COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

Andrew McGregor

Lecture 16

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.

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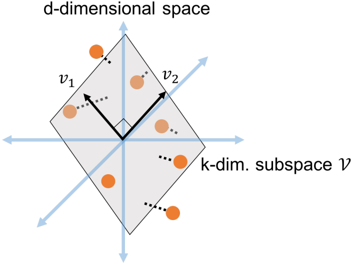
This Class:

- The best subspace $\mathcal{V}$ is the subspace spanned by the top k eigenvectors of $\mathbf{X}^T\mathbf{X}$. How good is this approximation?

RECAP: BASIC SET UP

Reminder of Set Up: Assume that $\vec{x}_1, \ldots, \vec{x}_n$ 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 $\vec{v}_1, \ldots, \vec{v}_k$ 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.

- $\mathbf{V}\mathbf{V}^T \in \mathbb{R}^{d \times d}$ is the projection matrix onto $\mathcal{V}$.
- $\mathbf{X} \approx \mathbf{X}(\mathbf{V}\mathbf{V}^T)$. Gives the closest approximation to $\mathbf{X}$ with rows in $\mathcal{V}$.

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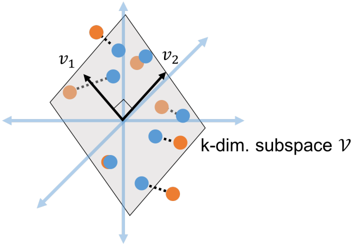

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If $\vec{x}_1, \ldots, \vec{x}_n$ are close to a k-dimensional subspace $\mathcal{V}$ with orthonormal basis $\mathbf{V} \in \mathbb{R}^{d \times k}$, the data matrix can be approximated as $\mathbf{X}\mathbf{V}\mathbf{V}^T$. $\mathbf{X}\mathbf{V}$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

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

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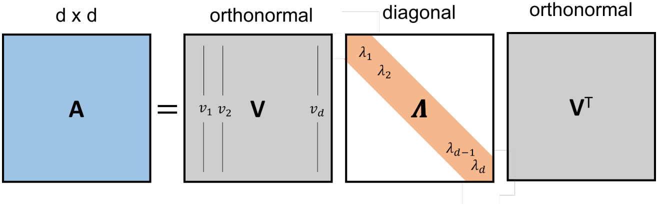
Yields eigendecomposition: $\mathbf{AVV}^T = \mathbf{A} = \mathbf{V\Lambda V}^T$.



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:

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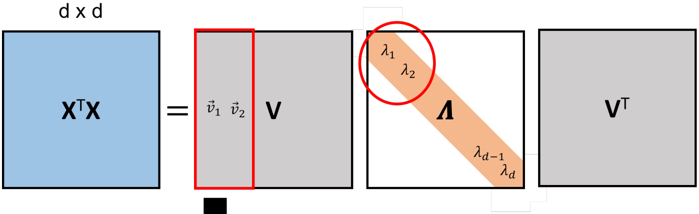
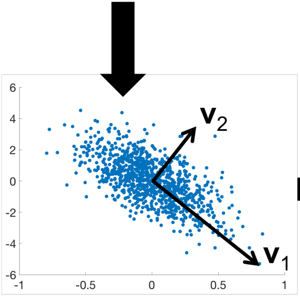
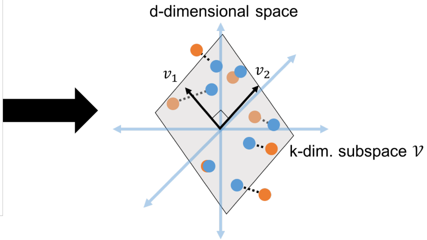
- $\vec{v}_j^T \mathbf{A} \vec{v}_j = \lambda_j \cdot \vec{v}_j^T \vec{v}_j = \lambda_j$, the j^{th} largest eigenvalue.
- The first k eigenvectors of $\mathbf{X}^T\mathbf{X}$ (corresponding to the largest k eigenvalues) are exactly the directions of greatest variance in $\mathbf{X}$ that we use for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


d x d
X^TX
=
$\vec{v}_1$ $\vec{v}_2$ V
λ_1
λ_2
Λ
λ_{d-1}
λ_d
V^T


v_2
v_1
6
4
2
0
-2
-4
-6
-1
-0.5
0
0.5
1


d-dimensional space
v_1
v_2
k-dim. subspace $\mathcal{V}$

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

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

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This is principal component analysis (PCA).

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- In Homework 3 we show matrix form of Pythagorus Theorem:

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

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

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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:

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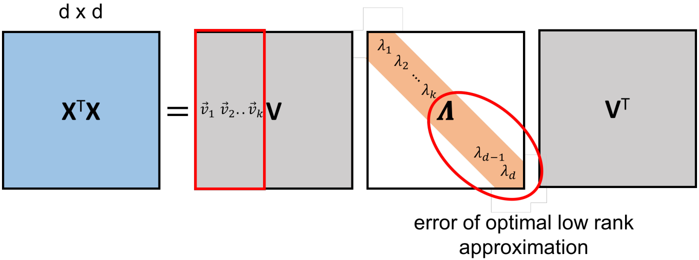

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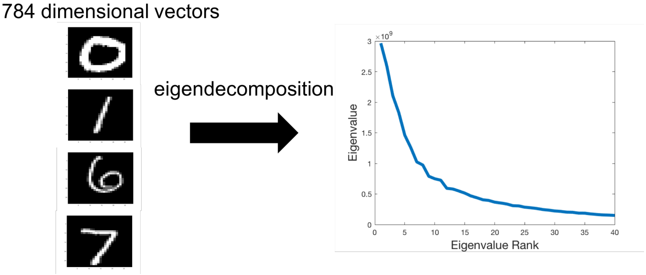

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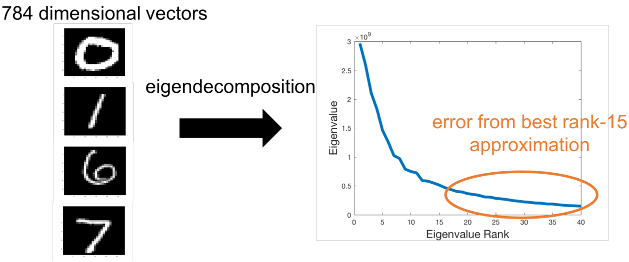

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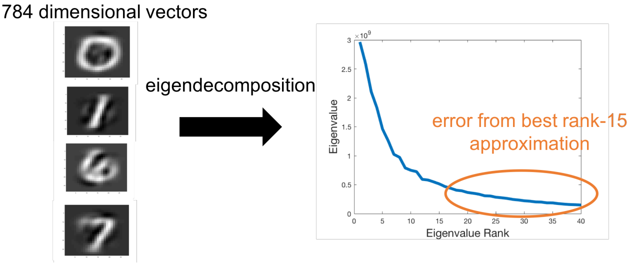

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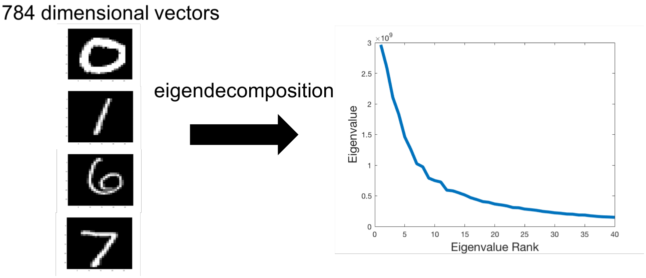

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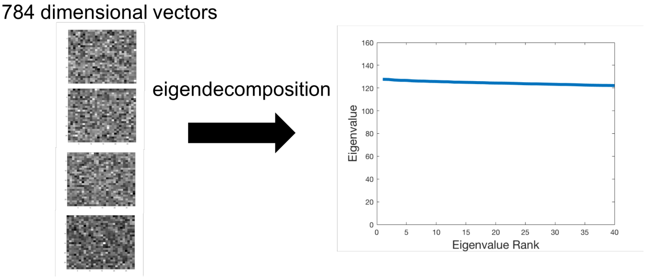

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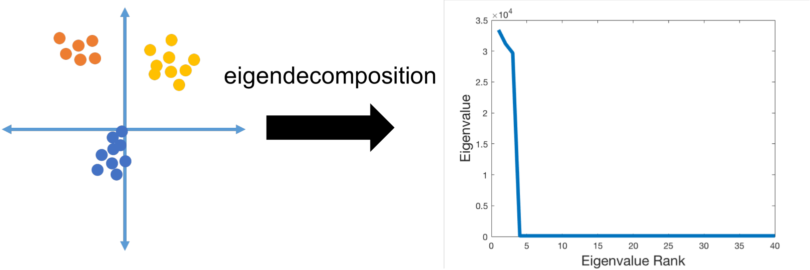

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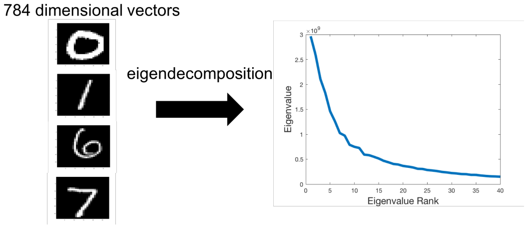

Exercise: Show that the eigenvalues of $\mathbf{X}^T\mathbf{X}$ are always positive.

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

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

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

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- Columns of $\mathbf{V}$ are the top eigenvectors of $\mathbf{X}^T\mathbf{X}$.
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- Error of best low-rank approximation is determined by the tail of $\mathbf{X}^T\mathbf{X}$'s eigenvalue spectrum.
- We'll return to the problem how to quickly compute the top eigenvectors of $\mathbf{X}^T\mathbf{X}$.