COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

Andrew McGregor

Lecture 15

Last Classes: Low-Rank Approximation

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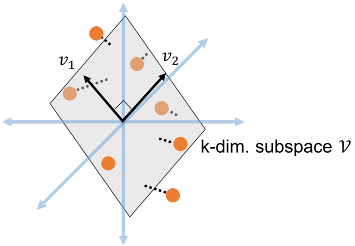
- The best subspace $\mathcal{V}$ is the subspace spanned by the top k eigenvectors of $\mathbf{X}^T\mathbf{X}$. How good is this approximation?

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 $\mathcal{V}$.
- $\mathbf{X}(\mathbf{V}\mathbf{V}^T)$ 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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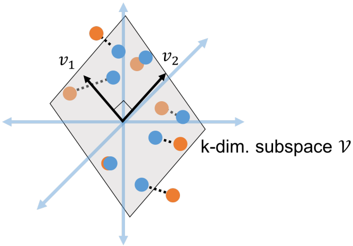

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If $\vec{x}_1, \ldots, \vec{x}_n$ are close to a k-dimensional subspace $\mathcal{V}$ with orthonormal basis $\mathbf{V} \in \mathbb{R}^{d \times k}$, the data matrix can be approximated as $\mathbf{X}\mathbf{V}\mathbf{V}^T$. $\mathbf{X}\mathbf{V}$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

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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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- That is, **A** just 'stretches' x.
- If **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 and $\mathbf{\Lambda}$ be the diagonal matrix with the corresponding eigenvalues on the diagonal.

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Yields eigendecomposition: $\mathbf{AVV}^T = \mathbf{A} = \mathbf{V\Lambda V}^T$ where the first inequality follows since rows of **A** are in span of the eigenvectors.

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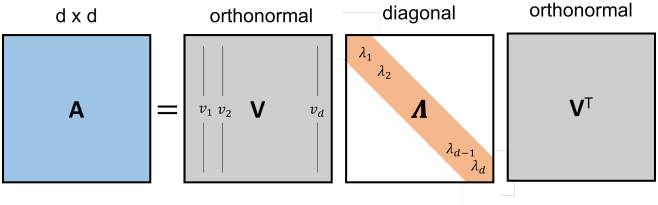

Typically order the eigenvectors in decreasing order:

$$\lambda_1 \geq \lambda_2 \geq \ldots \geq \lambda_d$$

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

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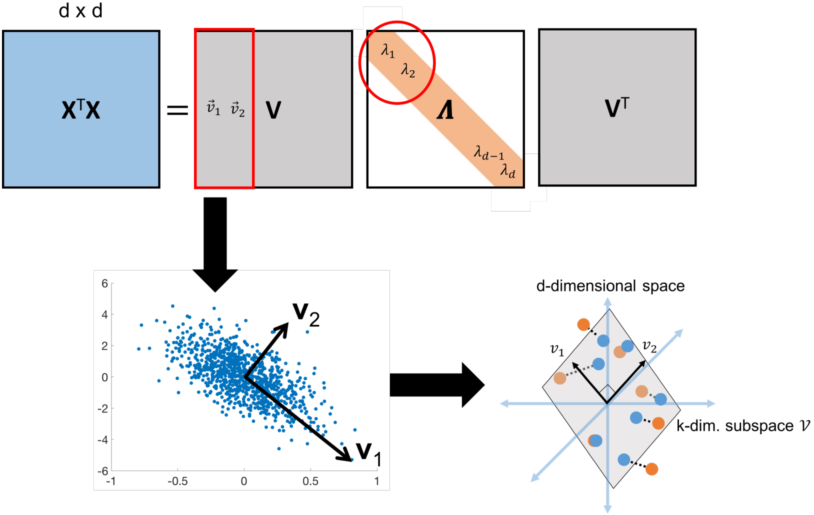
- $\vec{v}_j^T \mathbf{A} \vec{v}_j = \lambda_j \cdot \vec{v}_j^T \vec{v}_j = \lambda_j$, the j^{th} largest eigenvalue.
- The first k eigenvectors of $\mathbf{X}^T\mathbf{X}$ (corresponding to the largest k eigenvalues) are exactly the directions of greatest variance in $\mathbf{X}$ that we use for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

$$\vec{v}^T \mathbf{X}^T \mathbf{X} \vec{v} = \sum_i \langle \vec{v}, \vec{x}_i \rangle^2$$


d x d
X^TX
=
$\vec{v}_1$ $\vec{v}_2$ V
λ_1
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v_1
v_2
k-dim. subspace $\mathcal{V}$

LOW-RANK APPROX 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

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This is principal component analysis (PCA).

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- By applying the Pythagorus Theorem on each row:

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

and note $\|\mathbf{X}\mathbf{V}_k\mathbf{V}_k^T\|_F^2 = \|\mathbf{X}\mathbf{V}_k\|_F^2$ because $\mathbf{V}_k$ is orthonormal.

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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) and λ_i be the eigenvalue corresponding to $\vec{v}_i$.
Approximation error is:

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

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

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

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

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- 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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$$= \sum_{i=1}^{d} \lambda_i - \sum_{i=1}^{k} \vec{v}_i^T\mathbf{X}^T\mathbf{X}\vec{v}_i$$

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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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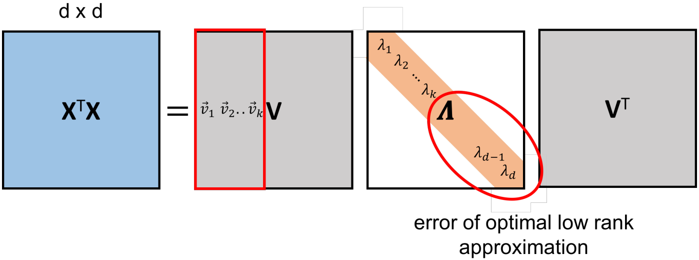

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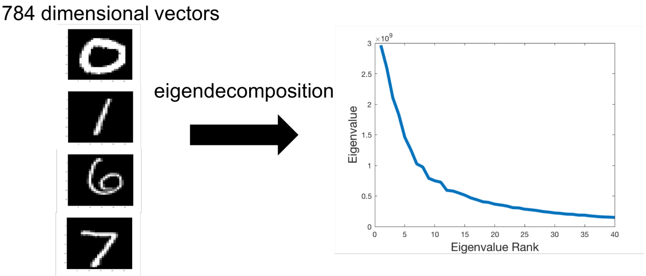

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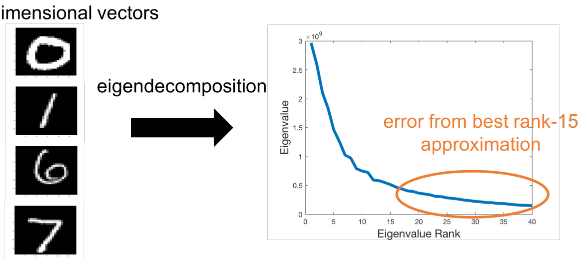

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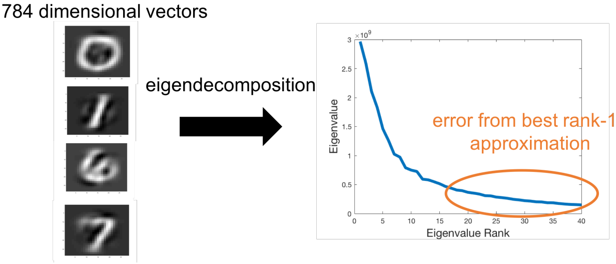

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SPECTRUM ANALYSIS

Plotting the spectrum of the covariance matrix $\mathbf{X}^T\mathbf{X}$ (its eigenvalues) shows how compressible $\mathbf{X}$ is using low-rank approximation (i.e., how close $\vec{x}_1, \ldots, \vec{x}_n$ are to a low-dimensional subspace).

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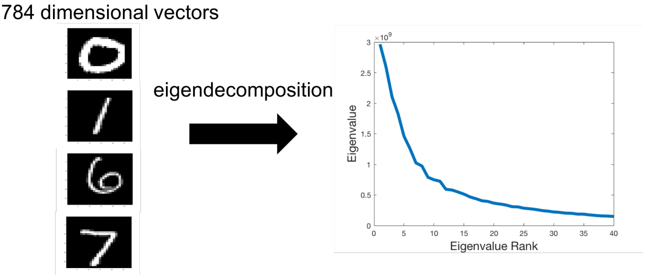

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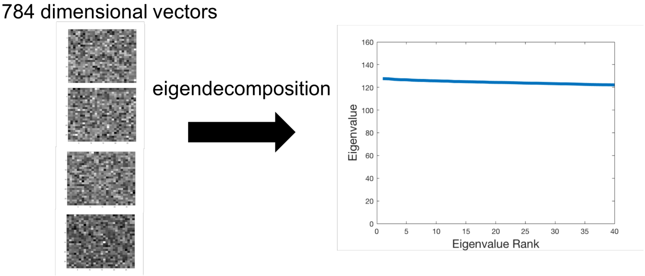

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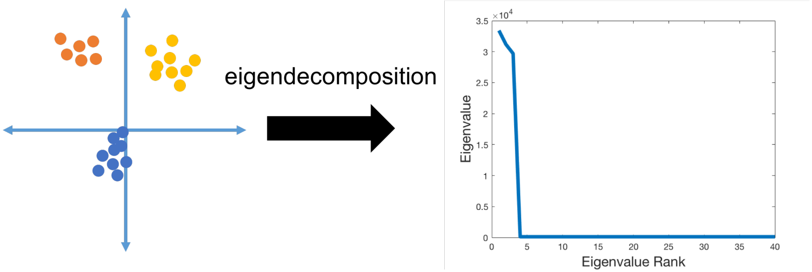

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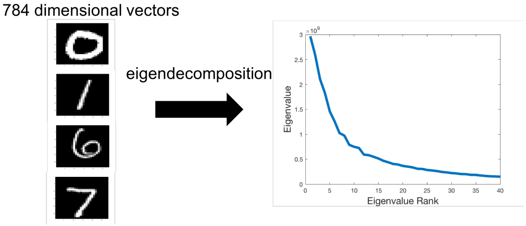

Exercise: Show that the eigenvalues of $\mathbf{X}^T\mathbf{X}$ are always positive. **Hint:** Use that $\lambda_j = \vec{v}_j^T \mathbf{X}^T \mathbf{X} \vec{v}_j$.

SUMMARY

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

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

- 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.

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