COMPSCI 514: Algorithms for Data Science

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University of Massachusetts Amherst. Fall 2022.

Lecture 16

Summary

Last Class: $\underbrace{V^T x_1}_{\mathbb{R}^k} \ldots V^T x_n$

- 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. $X = XVV^T$
- View as low-rank matrix factorization. Introduce concept of low-rank approximation.
- Idea of approximating a data matrix $\mathbf{X}$ with $\mathbf{X}\mathbf{V}\mathbf{V}^T$ when the data points lie close to the subspace spanned by $\mathbf{V}$'s columns.
- 'Dual view' of low-rank approximation: data points that can be approximately reconstructed from a few basis vectors vs. linearly dependent features.

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- 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.
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- 'Dual view' of low-rank approximation: data points that can be approximately reconstructed from a few basis vectors vs. linearly dependent features.

This Class:

- How to find an optimal orthogonal basis $\mathbf{V} \in \mathbb{R}^{d \times k}$ to minimize $\|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2$.

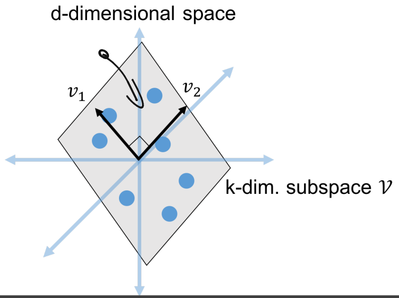
Low-Rank Factorizatoin

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

$$\begin{bmatrix} x_1^T \\ \vdots \\ x_n^T \end{bmatrix}$$

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

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

Low-Rank Approximation

Claim: If $\vec{x}_1, \ldots, \vec{x}_n$ lie 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:

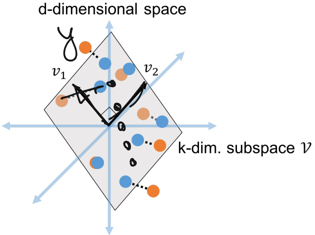
$$\arg\min_{B} f(B)$$

$$\mathbf{X} \approx \mathbf{X}\mathbf{V}\mathbf{V}^T$$

$$\begin{bmatrix} A \end{bmatrix}$$

$$\|A\|_F^2 = \sum_{i=1}^{n} \sum_{j=1}^{d} A_{ij}^2 = \sum_{i=1}^{n} \|a_i\|_2^2$$

$\|a_i\|_2^2$



$$\begin{array}{cc} & k \\ n & \begin{bmatrix} XV \end{bmatrix} \end{array}$$

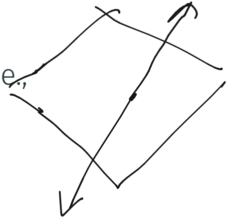
$\mathbf{X}\mathbf{V}\mathbf{V}^T$ has rank k. It is a low-rank approximation of $\mathbf{X}$.

$$\underbrace{\mathbf{X}\mathbf{V}\mathbf{V}^T}_{n \times d} = \underset{\mathbf{B} \text{ with rows in } \mathcal{V}}{\arg\min} \|\mathbf{X} - \mathbf{B}\|_F^2 = \sum_{i,j} (\mathbf{X}_{i,j} - \mathbf{B}_{i,j})^2. = \sum_{i=1}^{n} \|x_i^T - x_i^T V V^T\|_2^2$$

$$\sum_{i=1}^{n} \sum_{j=1}^{d}$$

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

Properties of Projection Matrices



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 $\vec{y} \in \mathbb{R}^d$.

$$V\underbrace{V^T V}_{I} V^T y = VV^T y$$

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).

$$VV^T - V\cancel{V^T V}V^T = 0$$

$[V^T V]_{i,j} = V_i^T V_j$

$$\|a+b\|_2^2 = (a+b)^T(a+b)$$
$$a^Ta + a^Tb + b^Ta + b^Tb$$
$$= \|a\|_2^2 + 2a^Tb + \|b\|_2^2$$

$$a^Tb = \langle a, b \rangle = b^Ta$$

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

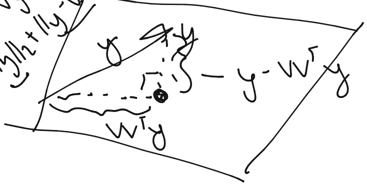
$$\|\vec{y}\|_2^2 = \|(\mathbf{V}\mathbf{V}^T)\vec{y}\|_2^2 + \|\vec{y} - (\mathbf{V}\mathbf{V}^T)\vec{y}\|_2^2.$$

$\boxed{\|VV^T y\|_2 \le \|y\|_2}$

$\|y\|_2 \le \|VV^T y\|_2 + \|y - VV^T y\|$

$\|VV^T y\|_2 \le \|y\|_2 + \|y - VV^T y\|$

$$\underbrace{VV^T}_{d \times d} \underbrace{y}_{d \times 1}$$



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

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

$\|VV^T y\|_2^2 + \|(I - VV^T) y\|_2^2 + 2\langle VV^T y, (I - VV^T) y\rangle$

$y^T \underbrace{VV^T (I - VV^T)}_{=0} y$

$y = Vc$

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 $\mathcal{V}$.

$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: 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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How do we find $\mathcal{V}$ (equivilantly $\mathbf{V}$)?

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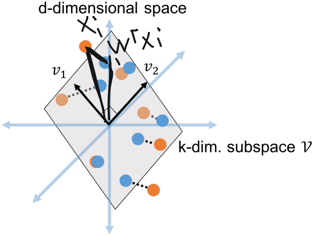
$$\|x_i^T - x_i^T VV^T\|_2^2$$

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

$$\|(I - VV^T)x_i\|_2^2 = \|x_i\|_2^2 - \|VV^T x_i\|_2^2$$



$$X = \begin{bmatrix} x_1^T \\ x_2^T \\ \vdots \\ x_n^T \end{bmatrix}$$

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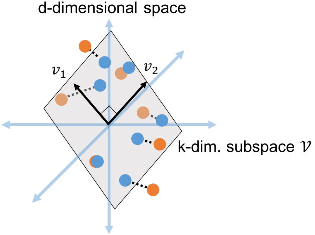
How do we find $\mathcal{V}$ (equivilantly $\mathbf{V}$)?

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

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



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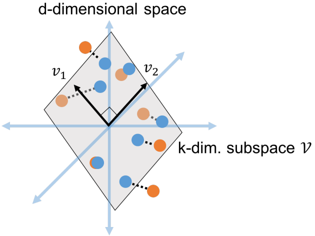
$\|X - XVV^T\|_F^2$ $\qquad$ $\|x_i - VV^T x_i\|_2^2$

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

$\min f(v) = 100 - g(v)$

$\max g(v)$



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

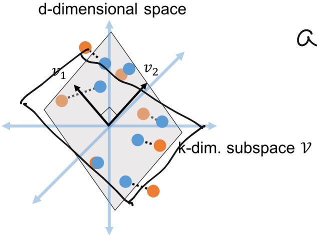
$\|X\|_F^2$ is fixed for any fixed scalar

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

$\|XVV^T\|_F^2$ depends on both X and V

Exercise!

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



$\arg\max_V \|\underbrace{XV}_{n \times k}\|_F^2$

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Solution via Eigendecomposition

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

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

$$\begin{array}{cc} & k \\ n & \begin{bmatrix} Xv_1 & Xv_2 & \cdots & Xv_k \\ & XV & & \end{bmatrix} \end{array}$$

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

Solution via Eigendecomposition

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

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

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

Solution via Eigendecomposition

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

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

$$\begin{array}{cc} & k \\ d & \begin{bmatrix} v_1 \cdots v_k \end{bmatrix} \end{array}$$

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

$$\underline{\vec{v}_1} = \underset{\vec{v} \text{ with } \|v\|_2 = 1}{\arg\max} \|\mathbf{X}\vec{v}\|_2^2. = (Xv)^T Xv = v^T X^T X v$$

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

Solution via Eigendecomposition

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

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

$\|Xv\|_2^2$

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Solution via Eigendecomposition

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

min $\|X - XVV^T\| \Leftrightarrow \max \|XV\|$

$\Leftrightarrow \max \|XV\|_F^2$

XVV^T

$XVV^TV = XV$

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

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

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

$\|Xv\|_2^2 = v^T X^T X v$

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

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

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

$M = X^T X$

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

$$\cdots$$

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

$\vec{v}_1, \ldots, \vec{v}_k$ are the top k eigenvectors of $\mathbf{X}^T\mathbf{X}$ by the *Courant-Fischer Principle.*

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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 $\vec{x}$).

if x is an eigenvector

cx is an eigenvector

$$A(cx) = c \cdot Ax = \lambda \cdot (cx)$$

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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 $\vec{x}$).

- That is, $\mathbf{A}$ just 'stretches' 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 $\vec{x}$).

$(X^TX)^T = X^T(X^T)^T = X^TX$

$A = A^T$ $\quad A_{ij} = A_{ji}$

$A \in \mathbb{R}^{d \times d}$

- 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.

$\text{rank}(X^TX) = k$ $\quad X^TX$

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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$$\mathbf{A}\underline{\mathbf{V}} = \begin{bmatrix} | & | & & | \\ \underbrace{\mathbf{A}\vec{v}_1}_{\lambda_1 v_1} & \underbrace{\mathbf{A}\vec{v}_2} & \cdots & \underbrace{\mathbf{A}\vec{v}_d} \\ | & | & & | \end{bmatrix}$$

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

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$$AV = V\Lambda$$

$$A = A\underbrace{VV^T}_{=I} = \underline{V\Lambda V^T}$$

Review of Eigenvectors and Eigendecomposition

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$V \in \mathbb{R}^{d \times d}$

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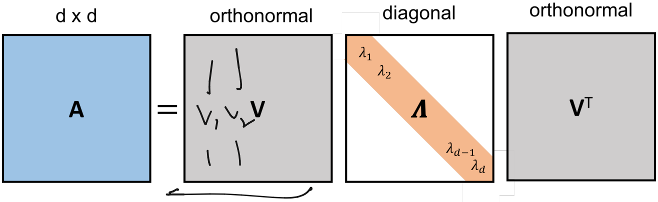
Yields eigendecomposition: $\underline{\mathbf{AVV}^T} = \underline{\mathbf{A}} = \underline{\mathbf{V\Lambda V}^T}$.

VV^T = projection onto subspace spanned by V's columns

Review of Eigenvectors and Eigendecomposition

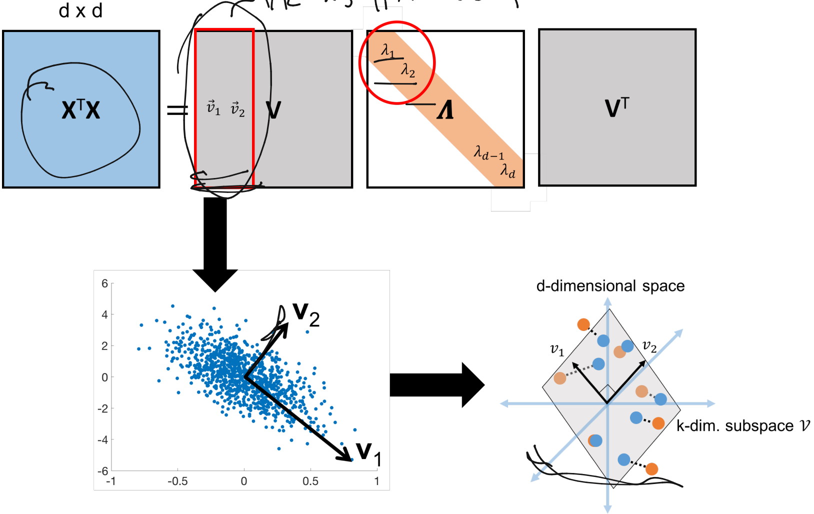
$\min_{V \in \mathbb{R}^{d \times k}} \|X - XVV^T\|_F^2$



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

Low-Rank Approximation via Eigendecomposition

$V_k = \arg\min \|X - XZZ^T\|_F^2$



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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How accurate is this low-rank approximation? Can understand using eigenvalues of $\mathbf{X}^T\mathbf{X}$.

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