COMPSCI 514: Algorithms for Data Science

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University of Massachusetts Amherst. Fall 2023.

Lecture 16

Logistics

~~75%~~ 78-80%

$\boxed{B}$

85%

- We released Problem Set 3 last night. It is due 11/17 at 11:59pm.
- Doing the first two Core Competency questions early might be helpful if you need linear algebra review.

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.

$[C][V^T]$

- View as low-rank matrix factorization. Introduce concept of low-rank approximation.
- 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.

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This Class:

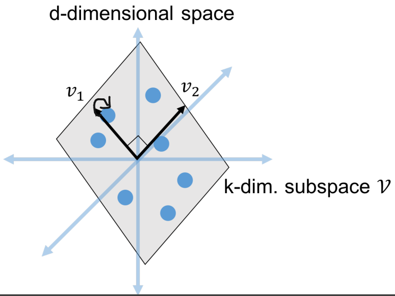
- 'Dual view' of low-rank approximation: data points that can be approximately reconstructed from a few basis vectors vs. linearly dependent features.
- How to find an optimal orthogonal basis $\mathbf{V} \in \mathbb{R}^{d \times k}$ to minimize $\|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2$. SVD, Eigendecomp, PCA

Low-Rank Factorization

Claim: If $\vec{x}_1, \ldots, \vec{x}_n$ 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

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

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

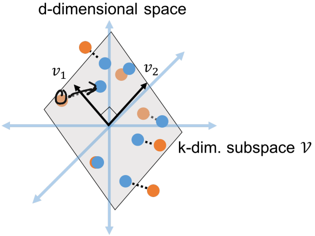


$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: orthogonal basis for subspace $\mathcal{V}$. $\mathbf{V} \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

Low-Rank Approximation

Claim: If $\vec{x}_1, \ldots, \vec{x}_n$ 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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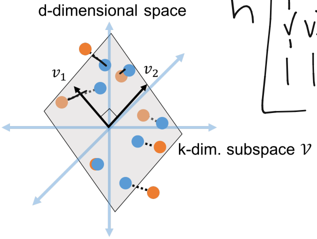
k $\quad$ $\vec{x}_i$ $\quad$ XV $\quad$ d $\quad$ x_i $\quad$ XVV^T

$n{\times}d \quad d{\times}k \quad k{\times}d$



$$\begin{array}{cc} & k \\ n & \begin{bmatrix} | & | & & | \\ v_1 & v_2 & \cdots & v_k \\ | & | & & | \end{bmatrix} \end{array}$$

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

$= I$

X not equal to

$W^T \in \mathbb{R}^{d \times d}$

$$\begin{array}{c} k \\ \begin{bmatrix} 1 & & & & & \\ & 1 & & & & \\ & & 1 & & & \\ & & & 0 & & \\ & & & & 0 & \\ & & & & & 0 \end{bmatrix} \end{array}$$

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

$XV \in \mathbb{R}^{n \times k}$

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Claim: If $\vec{x}_1, \ldots, \vec{x}_n$ 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:

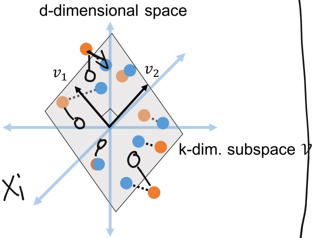
$\|M\|_F = \sqrt{\sum_i \sum_j m_{ij}^2}$

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

$\|M\|_F^2 = \sum_i \sum_j m_{ij}^2$

$\|M\|_F^2 = \sum_i \|m_{i,:}\|_2^2$

$\|X - XVV^T\|_F^2$



$x_i \in \mathbb{R}^d$

$\arg\min \|x_i - Vc\|_2^2 = V^T x_i$

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

$$\mathbf{X}\mathbf{V}\mathbf{V}^T = \underset{\mathbf{B} \text{ with rows in } \mathcal{V}}{\arg\min} \|\mathbf{X} - \mathbf{B}\|_F^2 = \sum_{i,j} (\mathbf{X}_{i,j} - \mathbf{B}_{i,j})^2. \quad = \sum \|X_{i,:} - B_{i,:}\|_2^2$$

B

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

So Far: If $\vec{x}_1, \ldots, \vec{x}_n$ 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:

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

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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Low-Rank Approximation

rows of X

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$\in \mathcal{V}$

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

$$\underbrace{\|\mathbf{V}\mathbf{V}^T\vec{x}_i - \mathbf{V}\mathbf{V}^T\vec{x}_j\|_2}_{\mathbb{R}^d} = \underbrace{\|\overbrace{\mathbf{V}^T\mathbf{V}}^{I}\mathbf{V}^T\vec{x}_i - \overbrace{\mathbf{V}^T\mathbf{V}}^{I}\mathbf{V}^T\vec{x}_j\|_2.}_{\mathbb{R}^k} = \|\mathbf{V}^T\vec{x}_i - \mathbf{V}^T\vec{x}_j\|_2.$$

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$$\begin{bmatrix} x_1^T \\ x_2^T \\ \vdots \\ x_n^T \end{bmatrix} VV^T = \begin{bmatrix} x_1^T VV^T \\ x_2^T VV^T \\ \vdots \end{bmatrix}$$

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

$$\|X - XVV^T\|_F^2$$

$$\overset{1\times d}{} \quad \overset{d \times d}{} \quad (x_i^T VV^T)^T$$

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

$$(VV^T)^T x_i$$

$$(V^T)^T V^T x_i$$

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

$$\overset{k\times d}{\begin{bmatrix} V^T \end{bmatrix}} \overset{d\times 1}{\begin{bmatrix} v_1 \end{bmatrix}}$$

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

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

$$V^T x_1, V^T x_2 \; \ldots$$

$$\begin{bmatrix} V \end{bmatrix} \begin{bmatrix} V^T \end{bmatrix} \begin{bmatrix} x_i \end{bmatrix}$$

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

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$\|VV^T(x_i-x_j)\|_2^2$

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

$(x_i-x_j)^T VV^T VV^T (x_i-x_j)$

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

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

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Quick 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 $\vec{y} \in \mathbb{R}^d$.

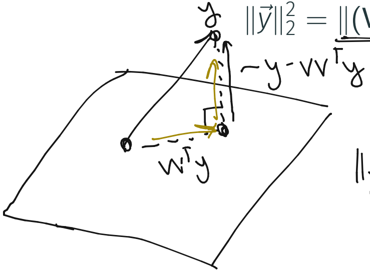
$V(\overset{I}{\cancel{V^T V}})V^T y$

$VV^T y$

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

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

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



want :D

$$\|y\|_2^2 = \|VV^Ty + (y - VV^Ty)\|_2^2$$

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

$$2y^TVV^T\underbrace{(I - VV^T)}_{0}y = 0$$

$$VV^T \cdot I - VV^TVV^T$$

$$VV^T - VV^T = 0$$

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

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

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

$\|a\|_2^2 + \|b\|_2^2 + 2\underbrace{a^Tb}_{0}$

A Step Back: Why Low-Rank Approximation?

Question: Why might we expect $\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$ to lie close to a k-dimensional subspace?

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- The rows of $\mathbf{X}$ can be approximately reconstructed from a basis of k vectors.

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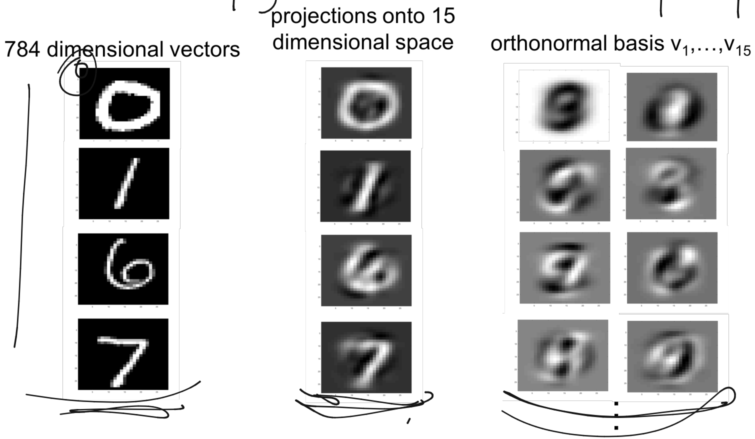
- The rows of X can be approximately reconstructed from a basis of k vectors.

784 15 784 15



Dual View of Low-Rank Approximation

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$$X \approx XVV^T$$

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Linearly Dependent Variables:

	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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10000* bathrooms+ 10* (sq. ft.) ≈ list price

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Best Fit Subspace

If $\vec{x}_1, \ldots, \vec{x}_n$ 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 $\mathcal{V}$.

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

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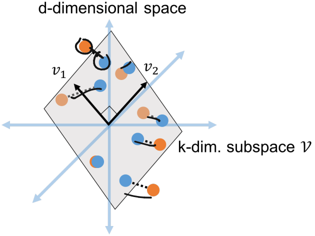
How do we find $\mathcal{V}$ (equivilantly $\mathbf{V}$)?

$x_1 \ldots x_n$ $VV^Tx_1 \ldots VV^Tx_n$ $\|(I-VV^T)x_i\|_2^2$

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

$\|x_i\|_2^2 - \|V^Tx_i\|_2^2$



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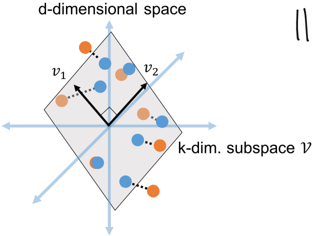
How do we find $\mathcal{V}$ (equivilantly $\mathbf{V}$)?

$\|x_i\|_2^2 = \|W^T x_i\|_2^2 + \|x_i - V V^T x\|_2^2$

$\|X - XVV^T\|_F^2 = \|X\|_F^2 - \|XVV^T\|_F^2$

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

$\|x_i - W^T x_i\|_2^2 = \|x_i\|_2^2 - \|W^T x_i\|_2^2$



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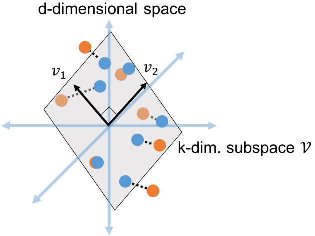
How do we find $\mathcal{V}$ (equivilantly $\mathbf{V}$)?

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



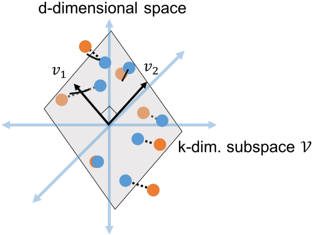
$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: orthogonal basis for subspace $\mathcal{V}$. $\mathbf{V} \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

Best Fit Subspace

If $\vec{x}_1, \ldots, \vec{x}_n$ 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 $\mathbf{XVV}^T$. $\mathbf{XV}$ gives optimal embedding of $\mathbf{X}$ in $\mathcal{V}$.

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

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



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

Solution via Eigendecomposition

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

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

$\|\mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2 = \sum \|\mathbf{V}\mathbf{V}^T x_i\|_2^2 = \sum \|\mathbf{V}^T x_i\|_2^2$

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

$$\begin{bmatrix} & & \\ & X & \\ & & \end{bmatrix} \begin{bmatrix} v_1 & v_2 & \cdots & v_k \end{bmatrix} = \begin{bmatrix} | & | & & | \\ Xv_1 & Xv_2 & \cdots & Xv_k \\ | & | & & | \end{bmatrix}$$

XV

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

Solution via Eigendecomposition

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

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

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

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

Solution via Eigendecomposition

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

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

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

$$\vec{v}_1 = \underset{\vec{v} \text{ with } \|v\|_2 = 1}{\arg\max} \|\mathbf{X}\vec{v}\|_2^2. = \langle Xv, Xv \rangle = v^T X^T X v$$

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

Solution via Eigendecomposition

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

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

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

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

Solution via Eigendecomposition

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

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

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

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

$\|Xv_2\|_2^2 \leq \|Xv_1\|_2^2$

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

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

Solution via Eigendecomposition

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

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

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

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

$$\cdots$$

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

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

Solution via Eigendecomposition

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

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

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

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

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

$$\cdots$$

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

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

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