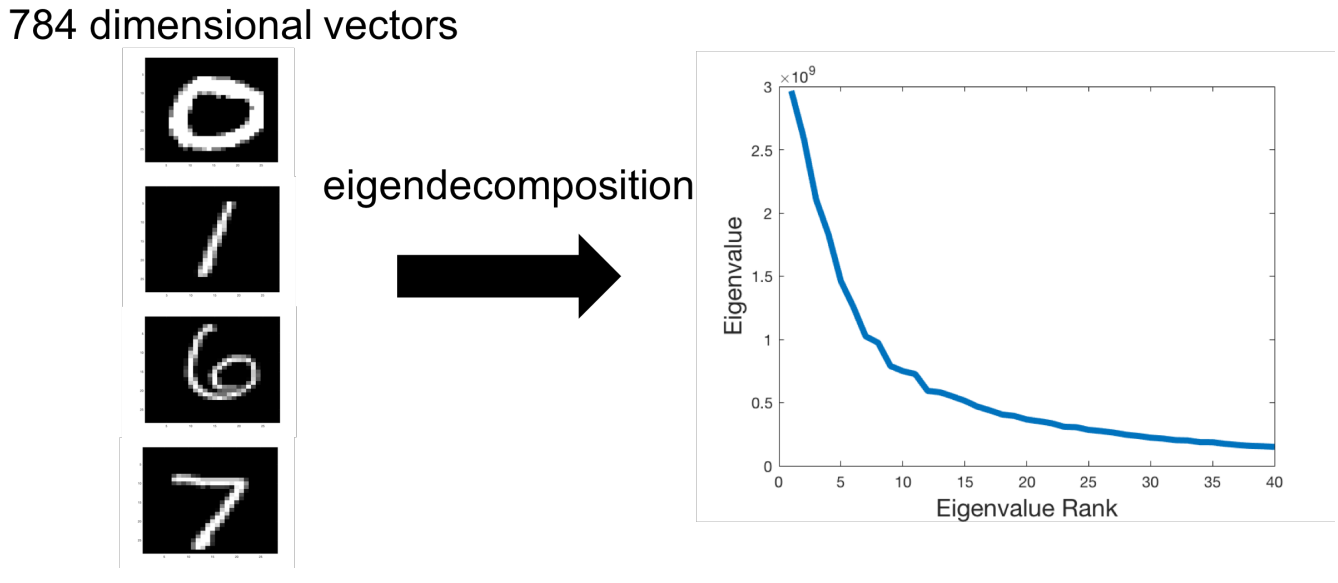
Spectrum Analysis

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).

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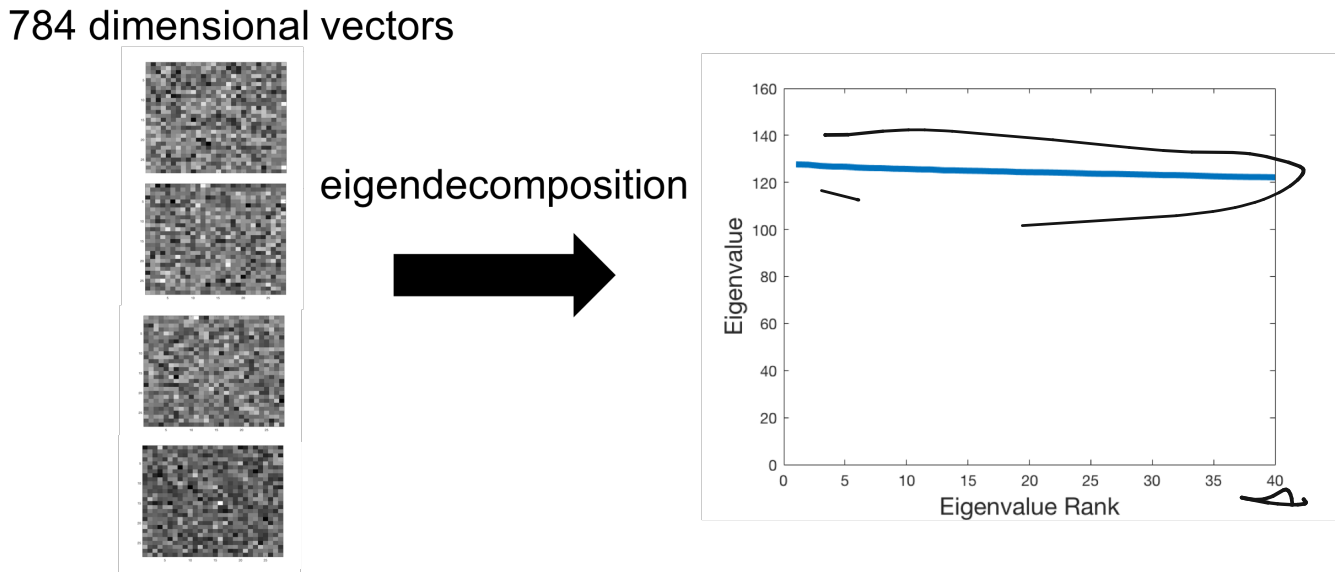
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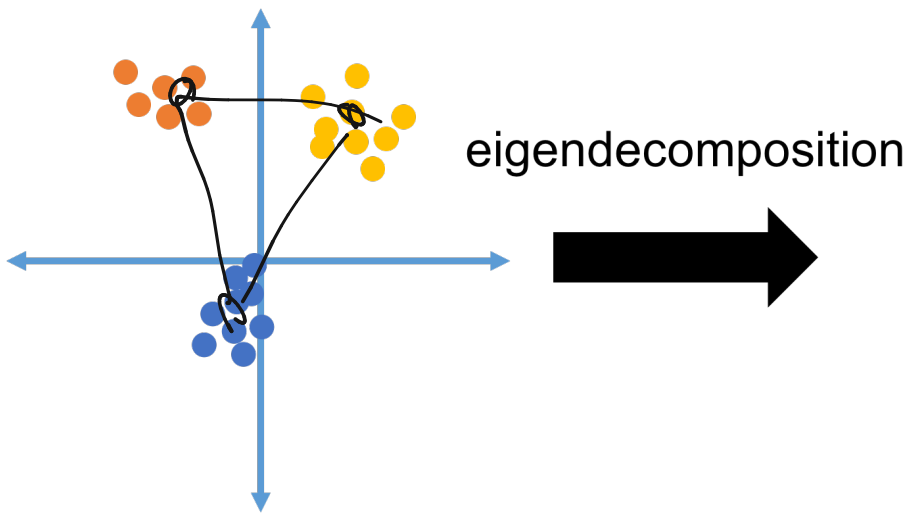
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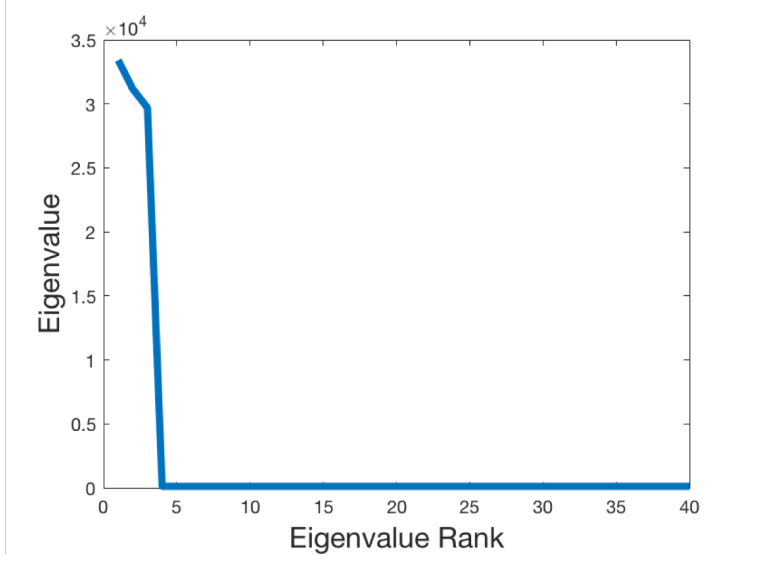


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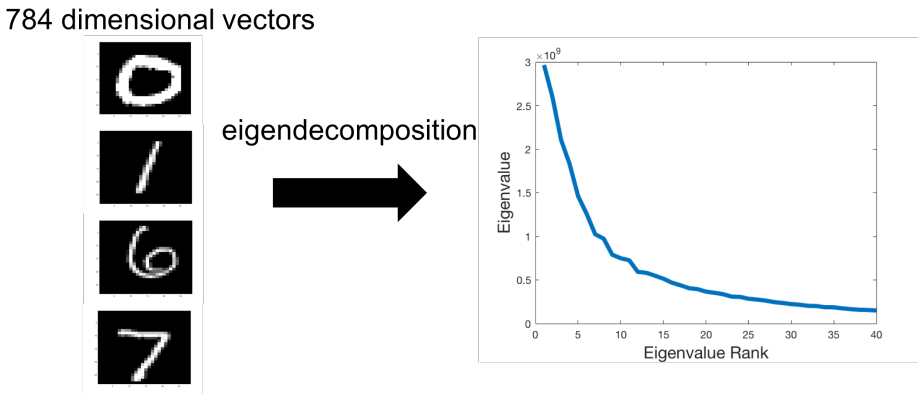
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Spectrum Analysis



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.

Midterm Review

Format = midterm 1

4-5 T/F questions. Give explanation

4-5 short numerical question (like in class quizzes)

2 "long form questions"

LSH

- minHash, simHash
- application to NN-search
- table + hash repetitions curve
- graph-based search high level.

JL related things

- low-distortion embeddings
- proof of distributional JL $\Rightarrow$ JL
- QJL $\langle g, \vec{v} \rangle = N(0, \|v\|_2^2)$

simHash $(\pi g, \text{sign}(\pi v)) \cdot \sqrt{\frac{2}{\pi}}$

Low Distortion Embeddings

Given $x_1 \dots x_n \in \mathbb{R}^d$

want $\tilde{x}_1 \dots \tilde{x}_n \in \mathbb{R}^m$ s.t. $\forall i, j$

$$\|\tilde{x}_i - \tilde{x}_j\|_2 \in (1 \pm \varepsilon)\|x_i - x_j\|_2$$

$$\|\Pi x_i - \Pi x_j\|_2$$

JL Lemma: If $\Pi \in \mathbb{R}^{d \times m}$ w/r. i.i.d. $N(0, 1/m)$

$m = O\left(\frac{\log n/\delta}{\varepsilon^2}\right)$ then

$\tilde{x}_i = \Pi x_i$ give a $(1 \pm \varepsilon)$ low distortion embedding

→ proved distributional JL lemma

$m = O\left(\frac{\log(1/\delta)}{\varepsilon^2}\right)$ we took a union bound over $\binom{n}{2}$ pairs

Distributional JL:

$\Pi \in \mathbb{R}^{m \times d}$ has i.i.d $N(0, 1/m)$ entries

$m = O\left(\frac{\log(1/\delta)}{\varepsilon^2}\right)$ for any $y \in \mathbb{R}^d$, w.p. $\geq 1 - \delta$

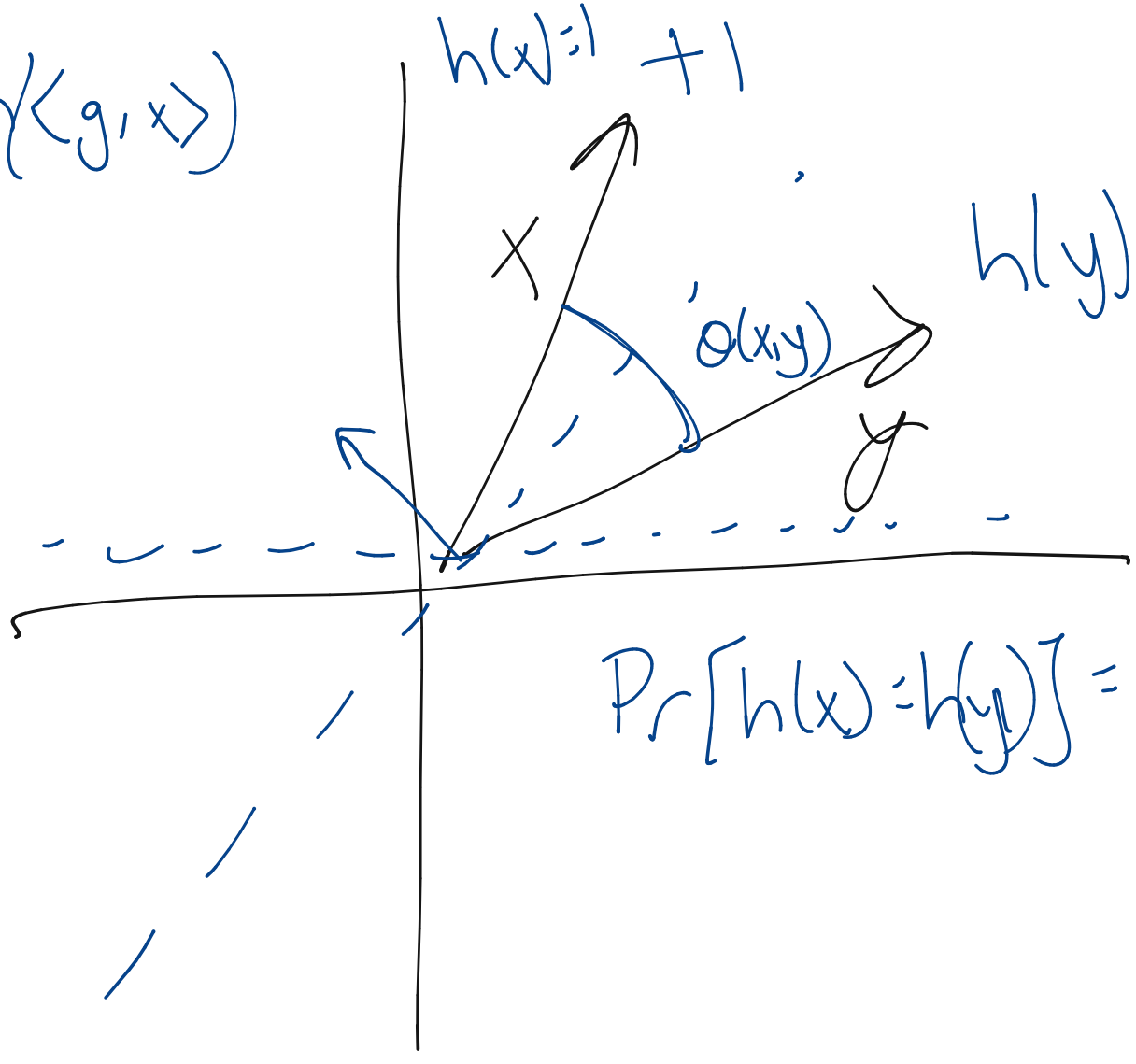
$$\|\Pi y\|_2 \in (1 \pm \varepsilon)\|y\|_2 \qquad y_{ij} = x_i - x_j$$

$\mathbb{E}\,\|\Pi y\|_2^2 = \|y\|_2^2$ (you should understand)

Concentrates around expectation using Chi-Squared concentration bound.

Midterm Review

$h(x) = sign(\langle g, x \rangle)$



$$Pr[h(x) = h(y)] = 1 - \frac{\theta(x,y)}{\pi}$$

Midterm Review