

COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

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University of Massachusetts Amherst. Spring 2020.

Lecture 15

Last Class: Low-Rank Approximation

- When data lies in a k -dimensional subspace \mathcal{V} , we can perfectly embed into k dimensions using an orthonormal span $\mathbf{V} \in \mathbb{R}^{d \times k}$. $\hat{\mathbf{x}}_i = \mathbf{V}^T \mathbf{x}_i$
- When data lies **close** to \mathcal{V} , the optimal embedding in that space is given by projecting onto that space.

$$\mathbb{R}^d \rightarrow \mathbb{R}^k$$

$$\boxed{\mathbf{X}\mathbf{V}\mathbf{V}^T} = \arg \min_{\mathbf{B} \text{ with rows in } \mathcal{V}} \|\mathbf{X} - \mathbf{B}\|_F^2.$$

(sum squared errors.)

Last Class: Low-Rank Approximation

- When data lies in a k -dimensional subspace \mathcal{V} , we can perfectly embed into k dimensions using an orthonormal span $\mathbf{V} \in \mathbb{R}^{d \times k}$.
- When data lies **close** to \mathcal{V} , the optimal embedding in that space is given by projecting onto that space.

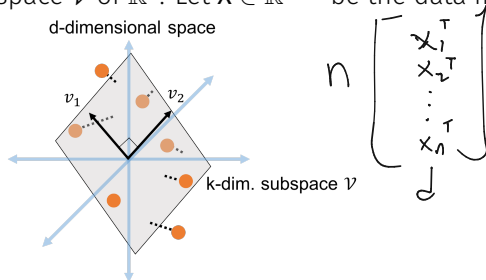
$$\mathbf{XV}^T = \underset{\mathbf{B} \text{ with rows in } \mathcal{V}}{\operatorname{arg\,min}} \quad \|\mathbf{X} - \mathbf{B}\|_F^2.$$

This Class: Finding \mathcal{V} via eigendecomposition.

- How do we find the best low-dimensional subspace to approximate \mathbf{X} ?
- PCA and its connection to eigendecomposition.

BASIC SET UP

Set Up: Assume that data points $\vec{x}_1, \dots, \vec{x}_n$ lie close to any k -dimensional subspace \mathcal{V} of \mathbb{R}^d . Let $\mathbf{X} \in \mathbb{R}^{n \times d}$ be the data matrix.



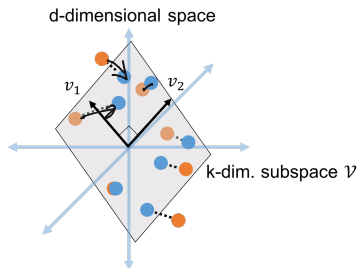
Let $\vec{v}_1, \dots, \vec{v}_k$ be an orthonormal basis for \mathcal{V} and $\mathbf{V} \in \mathbb{R}^{d \times k}$ be the matrix with these vectors as its columns.

- $\mathbf{W}\mathbf{W}^T \in \mathbb{R}^{d \times d}$ is the **projection matrix** onto \mathcal{V} .
- $\mathbf{X} \approx \underbrace{\left[\mathbf{X}(\mathbf{W}\mathbf{W}^T) \right]}_{\uparrow}$ Gives the closest approximation to \mathbf{X} with rows 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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- $\mathbf{X} \approx \mathbf{X}(\mathbf{W}\mathbf{W}^T)$. Gives the closest approximation to \mathbf{X} with rows in \mathcal{V} .

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DIMENSIONALITY REDUCTION AND LOW-RANK APPROXIMATION

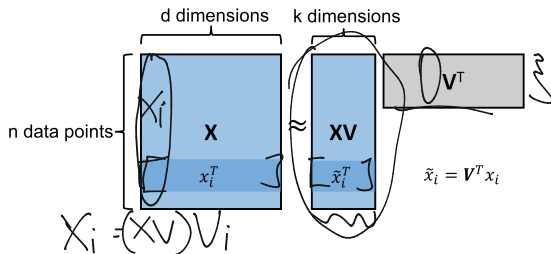
Low-Rank Approximation: Approximate $\underline{X} \approx \underline{XV}^T$.

$$X = XVV^T$$

$$x_i^T = \tilde{x}_i^T V^T$$

$$x_i = V\tilde{x}_i$$

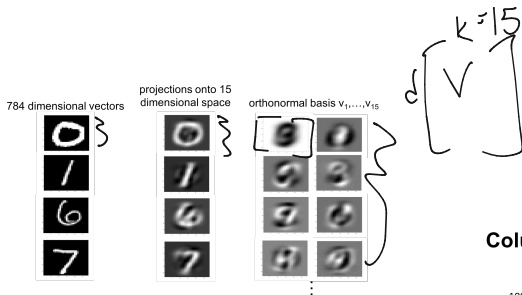
$$X_i = (XV)V_i$$



- XV^T is a **rank- k matrix** – all its rows fall in \mathcal{V} .
- X 's rows are approximately spanned by the columns of V .
- X 's columns are approximately spanned by the columns of XV .

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

DUAL VIEW OF LOW-RANK APPROXIMATION



Row (data point) compression

Column (feature) compression

$10000 * \text{bathrooms} + 10 * (\text{sq. ft.}) \approx \text{list price}$

	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

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} .

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

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BEST FIT SUBSPACE

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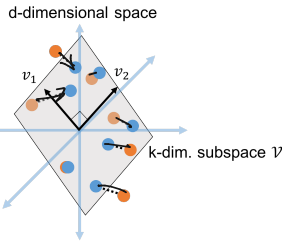
How do we find \mathcal{V} (equivalently \mathbf{V})?

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

$$d \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix} - [\mathbf{V}^T] \begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix} [\mathbf{x}_i]$$

$$\begin{bmatrix} n \\ \vdots \\ 1 \end{bmatrix} \begin{bmatrix} d \\ \vdots \\ 1 \end{bmatrix} \rightarrow \begin{bmatrix} n \\ \vdots \\ 1 \end{bmatrix} \begin{bmatrix} d \\ \vdots \\ 1 \end{bmatrix}$$

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

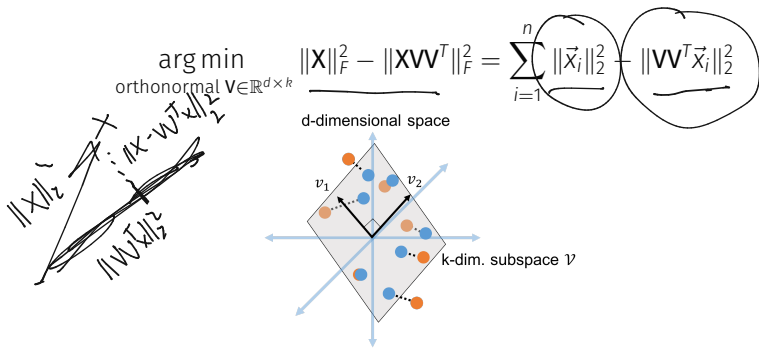


\mathbf{x}_i = column
 \mathbf{x}_i^T = row

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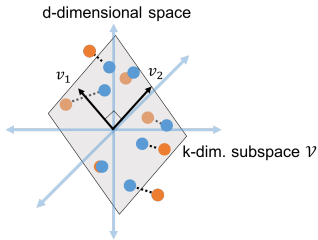


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$$\arg \min_{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}} \underbrace{\|\mathbf{X}\|_F^2}_{\text{d-dimensional space}} - \underbrace{\|\mathbf{XV}^T\|_F^2}_{\text{k-dim. subspace } \mathcal{V}} = \sum_{i=1}^n \|\vec{x}_i\|_2^2 - \|\mathbf{V}^T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

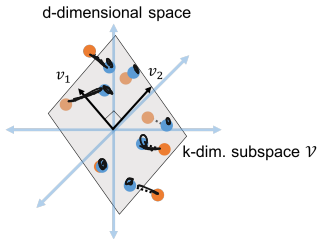


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$$\arg \max_{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}} \|\mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2 = \sum_{i=1}^n \|\mathbf{V}\mathbf{V}^T\vec{x}_i\|_2^2$$

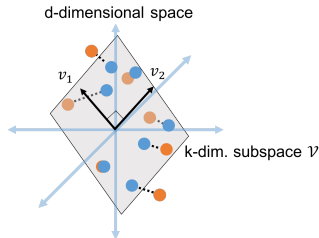


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Projection only reduces data point lengths and distances. Want to minimize this reduction.

BEST FIT SUBSPACE

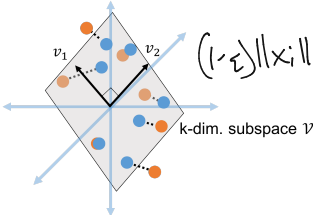
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How do we find \mathcal{V} (equivalently \mathbf{V})?

$$\mathbf{V}^T \mathbf{V} = \mathbf{I}$$

$$\arg \max_{\substack{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k} \\ \mathbf{V}^T \mathbf{V} = \mathbf{I}}} \|\mathbf{XV}^T\|_F^2 = \sum_{i=1}^n \underbrace{\|\mathbf{V}^T \vec{x}_i\|_2^2}_{\|\mathbf{V}^T \mathbf{x}_i\| \leq \|\mathbf{x}_i\|}$$

d-dimensional space



k-dim. subspace \mathcal{V}

$$(1-\epsilon)\|\mathbf{x}_i\| \leq \|\mathbf{V}^T \mathbf{x}_i\| \leq (1+\epsilon)\|\mathbf{x}_i\|$$

Projection only reduces data point lengths and distances. Want to minimize this reduction. How does this compare to JL random projection?

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

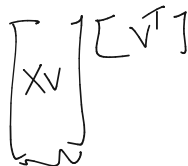
$$\arg \max_{\text{orthonormal } V \in \mathbb{R}^{d \times k}} \|XVV^T\|_F^2 = \sum_{i=1}^n \underbrace{\|V^T \vec{x}_i\|_2^2}_{\|V^T \vec{x}_i\|_2^2}$$

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$$= (\vec{v}_1^T \vec{x}_i)^2 + (\vec{v}_2^T \vec{x}_i)^2 + \dots + (\vec{v}_k^T \vec{x}_i)^2$$

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

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BEST FIT SUBSPACE

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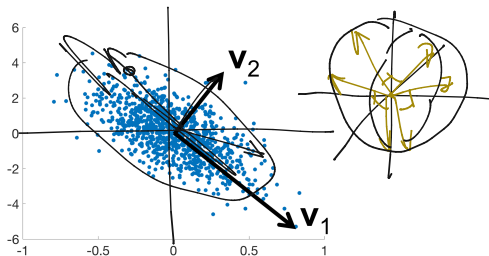
$$\arg \max_{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}} \|\mathbf{X}\mathbf{V}\|_F^2 = \sum_{i=1}^n \|\mathbf{V}^T \vec{x}_i\|_2^2 = \sum_{j=1}^k \left[\sum_{i=1}^n \langle \vec{v}_j, \vec{x}_i \rangle^2 \right]$$

$|\mathcal{L} = 1$

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

$d=3$
 $k=2$

$\left[\begin{array}{c} \mathbf{v}_1 \dots \mathbf{v}_k \end{array} \right]$

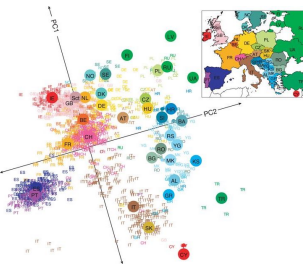


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SOLUTION VIA EIGENDECOMPOSITION

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

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



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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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$\|\mathbf{X}\mathbf{V}\|_F^2 = \|\mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2$
 $\sum_k \sum_n \|\mathbf{V}^T \vec{x}_i\|_2^2 = \sum_k \sum_n \langle \vec{v}_j, \vec{x}_i \rangle^2$

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

$\vec{v}_1, \dots, \vec{v}_k$ unit vectors $\vec{v}_1 = \arg \max_{\vec{v} \text{ with } \|\vec{v}\|_2=1} \|\mathbf{X}\vec{v}\|_2^2 = \sqrt{\mathbf{V}^T \mathbf{X}^T \mathbf{X} \mathbf{V}}$

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

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SOLUTION VIA EIGENDECOMPOSITION

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

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

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

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

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

$\vec{x}_1, \dots, \vec{x}_n \in \mathbb{R}^d$: 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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$$\vec{v}_k = \arg \max_{\vec{v} \text{ with } \|\vec{v}\|_2=1, \langle \vec{v}, \vec{v}_j \rangle = 0 \ \forall j < k} \vec{v}^T \mathbf{X}^T \mathbf{X} \vec{v}.$$


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These are exactly the top k eigenvectors 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, $\vec{v}_1, \dots, \vec{v}_k \in \mathbb{R}^d$: orthogonal basis for subspace \mathcal{V} . $\mathbf{V} \in \mathbb{R}^{d \times k}$: matrix with columns $\vec{v}_1, \dots, \vec{v}_k$.

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}).

$$\begin{bmatrix} \mathbf{A} \end{bmatrix} \begin{bmatrix} \vec{x} \end{bmatrix} = \lambda \begin{bmatrix} \vec{x} \end{bmatrix}$$

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$$\mathbf{AV} = \begin{matrix} \downarrow \\ \left[\begin{array}{cccc} | & | & \cdots & | \\ \mathbf{A}\vec{v}_1 & \mathbf{A}\vec{v}_2 & \cdots & \mathbf{A}\vec{v}_d \\ \underbrace{\quad} & | & | & | \\ \lambda_1 \vec{v}_1 & & & \end{array} \right] \end{matrix}$$

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

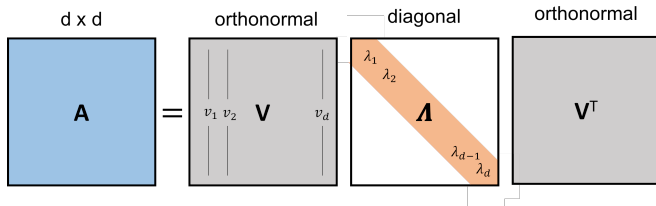
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Yields eigendecomposition: $\underline{\mathbf{AVV}^T} = \mathbf{A} = \underline{\mathbf{V}\mathbf{\Lambda}\mathbf{V}^T}$.

REVIEW OF EIGENVECTORS AND EIGENDECOMPOSITION



Typically order the eigenvectors in decreasing order:

$$\underline{\lambda_1} \geq \underline{\lambda_2} \geq \dots \geq \underline{\lambda_d}.$$

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

$$\left. \begin{aligned}
 \vec{v}_1 &= \arg \max_{\vec{v} \text{ with } \|\vec{v}\|_2=1} \vec{v}^T \mathbf{A} \vec{v}. \\
 \vec{v}_2 &= \arg \max_{\vec{v} \text{ with } \|\vec{v}\|_2=1, \langle \vec{v}, \vec{v}_1 \rangle = 0} \vec{v}^T \mathbf{A} \vec{v}. \\
 &\quad \dots \\
 \vec{v}_d &= \arg \max_{\vec{v} \text{ with } \|\vec{v}\|_2=1, \langle \vec{v}, \vec{v}_j \rangle = 0 \ \forall j < d} \vec{v}^T \mathbf{A} \vec{v}.
 \end{aligned} \right\}$$

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

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

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

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

$$\vec{v}_j^T A \vec{v}_j = \lambda_j$$

Singular value decomposition (SVD)

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v_1, \dots, v_k

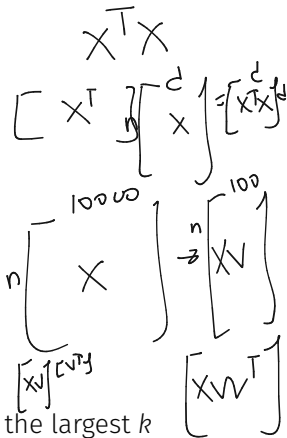
Span for subspace

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

top k eigenvectors of $X^T X$.

...

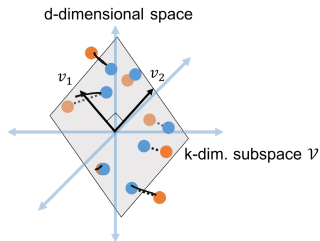
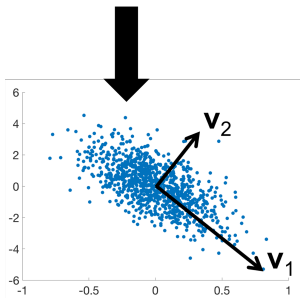
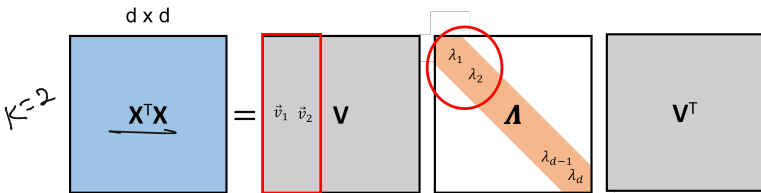
$$\vec{v}_d = \arg \max_{\vec{v} \text{ with } \|\vec{v}\|_2=1, \langle \vec{v}, \vec{v}_j \rangle = 0 \forall j < d} \vec{v}^T A \vec{v}.$$



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

LOW-RANK APPROXIMATION VIA EIGENDECOMPOSITION

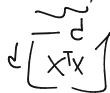
$$\min_V \|X - X\underline{V}V^T\|_F^2 \quad \text{How to find } V?$$



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

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



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

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

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

$$\mathbf{V}_k = \begin{bmatrix} \vec{v}_1 & \dots & \vec{v}_k \end{bmatrix}$$

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$$\|\mathbf{X} - \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T\|_F^2 = \|\mathbf{X}\|_F^2 - \underbrace{\|\mathbf{X}\mathbf{V}_k\mathbf{V}_k^T\|_F^2}_{\text{max.}}$$

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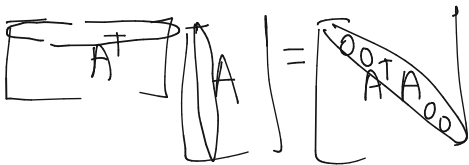
SPECTRUM ANALYSIS

Let $\vec{v}_1, \dots, \vec{v}_k$ be the top k eigenvectors of $X^T X$ (the top k ^{dot product} _{trick} principal components). Approximation error is:

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

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

$$\|A\|_F^2 = \text{tr}(A^T A)$$



$$\text{tr}(A^T A) = \sum_{i=1}^d (A^T A)_{i,i} = \sum \|a_i\|_2^2$$

(A^T A)_{i,i}

$$(A^T A)_{i,j} = \langle a_i, a_j \rangle$$

$$(A^T A)_{i,i} = \langle a_i, a_i \rangle = \|a_i\|_2^2$$

- For any matrix A , $\|A\|_F^2 = \sum_{i=1}^d \|\vec{a}_i\|_2^2 = \text{tr}(A^T A)$ (sum of diagonal entries = sum eigenvalues).

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

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

$$\|\mathbf{X} - \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T\|_F^2 = \underbrace{\text{tr}(\mathbf{X}^T\mathbf{X})} - \underbrace{\text{tr}(\mathbf{V}_k^T\mathbf{X}^T\mathbf{X}\mathbf{V}_k)}$$

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$$\begin{aligned} \|\mathbf{X} - \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T\|_F^2 &= \underbrace{\text{tr}(\mathbf{X}^T\mathbf{X})}_d - \underbrace{\text{tr}(\mathbf{V}_k^T\mathbf{X}^T\mathbf{X}\mathbf{V}_k)}_k \\ &= \sum_{i=1}^d \lambda_i(\mathbf{X}^T\mathbf{X}) - \sum_{i=1}^k \vec{v}_i^T \mathbf{X}^T \mathbf{X} \vec{v}_i \end{aligned}$$

- For any matrix \mathbf{A} , $\|\mathbf{A}\|_F^2 = \sum_{i=1}^d \|\vec{a}_i\|_2^2 = \text{tr}(\mathbf{A}^T\mathbf{A})$ (sum of diagonal entries = sum eigenvalues). $\sum \lambda_j(\mathbf{A}^T\mathbf{A})$

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$$\begin{aligned}
 \|\mathbf{X} - \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T\|_F^2 &= \text{tr}(\mathbf{X}^T\mathbf{X}) - \text{tr}(\mathbf{V}_k^T\mathbf{X}^T\mathbf{X}\mathbf{V}_k) \\
 &= \sum_{i=1}^d \lambda_i(\mathbf{X}^T\mathbf{X}) - \sum_{i=1}^k \underbrace{\vec{v}_i^T \mathbf{X}^T \mathbf{X} \vec{v}_i}_{\substack{\parallel \\ \vec{v}_i^T \mathbf{X}^T \mathbf{X} \vec{v}_i = \vec{v}_i^T (\lambda_i \vec{v}_i) = \lambda_i \vec{v}_i^T \vec{v}_i \\ = \lambda_i}} \\
 &= \sum_{i=1}^d \lambda_i(\mathbf{X}^T\mathbf{X}) - \sum_{i=1}^k \lambda_i(\mathbf{X}^T\mathbf{X})
 \end{aligned}$$

- For any matrix \mathbf{A} , $\|\mathbf{A}\|_F^2 = \sum_{i=1}^d \|\vec{a}_i\|_2^2 = \text{tr}(\mathbf{A}^T\mathbf{A})$ (sum of diagonal entries = sum eigenvalues).

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

$$\begin{aligned} \underbrace{\|\mathbf{X} - \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T\|_F^2} &= \text{tr}(\mathbf{X}^T\mathbf{X}) - \text{tr}(\mathbf{V}_k^T\mathbf{X}^T\mathbf{X}\mathbf{V}_k) \\ &= \sum_{i=1}^d \lambda_i(\mathbf{X}^T\mathbf{X}) - \sum_{i=1}^k \vec{v}_i^T \mathbf{X}^T\mathbf{X} \vec{v}_i \\ &= \sum_{i=1}^d \lambda_i(\mathbf{X}^T\mathbf{X}) - \sum_{i=1}^k \lambda_i(\mathbf{X}^T\mathbf{X}) = \underbrace{\sum_{i=k+1}^d \lambda_i(\mathbf{X}^T\mathbf{X})} \end{aligned}$$

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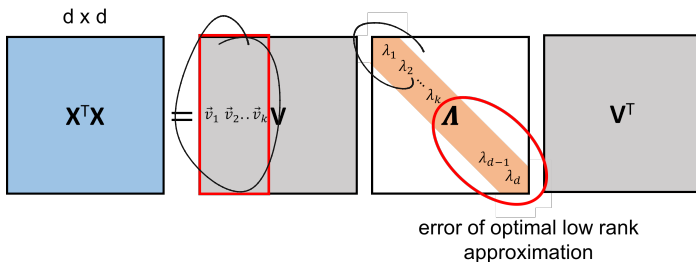
Claim: The error in approximating \mathbf{X} with the best rank k approximation (projecting onto the top k eigenvectors of $\mathbf{X}^T\mathbf{X}$ is:

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

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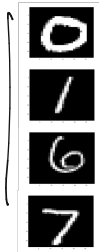
SPECTRUM ANALYSIS

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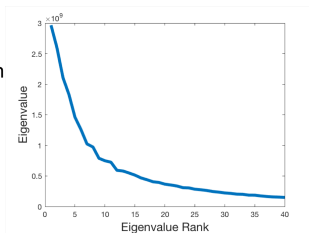
$$\|\mathbf{X} - \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T\|_F^2 = \sum_{i=k+1}^d \lambda_i(\mathbf{X}^T\mathbf{X})$$

*spectrum =
all eigenvalues*

784 dimensional vectors



eigendecomposition

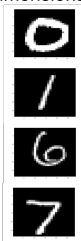


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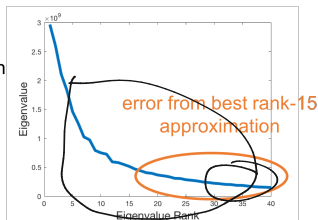
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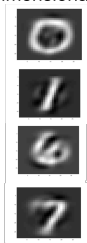
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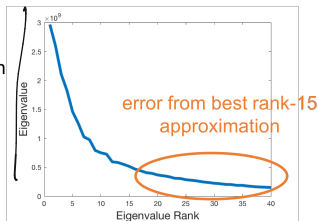
$(\mathbf{X}^T\mathbf{X})$
Symmetric.

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

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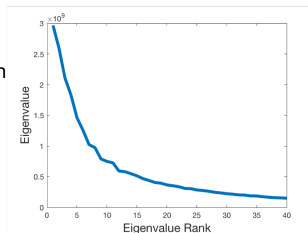
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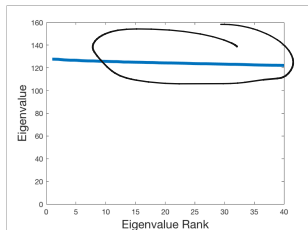
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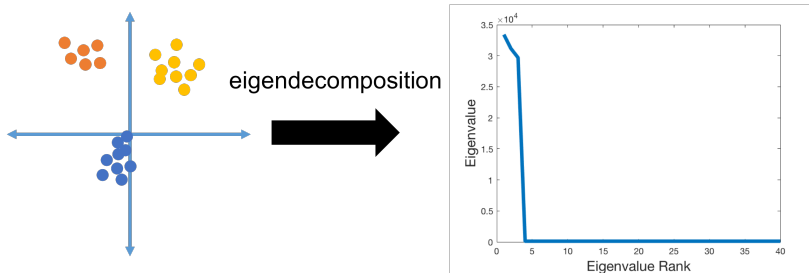
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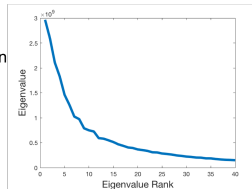


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eigendecomposition



Exercise: Show that the eigenvalues of $X^T X$ are always positive.

Hint: Use that $\lambda_j = \vec{v}_j^T X^T X \vec{v}_j$.

- Many (most) datasets can be approximated via projection onto a low-dimensional subspace.
- Find this subspace via a maximization problem:

$$\max_{\text{orthonormal } \mathbf{V}} \|\mathbf{XV}\|_F^2.$$

- 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 is determined by the tail of $\mathbf{X}^T\mathbf{X}$'s eigenvalue spectrum.

INTERPRETATION IN TERMS OF CORRELATION

Recall: Low-rank approximation is possible when our data features are correlated.

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

	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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Covariance becomes diagonal. I.e., all correlations have been removed. Maximal compression.

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Many faster iterative and randomized methods. Runtime is roughly $\tilde{O}(ndk)$ to output just the top k eigenvectors $\vec{v}_1, \dots, \vec{v}_k$.

- Will see in a few classes

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