COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

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University of Massachusetts Amherst. Fall 2021.

Lecture 15

Logistics:

- We have almost finished grading the midterm. Will return grades tomorrow evening and tests in class on Thursday.

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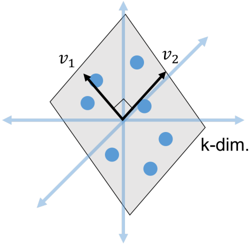
Last Class:

- 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.
  d×d
- Using that $\mathbf{V}^T\mathbf{V}$ is an identity matrix and $\mathbf{V}\mathbf{V}^T$ is a projection matrix to argue this, and understand low-rank matrix approximation.
- 'Dual view' of low-rank approximation: data points that can be reconstructed from a few basis vectors vs. linearly dependent features.

LAST CLASS: EMBEDDING WITH ASSUMPTIONS

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 $\mathbb{R}^d$.



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.

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

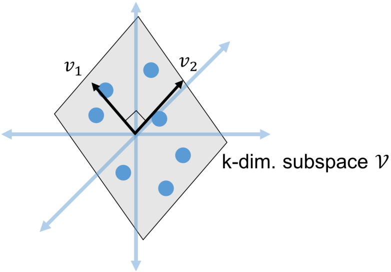
Letting $\tilde{x}_i = \mathbf{V}^T \vec{x}_i$, we have a perfect embedding from $\mathcal{V}$ into $\mathbb{R}^k$.

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

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

- $\mathbf{V}\mathbf{V}^T$ 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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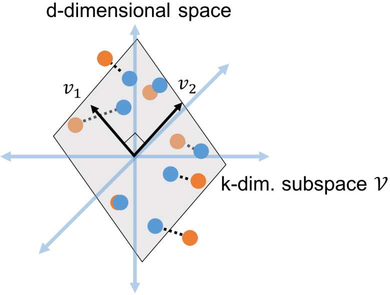

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Quick Exercise 1 : Show that $\mathbf{V}\mathbf{V}^T$ is idempotent. I.e., $(\mathbf{V}\mathbf{V}^T)(\mathbf{V}\mathbf{V}^T)\vec{y} = (\mathbf{V}\mathbf{V}^T)\vec{y}$ for any $\vec{y} \in \mathbb{R}^d$.

$$VV^T VV^T y = VV^T y \quad (V^T V = I)$$

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).

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

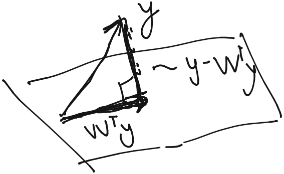
I is the d × d identity matrix $a^T a = \|a\|_2^2$

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

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

$I - VV^T \neq 0$

$I_{k \times k} - V^T V = 0$



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

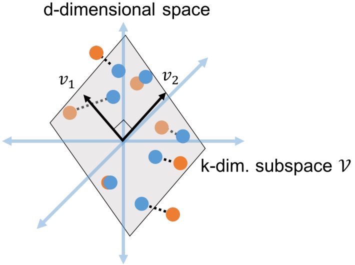
(A) $\|y\|_2^2 = \|VV^T y + (I - VV^T) y\|_2^2$

1xd dxd dxd dx1

(B) $y^T y = y^T (VV^T)^T VV^T y + y^T (I - VV^T)^T (I - VV^T) y + 2 y^T VV^T (I - VV^T) y$

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

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 $\mathbb{R}^d$.



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 $x_i \in \mathbb{R}^d$. The key idea behind low-rank approximation and principal component analysis (PCA).

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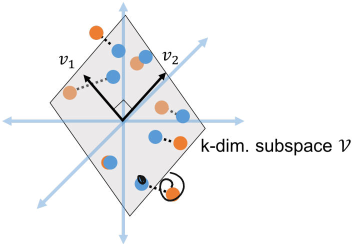

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- How do we find $\mathcal{V}$ and $\mathbf{V}$?
- How good is the embedding?

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 $\mathcal{V}$.

n×k

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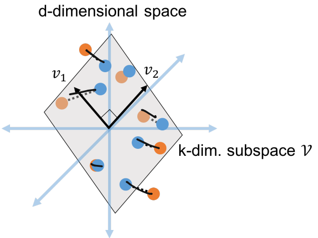
$$\underset{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}}{\arg\min} \|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2 = \sum_{i,j} (\mathbf{X}_{i,j} - (\mathbf{X}\mathbf{V}\mathbf{V}^T)_{i,j})^2 = \sum_{i=1}^{n} \|\vec{x}_i - \mathbf{V}\mathbf{V}^T\vec{x}_i\|_2^2$$

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



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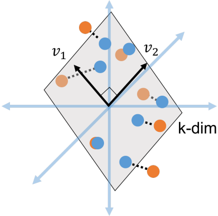

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as large as possible

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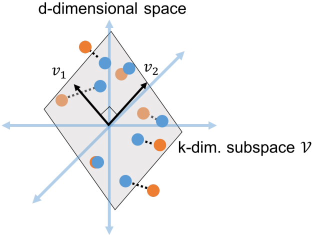

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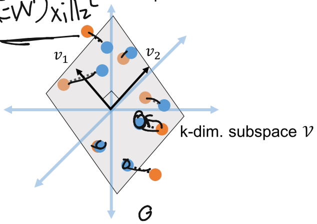

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$\|XVV^T\|_F^2$

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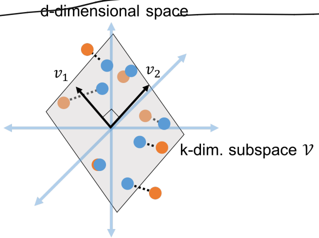

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$(Xv)^T(Xv) = v^T X^T X v$

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SOLUTION VIA EIGENDECOMPOSITION

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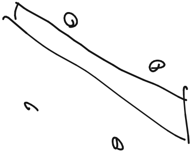

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$$\cdots$$

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

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— top eigenvecto of X^TX

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

— second eigenvect of X^TX

$$\cdots$$

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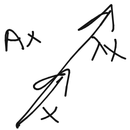
These are exactly the top k eigenvectors of $\mathbf{X}^T\mathbf{X}$.

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

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

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

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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d×d

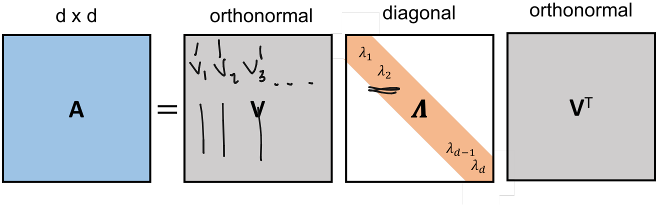
- That is, $\mathbf{A}$ just 'stretches' x.
- If $\mathbf{A}$ is symmetric, can find d orthonormal eigenvectors $\vec{v}_1, \ldots, \vec{v}_d$. Let $\mathbf{V} \in \mathbb{R}^{d \times d}$ have these vectors as columns.

$$\mathbf{AV}^T = \begin{bmatrix} | & | & & | \\ \mathbf{A}\vec{v}_1 & \mathbf{A}\vec{v}_2 & \cdots & \mathbf{A}\vec{v}_d \\ | & | & & | \end{bmatrix} = \begin{bmatrix} | & | & & | \\ \lambda_1\vec{v}_1 & \lambda_2\vec{v}_2 & \cdots & \lambda\vec{v}_d \\ | & | & & | \end{bmatrix} = \mathbf{V\Lambda} V^T$$

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

"projects onto $\mathbb{R}^d$"

$VV^T = I$



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

Courant-Fischer Principal: For symmetric $\mathbf{A}$, the eigenvectors are given via the greedy optimization:

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

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

$$\cdots$$

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

$Av = \lambda v \qquad A(c \cdot v) = \lambda \cdot c \cdot v$

Courant-Fischer Principal: For symmetric A, the eigenvectors are given via the greedy optimization:

$\|a\|_2^2 = a^T a$

$$\vec{v}_1 = \underset{\vec{v} \text{ with } \|v\|_2=1}{\arg\max} \vec{v}^T A \vec{v}. \quad = v_1^T A v_1 = \lambda_1$$

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$$\cdots$$

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$\|v_j\|_2^2 = 1$

eigenvectors have unit norm

- $\vec{v}_j^T A \vec{v}_j = \lambda_j \cdot \vec{v}_j^T \vec{v}_j = \lambda_j$, the j^{th} largest eigenvalue.

$Av_j = \lambda_j \cdot v_j$

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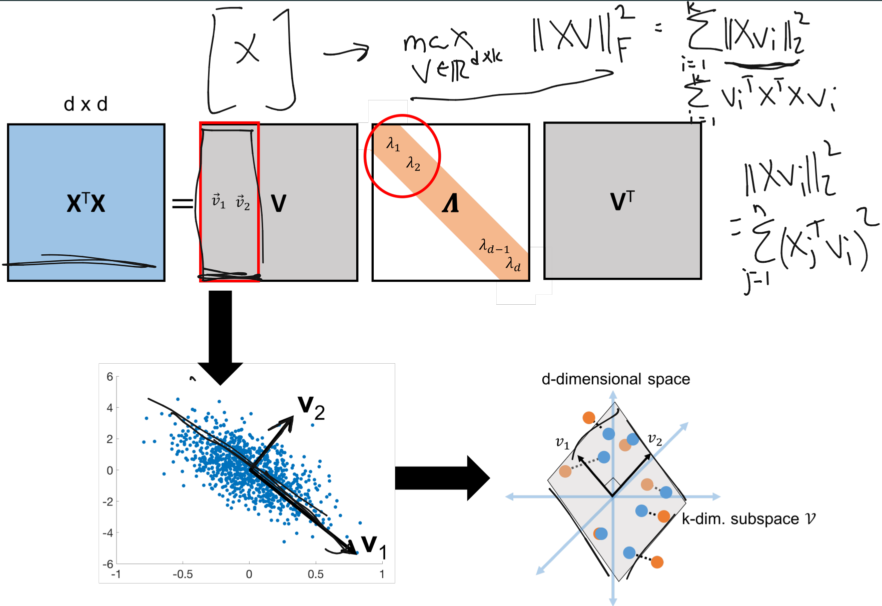
$A = X^T X$

- $\vec{v}_j^T \mathbf{A} \vec{v}_j = \lambda_j \cdot \vec{v}_j^T \vec{v}_j = \lambda_j$, the j^{th} largest eigenvalue.
- The first k eigenvectors of $\mathbf{X}^T\mathbf{X}$ (corresponding to the largest k eigenvalues) are exactly the directions of greatest variance in $\mathbf{X}$ that we use for low-rank approximation.

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

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

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

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This is principal component analysis (PCA).

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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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