COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

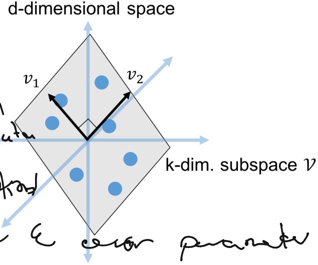
Cameron Musco
University of Massachusetts Amherst. Fall 2020.
Lecture 14

~~Midterm:~~

- Problem Set 2 grades are posted in Gradescope.
- Mean/median were 28/35.
- I posted Problem Set 3 last night. Due Friday 10/23 at 8pm.
- We are working on grading the midterm this week.
- Final will be Thursday/Friday, 12/3-12/4. Same set up as the midterm.
- Quizzes will resume this week.

Set Up: Assume that data points $\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$ lie in some k-dimensional subspace $\mathcal{V}$ of $\mathbb{R}^d$.

Different from JL?
- V is not random
  - Π in JL was random and chosen ind. of data
- JL makes no assumptions
- For JL we have some ε error parameter



Let $\vec{v}_1, \ldots, \vec{v}_k$ be an orthonormal basis for $\mathcal{V}$ and $\mathbf{V} \in \mathbb{R}^{d\times k}$ be the matrix with these vectors as its columns.

$$\|\mathbf{V}^T\vec{x}_i - \mathbf{V}^T\vec{x}_j\|_2^2 = \|\vec{x}_i - \vec{x}_j\|_2^2.$$

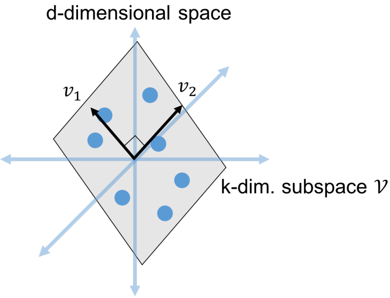
Letting $\tilde{x}_i = \mathbf{V}^T\vec{x}_i$, we have a perfect embedding from $\mathcal{V}$ into $\mathbb{R}^k$.

PROJECTION VIEW

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

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

- $\mathbf{V}\mathbf{V}^T$ 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 $\vec{v}_1, \ldots, \vec{v}_k$.

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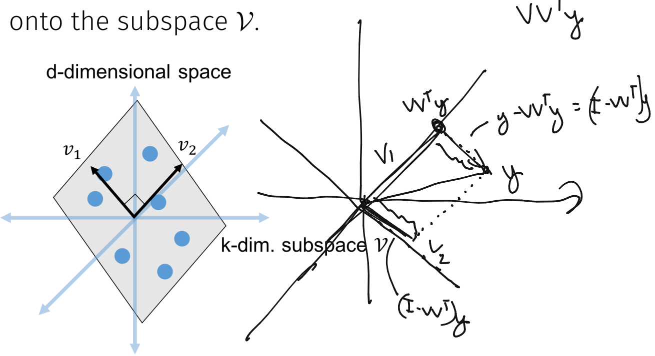

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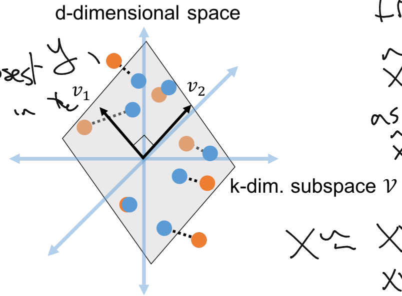

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- After projection, you are in subspace
- If project points in subspace, then nothing should happen

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 is orthonormal

$V^TV = I$

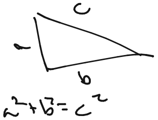
$(VV^T)(VV^T)y = VV^TVV^Ty = VV^Ty$

Why does this make sense intuitively?

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).

$VV^T(I - VV^T) = VV^T - VV^TVV^T = VV^T - VV^T = 0.$

Give the Pythagorean Theorem: Show that for any $\vec{y} \in \mathbb{R}^d$,



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

$\|y - VV^Ty\|_2^2$

$\|VV^Ty\|_2^2 = \|VV^Ty\|$

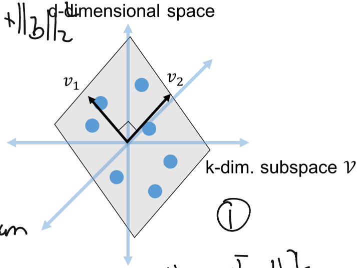
EMBEDDING WITH ASSUMPTIONS

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

Main Focus of Today: Assume that data points $\vec{x}_1, \ldots, \vec{x}_n$ lie close to any k-dimensional subspace $\mathcal{V}$ of $\mathbb{R}^d$.

$\|a+b\|_2^2 \neq \|a\|_2^2 + \|b\|_2^2$ in general

$[\,y^T\,][\,y\,] = [\|y\|_2^2]$



$(I - VV^T)^T = I^T - (VV^T)^T = I - (V^T)^T V^T = I - VV^T$

Proof of Pythagorean Theorem:

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

$\|y\|_2^2 = y^Ty$

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

① $y^TVV^TVV^Ty$ + ② $y^T(I-VV^T)(I-VV^T)y$ + ③ $2y^TVV^T(I-VV^T)y$

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

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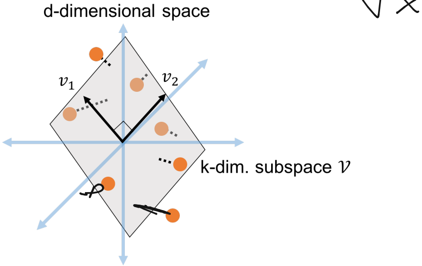

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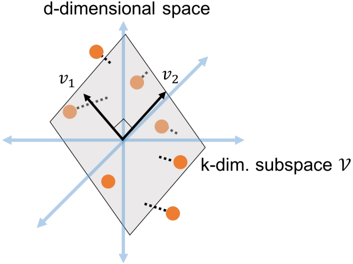

Letting $\vec{v}_1, \ldots, \vec{v}_k$ be an orthonormal basis for $\mathcal{V}$ and $\mathbf{V} \in \mathbb{R}^{d \times k}$ be the matrix with these vectors as its columns, $\mathbf{V}^T \vec{x}_i \in \mathbb{R}^k$ is still a good embedding for $x_i \in \mathbb{R}^d$.

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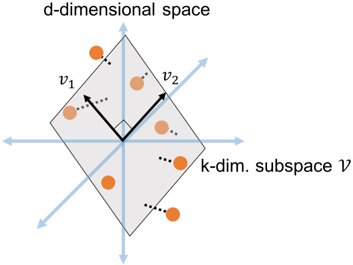

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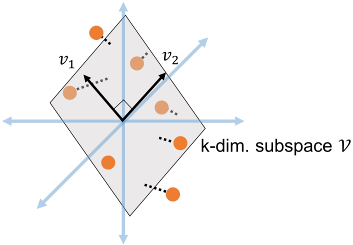

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- How do we find $\mathcal{V}$ and $\mathbf{V}$?
- How good is the embedding?

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?

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?

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

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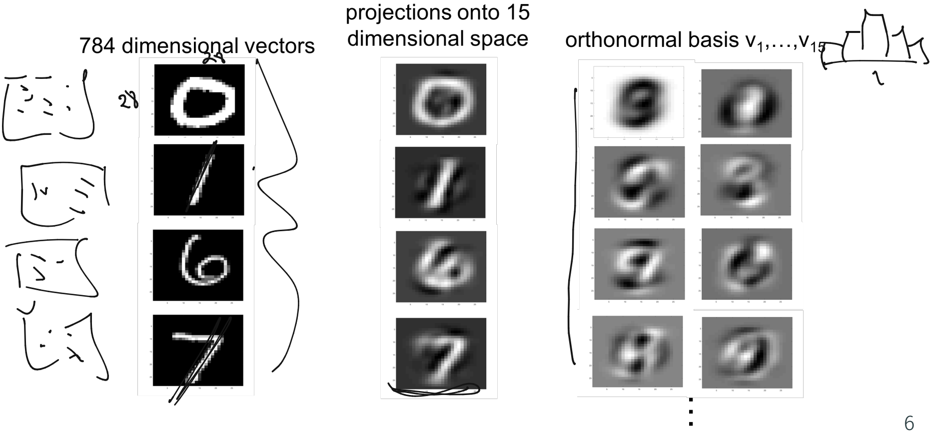

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$X \approx XVV^T$

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- Equivalently, the columns of X are approx. spanned by k vectors.

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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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$n \times d$ $\quad$ $n \times k$

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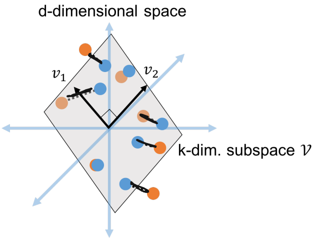
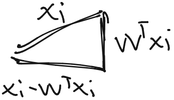
$$\underset{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}}{\arg\min} \|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2 = \sum_{i,j} (\mathbf{X}_{i,j} - (\mathbf{X}\mathbf{V}\mathbf{V}^T)_{i,j})^2 = \sum_{i=1}^{n} \|\vec{x}_i - \mathbf{V}\mathbf{V}^T\vec{x}_i\|_2^2$$





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original   projected data $\|x_i - VV^T x_i\|_2^2$

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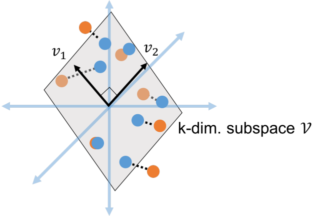

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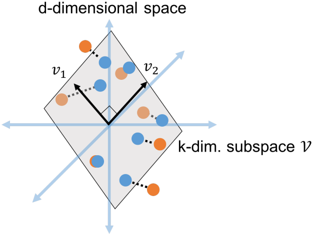

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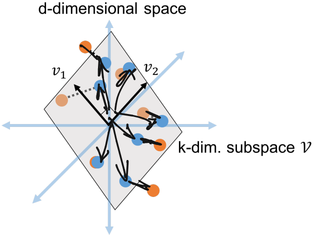

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$\mathbf{V}$ minimizing $\|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2$ is given by:

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

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

in our subspace

$\|VV^T x_i\|_2^2 = \|V^T x_i\|_2^2$

$\|VV^T x_i\|_2^2 = x_i^T VV^T VV^T x_i$

$= x_i^T VV^T x_i$

$= \|V^T x_i\|_2^2$

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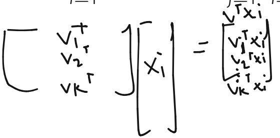

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$\mathbf{V}$ minimizing $\|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2$ is given by:

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

Columns of $\mathbf{V}$ are 'directions of greatest variance' in the data.

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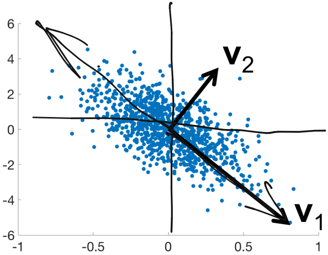
Columns of $\mathbf{V}$ are 'directions of greatest variance' in the data.

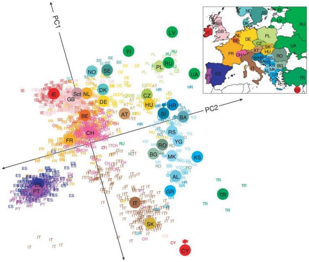


$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: orthogonal basis for subspace $\mathcal{V}$. $\mathbf{V} \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \ldots, \vec{v}_k$.

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

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

Columns of **V** are 'directions of greatest variance' in the data.



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

SUMMARY

- Many datasets lie close to a k-dimensionsal subspace.
- Can take advantage of this to do data-dependent linear dimensionality reduction (low-rank approximation).
- Dual view: both rows (data points) and columns (features) are approximated spanned by a small number of vectors.

SUMMARY

- Many datasets lie close to a k-dimensionsal subspace.
- Can take advantage of this to do data-dependent linear dimensionality reduction (low-rank approximation).
- Dual view: both rows (data points) and columns (features) are approximated spanned by a small number of vectors.

- **Step 1:** Find this subspace by finding the directions of greatest variance in the data. I.e., maximize $\|\mathbf{XV}\|_F^2$.
- **Step 2:** Get best approximation to the data points in this subspace via projection matrix $\mathbf{VV}^T$. $\mathbf{V} \in \mathbb{R}^{d \times k}$ used as linear mapping from d-dimensional to k-dimensional space.

$XVV^T \approx X$ $\qquad$ $n\,XV\,k$