


COMPSCI 514: Algorithms for Data Science

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University of Massachusetts Amherst. Fall 2024.

Lecture 15

- We released Problem Set 3 on Friday. It is due Friday 11/8 at 11:59pm.
- Midterm grade have been posted. The average was good – around an 80%.

- Reach out to me if you are concerned about your midterm grade or your grade in the class overall.

Quiz Questions/Concerns

- Linear algebra review.
- Concerns about grades.
- Participation grade.

$\approx 78-80 \approx B$

-ec on problem sets

Summary

Last Class:

- No-distortion embeddings for data lying in a k -dimensional subspace via an orthonormal basis $\mathbf{V} \in \mathbb{R}^{d \times k}$ for that subspace.
- View as low-rank matrix factorization. Introduce concept of low-rank approximation. $\mathbf{X} = \mathbf{C}\mathbf{V}^T = \underbrace{\mathbf{X}\mathbf{V}}_{\mathbf{C}}\mathbf{V}^T$
- Idea of approximating a data matrix \mathbf{X} with $\mathbf{X}\mathbf{V}\mathbf{V}^T$ when the data points lie close to the subspace spanned by \mathbf{V} 's columns.

$$\| \underbrace{V^T x_i - V^T x_j}_{\mathbb{R}^k} \|_2 = \| \underbrace{x_i - x_j}_{\mathbb{R}^d} \|$$

Summary

Last Class:

- No-distortion embeddings for data lying in a k -dimensional subspace via an orthonormal basis $\mathbf{V} \in \mathbb{R}^{d \times k}$ for that subspace.
- View as low-rank matrix factorization. Introduce concept of low-rank approximation.
- Idea of approximating a data matrix \mathbf{X} with \mathbf{XV}^T when the data points lie close to the subspace spanned by \mathbf{V} 's columns.

This Class:

- Finding an optimal orthogonal basis $\mathbf{V} \in \mathbb{R}^{d \times k}$ to minimize $\|\mathbf{X} - \mathbf{XV}^T\|_F^2$ when our data does not exactly lie in a low-dimensional subspace, via eigendecomposition.
- Measuring the error of the optimal low-rank approximation via covariance matrix eigenvalues.

Low-Rank Factorization

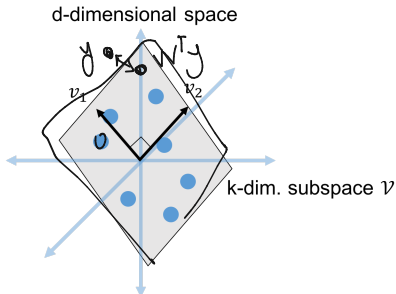
Claim: If $\vec{x}_1, \dots, \vec{x}_n$ lie in a k -dimensional subspace \mathcal{V} with orthonormal basis $\mathbf{V} \in \mathbb{R}^{d \times k}$, the data matrix can be written as

$$\begin{matrix} \downarrow \\ \left[\begin{array}{c|c|c|c} | & | & | & | \\ \hline v_1 & v_2 & \dots & v_k \\ \hline | & | & | & | \end{array} \right] \end{matrix}$$

$$\mathbf{X} = \mathbf{X}\mathbf{V}\mathbf{V}^T \text{ (implies } \text{rank}(\mathbf{X}) \leq k \text{)}$$

$\mathbf{V}\mathbf{V}^T$: projection matrix onto subspace

$\mathbf{V}\mathbf{V}^T$ is a **projection matrix**, which projects the rows of \mathbf{X} (the data points $\vec{x}_1, \dots, \vec{x}_n$) onto the subspace \mathcal{V} .

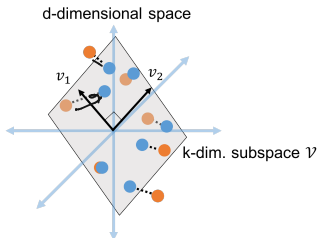


$\vec{x}_1, \dots, \vec{x}_n \in \mathbb{R}^d$: data points, $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \dots, \vec{v}_k \in \mathbb{R}^d$: orthogonal basis for subspace \mathcal{V} . $\mathbf{V} \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \dots, \vec{v}_k$.

Low-Rank Approximation

Claim: If $\vec{x}_1, \dots, \vec{x}_n$ lie close to a k -dimensional subspace \mathcal{V} with orthonormal basis $\mathbf{V} \in \mathbb{R}^{d \times k}$, the data matrix can be approximated as:

$$\mathbf{X} \approx \mathbf{X}\mathbf{V}\mathbf{V}^T$$



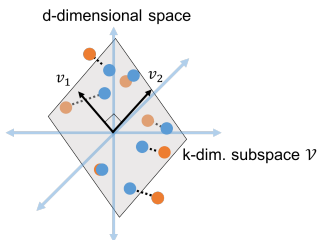
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Low-Rank Approximation

Claim: If $\vec{x}_1, \dots, \vec{x}_n$ lie **close** to a k -dimensional subspace \mathcal{V} with orthonormal basis $\mathbf{V} \in \mathbb{R}^{d \times k}$, the data matrix can be **approximated** as:

$$\mathbf{X} \approx \mathbf{X}\mathbf{V}\mathbf{V}^T$$

$$n \begin{bmatrix} k \\ \mathbf{X}\mathbf{V} \end{bmatrix} \begin{bmatrix} d \\ \mathbf{V}^T \end{bmatrix} k$$



Note: $\mathbf{X}\mathbf{V}\mathbf{V}^T$ has rank k . It is a **low-rank approximation** of \mathbf{X} .

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

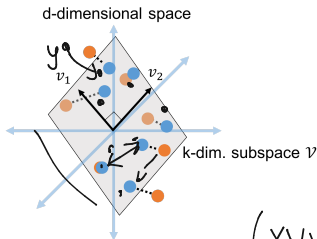
Low-Rank Approximation

Claim: If $\vec{x}_1, \dots, \vec{x}_n$ lie **close** to a k -dimensional subspace \mathcal{V} with orthonormal basis $\mathbf{V} \in \mathbb{R}^{d \times k}$, the data matrix can be **approximated** as:

$$(\mathbf{A}\mathbf{B})^T = \mathbf{B}^T \mathbf{A}^T$$

$$\mathbf{X} \approx \mathbf{X}\mathbf{V}\mathbf{V}^T$$

$$\downarrow \begin{bmatrix} d \\ d \end{bmatrix} \begin{bmatrix} d \times 1 \\ d \times 1 \end{bmatrix} = \begin{bmatrix} d \times 1 \\ d \times 1 \end{bmatrix}$$



$$\begin{bmatrix} \mathbf{X} \\ \mathbf{X}^T \end{bmatrix} \begin{bmatrix} \mathbf{V}^T \\ \mathbf{V}^T \end{bmatrix} = \begin{bmatrix} \mathbf{X}\mathbf{V}^T \\ \mathbf{X}^T\mathbf{V} \end{bmatrix}$$

$$(\mathbf{X}\mathbf{V}\mathbf{V}^T)^T = (\mathbf{V}^T)^T \mathbf{X}^T = \mathbf{V} \mathbf{X}^T$$

Finally
 $\mathbf{V}^T \mathbf{y} \approx \mathbf{y}$
 subsp. \mathcal{V}

Note: $\mathbf{X}\mathbf{V}\mathbf{V}^T$ has rank k . It is a **low-rank approximation** of \mathbf{X} .

$$\underline{\mathbf{X}\mathbf{V}\mathbf{V}^T} = \arg \min_{\mathbf{B} \text{ with rows in } \mathcal{V}} \|\mathbf{X} - \mathbf{B}\|_F^2 = \sum_{i,j} (\mathbf{X}_{i,j} - \mathbf{B}_{i,j})^2.$$

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

Low-Rank Approximation

So Far: If $\vec{x}_1, \dots, \vec{x}_n$ lie close to a k -dimensional subspace \mathcal{V} with orthonormal basis $\mathbf{V} \in \mathbb{R}^{d \times k}$, the data matrix can be approximated as:

$$\underline{\mathbf{X} \approx \mathbf{X}\mathbf{V}\mathbf{V}^T}.$$

This is the closest approximation to \mathbf{X} with rows in \mathcal{V} (i.e., in the column span of \mathbf{V}).

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This is the closest approximation to \mathbf{X} with rows in \mathcal{V} (i.e., in the column span of \mathbf{V}).

- Letting $\underbrace{\mathbf{V}\mathbf{V}^T}_{\text{size } 1} \vec{x}_i, \underbrace{\mathbf{V}\mathbf{V}^T}_{\text{size } 1} \vec{x}_j$ be the i^{th} and j^{th} projected data points,
$$\|\underbrace{\mathbf{V}\mathbf{V}^T \vec{x}_i}_{\text{size } 1} - \underbrace{\mathbf{V}\mathbf{V}^T \vec{x}_j}_{\text{size } 1}\|_2 = \|\mathbf{V}^T \mathbf{V} \mathbf{V}^T \vec{x}_i - \mathbf{V}^T \mathbf{V} \mathbf{V}^T \vec{x}_j\|_2 = \|\mathbf{V}^T \vec{x}_i - \mathbf{V}^T \vec{x}_j\|_2.$$

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

This is the closest approximation to \mathbf{X} with rows in \mathcal{V} (i.e., in the column span of \mathbf{V}).

- Letting $\mathbf{W}\mathbf{V}^T\vec{x}_i, \mathbf{W}\mathbf{V}^T\vec{x}_j$ be the i^{th} and j^{th} projected data points,

$$\|\mathbf{W}\mathbf{V}^T\vec{x}_i - \mathbf{W}\mathbf{V}^T\vec{x}_j\|_2 = \|\mathbf{V}^T\mathbf{W}\mathbf{V}^T\vec{x}_i - \mathbf{V}^T\mathbf{W}\mathbf{V}^T\vec{x}_j\|_2 = \|\mathbf{V}^T\vec{x}_i - \mathbf{V}^T\vec{x}_j\|_2.$$

- I.e., we can use the rows of $\mathbf{X}\mathbf{V} \in \mathbb{R}^{n \times k}$ as a compressed approximate data set.

$\vec{x}_1, \dots, \vec{x}_n \in \mathbb{R}^d$: 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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This is the closest approximation to \mathbf{X} with rows in \mathcal{V} (i.e., in the column span of \mathbf{V}).

$$\|\mathbf{V}^T \mathbf{x} - \mathbf{V}^T \mathbf{y}\| \neq \|\mathbf{x} - \mathbf{y}\|$$

- Letting $\mathbf{W}\mathbf{V}^T \vec{x}_i$, $\mathbf{W}\mathbf{V}^T \vec{x}_j$ be the i^{th} and j^{th} projected data points,

$$\|\mathbf{W}\mathbf{V}^T \vec{x}_i - \mathbf{W}\mathbf{V}^T \vec{x}_j\|_2 = \|\underbrace{\mathbf{V}^T \mathbf{V}}_{\mathbf{I}} \mathbf{V}^T \vec{x}_i - \underbrace{\mathbf{V}^T \mathbf{V}}_{\mathbf{I}} \mathbf{V}^T \vec{x}_j\|_2 = \|\mathbf{V}^T \vec{x}_i - \mathbf{V}^T \vec{x}_j\|_2.$$

- I.e., we can use the rows of $\mathbf{X}\mathbf{V} \in \mathbb{R}^{n \times k}$ as a compressed approximate data set.

$$\text{original } n \begin{bmatrix} d \\ \mathbf{X} \end{bmatrix} \rightarrow n \begin{bmatrix} d \\ \mathbf{X}\mathbf{V} \end{bmatrix} \rightarrow n \begin{bmatrix} k \\ \mathbf{X}\mathbf{V} \end{bmatrix} \text{ (compressed)}$$

Key question is how to find the subspace \mathcal{V} and correspondingly \mathbf{V} .

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

Properties of Projection Matrices

Quick Exercise 1: Show that $\mathbf{W}\mathbf{W}^T$ is idempotent. I.e.,

$(\mathbf{W}\mathbf{W}^T)(\mathbf{W}\mathbf{W}^T)\vec{y} = (\mathbf{W}\mathbf{W}^T)\vec{y}$ for any $\vec{y} \in \mathbb{R}^d$.

$$\underbrace{\mathbf{W}\mathbf{W}^T\mathbf{W}\mathbf{W}^T}_{\mathbf{I}}\vec{y} = \mathbf{W}\mathbf{W}^T\vec{y} \quad \text{V is orthogonal so } \mathbf{V}\mathbf{V} = \mathbf{I}_{k,k}$$

Quick Exercise 2: Show that $\mathbf{W}\mathbf{W}^T(\mathbf{I} - \mathbf{W}\mathbf{W}^T) = \mathbf{0}$ (the projection is orthogonal to its complement).

$$\begin{aligned} (\mathbf{W}\mathbf{W}^T\vec{y})^T &= \vec{y}^T(\mathbf{W}\mathbf{W}^T)^T \\ \vec{y}^T(\mathbf{W}\mathbf{W}^T)^T &= \vec{y}^T\mathbf{W}\mathbf{W}^T \\ (\mathbf{W}\mathbf{W}^T)^T &= \mathbf{W}\mathbf{W}^T \end{aligned}$$

$$\begin{aligned} \mathbf{W}\mathbf{W}^T \cdot \mathbf{I} - \mathbf{W}\mathbf{W}^T \cdot \mathbf{W}\mathbf{W}^T \\ = \mathbf{W}\mathbf{W}^T - \mathbf{W}\mathbf{W}^T &= \mathbf{0} \end{aligned}$$

k -dim subspace V
↳ set of all vectors $x = c_1\hat{v}_1 + c_2\hat{v}_2 + \dots + c_k\hat{v}_k$
for any coefficients $c_1, \dots, c_k \in \mathbb{R}$

Pythagorean Theorem

Pythagorean Theorem: For any orthonormal $V \in \mathbb{R}^{d \times k}$ and any

$\vec{y} \in \mathbb{R}^d$,

$$\|a+b\|_2^2$$

$$\langle a+b, a+b \rangle$$

$$\langle a, a \rangle + \langle b, b \rangle$$

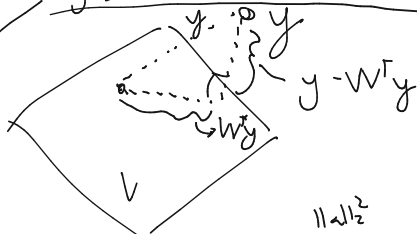
$$+ 2\langle a, b \rangle$$

$$\|a\|_2^2 + \|b\|_2^2$$

$$+ 2a^T b$$

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

$$\|y\|_2^2 = \|V^T y\|_2^2 + \|(I - VV^T)y\|_2^2$$



$$V^T a = V V^T b$$

~~$a = b$~~


$$a = b$$

$$\|V^T y + (I - VV^T)y\|_2^2 = \|V^T y\|_2^2 + \|(I - VV^T)y\|_2^2 + 2y^T V^T (I - VV^T)y$$

$$V V^T y + y - V V^T y = y \quad \|y\|_2^2 = \|V^T y\|_2^2 + \|(I - V^T)y\|_2^2$$

Best Fit Subspace

If $\vec{x}_1, \dots, \vec{x}_n$ are close to a k -dimensional subspace \mathcal{V} with orthonormal basis $\mathbf{V} \in \mathbb{R}^{d \times k}$, the data matrix can be approximated as $\mathbf{XV}\mathbf{V}^T$. \mathbf{XV} gives optimal embedding of \mathbf{X} in \mathcal{V} .



$\vec{x}_1, \dots, \vec{x}_n \in \mathbb{R}^d$: 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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If $\vec{x}_1, \dots, \vec{x}_n$ are close to a k -dimensional subspace \mathcal{V} with orthonormal basis $\mathbf{V} \in \mathbb{R}^{d \times k}$, the data matrix can be approximated as $\mathbf{X}\mathbf{V}\mathbf{V}^T$. $\mathbf{X}\mathbf{V}$ gives optimal embedding of \mathbf{X} in \mathcal{V} .

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

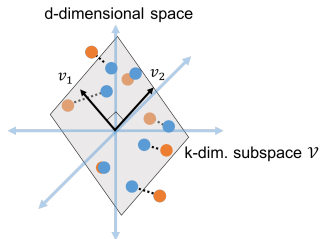
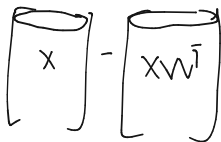
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How do we find \mathcal{V} (equivalently \mathbf{V})?

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



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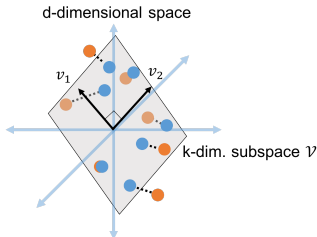
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$$\|\vec{x}_i\|_2^2 = \|\vec{x}_i \mathbf{V}^T\|_2^2 + \|\mathbf{V}^T \vec{x}_i\|_2^2$$

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

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



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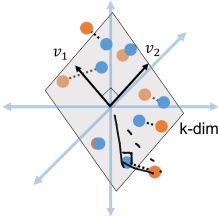
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$$\arg \min_{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}} \|\mathbf{X} - \mathbf{XV}^T\|_F^2 = \sum_{i=1}^n \|\vec{x}_i - \mathbf{V}^T \vec{x}_i\|_2^2$$

d-dimensional space



$\|\mathbf{X} - \mathbf{V}^T \mathbf{X}\|_F^2 = \sum_{i=1}^n \|\vec{x}_i - \mathbf{V}^T \vec{x}_i\|_2^2$
 pythagorem
 $\sum_{i=1}^n \|\vec{x}_i\|_2^2 - \sum_{i=1}^n \|\mathbf{V}^T \vec{x}_i\|_2^2$
 $\|\mathbf{X}\|_F^2 - \|\mathbf{XV}\|_F^2$

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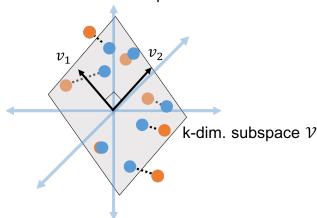
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How do we find \mathcal{V} (equivilantly \mathbf{V})?

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

$\underbrace{\hspace{10em}}_{\text{d-dimensional space}} \quad \underbrace{\hspace{10em}}$



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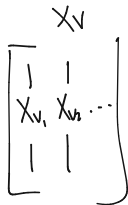
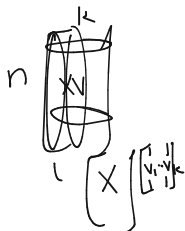
Solution via Eigendecomposition

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

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

$$\arg \max_V \|XVV^T\|_F^2 = \sum_{i=1}^n \|VV^T x_i\|_2^2 = \sum_{i=1}^n \|V^T x_i\|_2^2$$

$$\|VV^T x_i\|_2^2 = x_i^T \underbrace{VV^T}_{\substack{I \\ x_i^T V V^T x_i}} x_i = \|V^T x_i\|_2^2$$



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Solution via Eigendecomposition

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

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

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

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

Solution via Eigendecomposition

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

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

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

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

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

Solution via Eigendecomposition

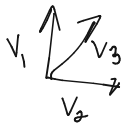
\mathbf{V} minimizing $\|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2$ is given by:

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

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

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$$\vec{v}_2 = \arg \max_{\vec{v} \text{ with } \|\vec{v}\|_2=1, \langle \vec{v}, \vec{v}_1 \rangle = 0} \|\mathbf{X}\vec{v}\|_2^2$$



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

Solution via Eigendecomposition

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

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

$$\begin{bmatrix} \mathbf{X} \\ \mathbf{V} \end{bmatrix} = \begin{bmatrix} \mathbf{X} \\ \mathbf{X}\mathbf{V} \end{bmatrix}$$

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

$$\left. \begin{aligned} \vec{v}_1 &= \arg \max_{\vec{v} \text{ with } \|\vec{v}\|_2=1} \|\mathbf{X}\vec{v}\|_2^2 = \sqrt{\lambda_1} \mathbf{X}^T \mathbf{X} \mathbf{V}_1 \\ \vec{v}_2 &= \arg \max_{\substack{\vec{v} \text{ with } \|\vec{v}\|_2=1, \\ \langle \vec{v}, \vec{v}_1 \rangle = 0}} \|\mathbf{X}\vec{v}\|_2^2 = \sqrt{\lambda_2} \mathbf{X}^T \mathbf{X} \mathbf{V}_2 \\ &\dots \\ \vec{v}_k &= \arg \max_{\substack{\vec{v} \text{ with } \|\vec{v}\|_2=1, \\ \langle \vec{v}, \vec{v}_j \rangle = 0 \ \forall j < k}} \|\mathbf{X}\vec{v}\|_2^2 = \sqrt{\lambda_k} \mathbf{X}^T \mathbf{X} \mathbf{V}_k \end{aligned} \right\}$$

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

Solution via Eigendecomposition

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

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

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

eigenvectors of $\mathbf{X}^T\mathbf{X}$



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

$$\vec{v}_2 = \arg \max_{\vec{v} \text{ with } \|\vec{v}\|_2=1, \langle \vec{v}, \vec{v}_1 \rangle = 0} \|\mathbf{X}\vec{v}\|_2^2$$

...

$$\vec{v}_k = \arg \max_{\vec{v} \text{ with } \|\vec{v}\|_2=1, \langle \vec{v}, \vec{v}_j \rangle = 0 \forall j < k} \|\mathbf{X}\vec{v}\|_2^2.$$

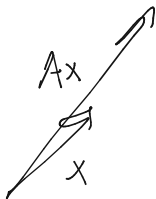
$\vec{v}_1, \dots, \vec{v}_k$ are the top k eigenvectors of $\mathbf{X}^T\mathbf{X}$ by the *Courant-Fischer Principle*.

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

Review of Eigenvectors and Eigendecomposition

$$\downarrow \begin{bmatrix} n & 1 \\ x^T & x \end{bmatrix}^n = \begin{bmatrix} x^T & x \end{bmatrix}$$

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}).



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}).

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

Review of Eigenvectors and Eigendecomposition

$$\underline{(X^T X)^T} = X^T X$$

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}).

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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.

Review of Eigenvectors and Eigendecomposition

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$$\begin{array}{cccc} \lambda_1 \vec{v}_1 & \lambda_2 \vec{v}_2 & \dots & \lambda_d \vec{v}_d \\ \uparrow & | & | & | \\ \mathbf{A}\vec{v}_1 & \mathbf{A}\vec{v}_2 & \dots & \mathbf{A}\vec{v}_d \\ | & | & | & | \end{array}$$
$$\mathbf{A}\mathbf{V} = \begin{bmatrix} \uparrow & | & | & | \\ \mathbf{A}\vec{v}_1 & \mathbf{A}\vec{v}_2 & \dots & \mathbf{A}\vec{v}_d \\ | & | & | & | \end{bmatrix}$$

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}).

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$$\mathbf{AV} = \begin{bmatrix} | & | & | & | \\ \mathbf{A}\vec{v}_1 & \mathbf{A}\vec{v}_2 & \cdots & \mathbf{A}\vec{v}_d \\ | & | & | & | \end{bmatrix} = \begin{bmatrix} | & | & | & | \\ \lambda_1\vec{v}_1 & \lambda_2\vec{v}_2 & \cdots & \lambda_d\vec{v}_d \\ | & | & | & | \end{bmatrix}$$

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}).

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

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}).

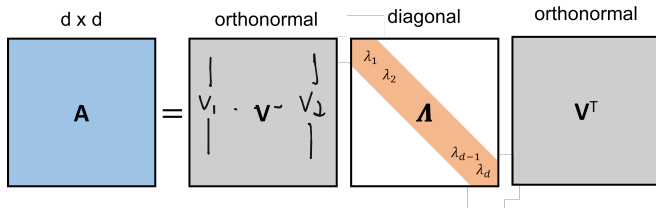
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Yields eigendecomposition: $\mathbf{AVV}^T = \mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T$.

eigendecomp.

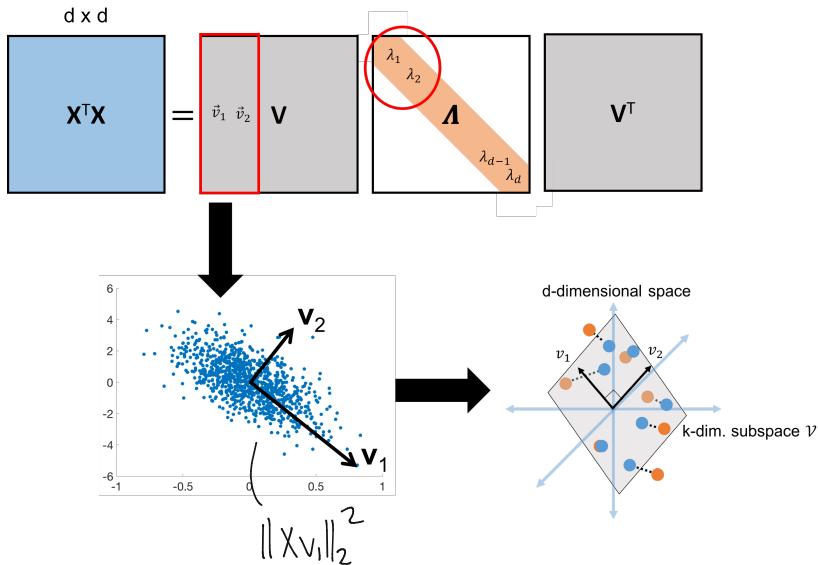
Review of Eigenvectors and Eigendecomposition



Typically order the eigenvectors in decreasing order:

$$\lambda_1 \geq \lambda_2 \geq \lambda_{\mu} \geq \lambda_d$$

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

Optimal low-rank approximation

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

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

Low-Rank Approximation via Eigendecomposition

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How accurate is this low-rank approximation?

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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

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

This is principal component analysis (PCA).

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

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