COMPSCI 514: Algorithms for Data Science

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University of Massachusetts Amherst. Spring 2026.
Lecture 14

Logistics

- Problem Set 3 due next Friday 4/10 at 11:59pm.
- Quiz due Monday at 8pm.

Summary

Last Class:

- 'Dual view' of low-rank approximation – rows and columns both approximately lie in a low-dimensional subspace.
- Finding an optimal orthogonal basis $\mathbf{V} \in \mathbb{R}^{d \times k}$ to minimize $\|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2$ when the data does not exactly lie in a low-dimensional subspace.
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This Class:

- Wrap up optimal low-rank approximation.
- Singular value decomposition (SVD) and its connection to low-rank approximation.

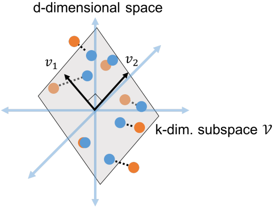
Best Fit Subspace

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 $\mathcal{V}$.

We can find $\mathbf{V}$ by solving the optimization problem:

Projection onto V

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



$\vec{x}_1, \ldots, \vec{x}_n \in \mathbb{R}^d$: data points, $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\vec{v}_1, \ldots, \vec{v}_k \in \mathbb{R}^d$: 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

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

$$\vec{v}_1 = \underset{\vec{v} \text{ with } \|v\|_2 = 1}{\arg\max} \|\mathbf{X}\vec{v}\|_2^2$$

$$\vec{v}_2 = \underset{\vec{v} \text{ with } \|v\|_2 = 1,\ \langle \vec{v}, \vec{v}_1 \rangle = 0}{\arg\max} \|\mathbf{X}\vec{v}\|_2^2$$

$$\cdots$$

$$\vec{v}_k = \underset{\vec{v} \text{ with } \|v\|_2 = 1,\ \langle \vec{v}, \vec{v}_j \rangle = 0\ \forall j < k}{\arg\max} \|\mathbf{X}\vec{v}\|_2^2.$$

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

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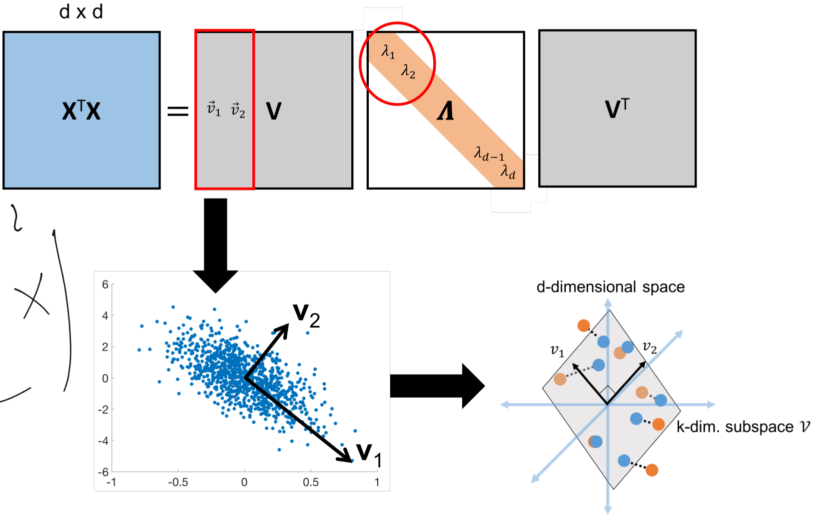
Low-Rank Approximation via Eigendecomposition



Low-Rank Approximation via Eigendecomposition

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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Error of Optimal Low-Rank Approximation:

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

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Error of Optimal Low-Rank Approximation:

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

So plotting the eigenvalue spectrum of $\mathbf{X}^T\mathbf{X}$ shows how compressible $\mathbf{X}$ is using low-rank approximation.

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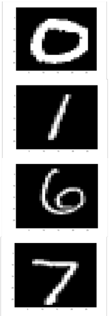
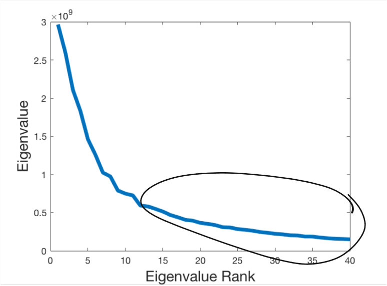
Spectrum Analysis

784 dimensional vectors



eigendecomposition



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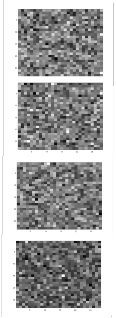

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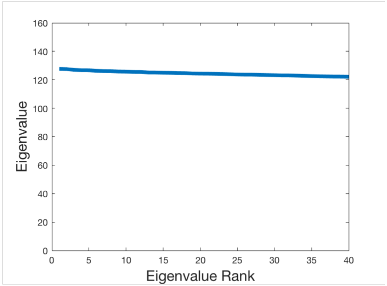

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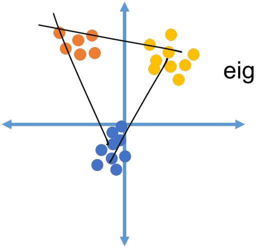

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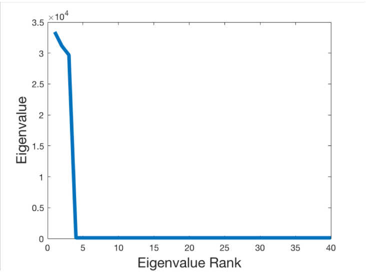

Summary

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

Linear Algebra Proofs/Practice

Prove that $\|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2 = \|\mathbf{X}\|_F^2 - \|\mathbf{X}\mathbf{V}\|_F^2$. → used to calculate $\min \|X - XV_kV_k^T\|_F$

$= \|X\|_F^2 - \|XW^T\|_F^2$

used to convert $\min \|X - XW\|$ to $\max \|XV\|$

$\|A - B\| \neq \|A\| - \|B\|$

$$\|X - XVV^T\|_F^2 = \operatorname{tr}\left((X - XVV^T)(X - XVV^T)^T\right)$$

$$\operatorname{tr}\left((X - XVV^T)(X^T - VV^TX^T)\right)$$

$$\operatorname{tr}\left(XX^T - XVV^TX^T - XVV^TX^T + XV\underbrace{V^TV}_{I}V^TX\right)$$

$$\operatorname{tr}\left(XX^T - XVV^TX^T\right)$$

$$\operatorname{tr}(XX^T) - \operatorname{tr}(XVV^TX^T)$$

$$\|X\|_F^2 - \|XV\|_F^2$$

Use that for any matrix $\mathbf{A}$, $\|\mathbf{A}\|_F^2 = \operatorname{tr}(\mathbf{A}^T\mathbf{A}) = \operatorname{tr}(\mathbf{A}\mathbf{A}^T)$.

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

Some Linear Algebra Practice

Show that for symmetric A, the trace is the sum of eigenvalues: $\operatorname{tr}(\mathsf{A}) = \sum_{i=1}^{n} \lambda_i(\mathsf{A})$. $= \sum A_{ii}$

$\to \|X - XV_k V_k^T\|_F^2 = \sum_{i=k+1}^{n} \lambda_i$

$$\operatorname{tr}(A) = \operatorname{tr}(V \Lambda V^T)$$

$$= \operatorname{tr}(V^T V \Lambda)$$

$$= \operatorname{tr}(\Lambda)$$

$$= \sum_{i=1}^{n} \lambda_i \quad \checkmark$$

$M = V\Lambda$
$N = V^T$

$$\begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{bmatrix}$$

$[m][n] \quad [n][m]$

Use the cyclic property of trace, that for any MN, $\operatorname{tr}(\mathsf{MN}) = \operatorname{tr}(\mathsf{NM})$.

Some Linear Algebra Practice

Show that for any X, the eigenvalues of $X^T X$ are non-negative.

symmetric

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

symmetric matrix A $d \times d$

$\downarrow$

d real eigenvalues

$A = A^T$

$X^T X v = \lambda v$

goal to show: $\lambda \geq 0$

≥ 0

$v^T X^T X v = v^T (\lambda v)$

$= \lambda \cdot \underbrace{v^T v}_{\|v\|_2^2 = 1}$

$0 \leq \|Xv\|_2^2 = \lambda$

Some Linear Algebra Practice

Prove the first step of Courant Fischer: the top eigenvector $\vec{v}_1$ of a matrix $\mathbf{A}$ is given by

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

$V_1 \ldots V_d$ be the eigenvectors of A

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

$$\vec{V} = c_1 \cdot \vec{V}_1 + c_2 \vec{V}_2 \cdots c_d \vec{V}_d$$

$$V^T A V = \left(\sum c_i \vec{v}_i\right)^T A \left(\sum_{i=1}^{d} c_i v_i\right)$$

$$= \sum_{i=1}^{d} c_i v_i^T \sum_{i=1}^{d} A \cdot c_i v_i$$

$$\sum_{i=1}^{d} c_i v_i^T \sum_{i=1}^{d} c_i \lambda_i v_i$$

$$\sum_{i=1}^{d} c_i v_i^T c_i \lambda_i v_i = \sum_{i=1}^{d} c_i^2 \lambda_i$$

$Av_i = \lambda_i v_i$

$c_j v_j^T \cdot c_i \lambda_i v_i$

$c_j c_i \lambda_i \underbrace{v_j^T v_i}_{0}$

$c_1 = 1$

$V = V_1$

Singular Value Decomposition

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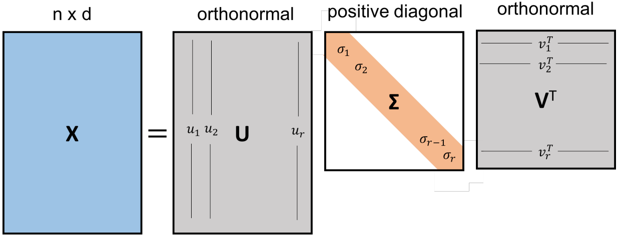
The Singular Value Decomposition (SVD) generalizes the eigendecomposition to asymmetric (even rectangular) matrices.

Singular Value Decomposition

The Singular Value Decomposition (SVD) generalizes the eigendecomposition to asymmetric (even rectangular) matrices. Any matrix $\mathbf{X} \in \mathbb{R}^{n\times d}$ with $\text{rank}(\mathbf{X}) = r$ can be written as $\mathbf{X} = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T$.

- $\mathbf{U}$ has orthonormal columns $\vec{u}_1, \ldots, \vec{u}_r \in \mathbb{R}^n$ (left singular vectors).
- $\mathbf{V}$ has orthonormal columns $\vec{v}_1, \ldots, \vec{v}_r \in \mathbb{R}^d$ (right singular vectors).
- $\boldsymbol{\Sigma}$ is diagonal with elements $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_r > 0$ (singular values).



Connection of the SVD to Eigendecomposition

Writing $\mathbf{X} \in \mathbb{R}^{n \times d}$ in its singular value decomposition $\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$:

$$\mathbf{X}^T\mathbf{X} = (U\Sigma V^T)^T U\Sigma V^T$$

$$= V\Sigma \underbrace{U^T U}_{= I} \Sigma V^T$$

$$= V\Sigma^2 V^T \quad \text{(eigendecomposition of } X^T X\text{)}$$

$$\lambda_i(X^T X) = \sigma_i(X)^2$$

$$XX^T = U\Sigma V^T V \Sigma U^T$$

$$U\Sigma^2 U^T \quad \text{(eigendecomp of } XX^T\text{)}$$

$\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\mathbf{U} \in \mathbb{R}^{n \times \text{rank}(\mathbf{X})}$: matrix with orthonormal columns $\vec{u}_1, \vec{u}_2, \ldots$ (left singular vectors), $\mathbf{V} \in \mathbb{R}^{d \times \text{rank}(\mathbf{X})}$: matrix with orthonormal columns $\vec{v}_1, \vec{v}_2, \ldots$ (right singular vectors), $\mathbf{\Sigma} \in \mathbb{R}^{\text{rank}(\mathbf{X}) \times \text{rank}(\mathbf{X})}$: positive diagonal matrix containing singular values of $\mathbf{X}$.

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Similarly: $\mathbf{X}\mathbf{X}^T = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T\mathbf{V}\boldsymbol{\Sigma}\mathbf{U}^T = \mathbf{U}\boldsymbol{\Sigma}^2\mathbf{U}^T$.

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Similarly: $\mathbf{X}\mathbf{X}^T = \mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T\mathbf{V}\boldsymbol{\Sigma}\mathbf{U}^T = \mathbf{U}\boldsymbol{\Sigma}^2\mathbf{U}^T$.

The left and right singular vectors are the eigenvectors of the covariance matrix $\mathbf{X}^T\mathbf{X}$ and the gram matrix $\mathbf{X}\mathbf{X}^T$ respectively.

$\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\mathbf{U} \in \mathbb{R}^{n \times \text{rank}(\mathbf{X})}$: matrix with orthonormal columns $\vec{u}_1, \vec{u}_2, \ldots$ (left singular vectors), $\mathbf{V} \in \mathbb{R}^{d \times \text{rank}(\mathbf{X})}$: matrix with orthonormal columns $\vec{v}_1, \vec{v}_2, \ldots$ (right singular vectors), $\boldsymbol{\Sigma} \in \mathbb{R}^{\text{rank}(\mathbf{X}) \times \text{rank}(\mathbf{X})}$: positive diagonal matrix containing singular values of $\mathbf{X}$.

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The left and right singular vectors are the eigenvectors of the covariance matrix $\mathbf{X}^T\mathbf{X}$ and the gram matrix $\mathbf{X}\mathbf{X}^T$ respectively.

So, letting $\mathbf{V}_k \in \mathbb{R}^{d \times k}$ have columns equal to $\vec{v}_1, \ldots, \vec{v}_k$, we know that $\mathbf{X}\mathbf{V}_k\mathbf{V}_k^T$ is the best rank-k approximation to $\mathbf{X}$ (given by PCA).

$\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\mathbf{U} \in \mathbb{R}^{n \times \text{rank}(\mathbf{X})}$: matrix with orthonormal columns $\vec{u}_1, \vec{u}_2, \ldots$ (left singular vectors), $\mathbf{V} \in \mathbb{R}^{d \times \text{rank}(\mathbf{X})}$: matrix with orthonormal columns $\vec{v}_1, \vec{v}_2, \ldots$ (right singular vectors), $\boldsymbol{\Sigma} \in \mathbb{R}^{\text{rank}(\mathbf{X}) \times \text{rank}(\mathbf{X})}$: positive diagonal matrix containing singular values of $\mathbf{X}$.

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$$\mathbf{X}^T\mathbf{X} = \mathbf{V}\boldsymbol{\Sigma}\mathbf{U}^T\mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T = \mathbf{V}\boldsymbol{\Sigma}^2\mathbf{V}^T \text{ (the eigendecomposition)}$$ $V \Sigma U^T$

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U_k

The left and right singular vectors are the eigenvectors of the covariance matrix $\mathbf{X}^T\mathbf{X}$ and the gram matrix $\mathbf{X}\mathbf{X}^T$ respectively. $X^T U_k V_k^T$

So, letting $\mathbf{V}_k \in \mathbb{R}^{d \times k}$ have columns equal to $\vec{v}_1, \ldots, \vec{v}_k$, we know that $\mathbf{X}\mathbf{V}_k\mathbf{V}_k^T$ is the best rank-k approximation to $\mathbf{X}$ (given by PCA).

What about $\mathbf{U}_k\mathbf{U}_k^T\mathbf{X}$ where $\mathbf{U}_k \in \mathbb{R}^{n \times k}$ has columns equal to $\vec{u}_1, \ldots, \vec{u}_k$?

$U_k U_k^T X = X V_k V_k^T$ = best rank-k approx

> $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\mathbf{U} \in \mathbb{R}^{n \times \text{rank}(\mathbf{X})}$: matrix with orthonormal columns $\vec{u}_1, \vec{u}_2, \ldots$ (left singular vectors), $\mathbf{V} \in \mathbb{R}^{d \times \text{rank}(\mathbf{X})}$: matrix with orthonormal columns $\vec{v}_1, \vec{v}_2, \ldots$ (right singular vectors), $\boldsymbol{\Sigma} \in \mathbb{R}^{\text{rank}(\mathbf{X}) \times \text{rank}(\mathbf{X})}$: positive diagonal matrix containing singular values of $\mathbf{X}$.

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What about $\mathbf{U}_k\mathbf{U}_k^T\mathbf{X}$ where $\mathbf{U}_k \in \mathbb{R}^{n \times k}$ has columns equal to $\vec{u}_1, \ldots, \vec{u}_k$?
Gives exactly the same approximation!

> $\mathbf{X} \in \mathbb{R}^{n \times d}$: data matrix, $\mathbf{U} \in \mathbb{R}^{n \times \text{rank}(\mathbf{X})}$: matrix with orthonormal columns $\vec{u}_1, \vec{u}_2, \ldots$ (left singular vectors), $\mathbf{V} \in \mathbb{R}^{d \times \text{rank}(\mathbf{X})}$: matrix with orthonormal columns $\vec{v}_1, \vec{v}_2, \ldots$ (right singular vectors), $\mathbf{\Sigma} \in \mathbb{R}^{\text{rank}(\mathbf{X}) \times \text{rank}(\mathbf{X})}$: positive diagonal matrix containing singular values of $\mathbf{X}$.

The SVD and Optimal Low-Rank Approximation

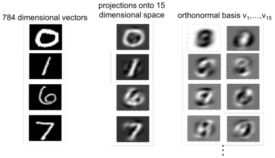
The best low-rank approximation to $\mathbf{X}$:

$\mathbf{X}_k = \arg\min_{\text{rank}-k\ \mathbf{B} \in \mathbb{R}^{n \times d}} \|\mathbf{X} - \mathbf{B}\|_F$ is given by:

$$\mathbf{X}_k = \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T = \mathbf{U}_k\mathbf{U}_k^T\mathbf{X}$$

Correspond to projecting the rows (data points) onto the span of $\mathbf{V}_k$ or the columns (features) onto the span of $\mathbf{U}_k$

Row (data point) compression



Column (feature) compression

10000* bathrooms+ 10* (sq. ft.) ≈ 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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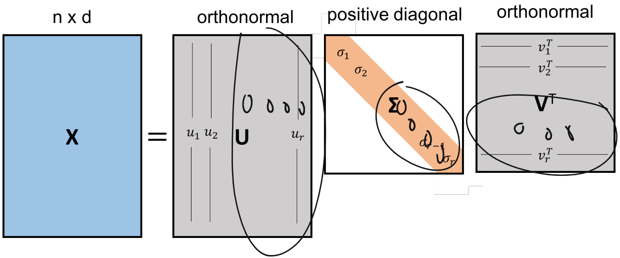

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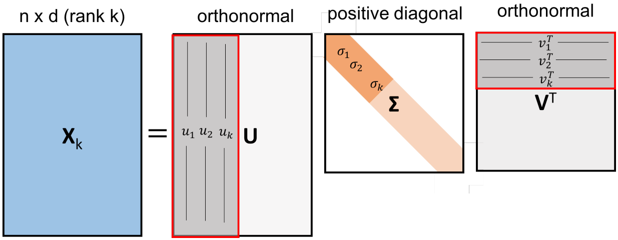

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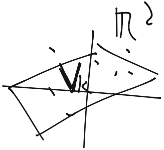
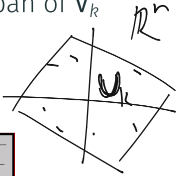
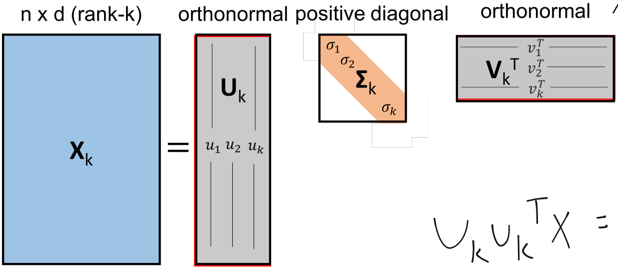


Correspond to projecting the rows (data points) onto the span of $\mathbf{V}_k$ or the columns (features) onto the span of $\mathbf{U}_k$





$U_k U_k^T X = X V_k V_k^T$

X symmetric

$V \Lambda V^T$

$U \Sigma V^T$

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I'll show analogous

Want to prove $A = B$
$CA = CB$

$$XV_kV_k^T = U_k\Sigma_kV_k^T$$

$$U\Sigma \underbrace{V^TV_k}V_k^T \quad k<r \quad = U\begin{bmatrix}\sigma_1 & & \\ & \ddots & \\ & & \sigma_r\end{bmatrix}\begin{bmatrix} I \\ \cdots \\ 0\end{bmatrix} V_k^T$$

$$\begin{bmatrix} v_1^T \\ \vdots \\ v_r^T\end{bmatrix}\begin{bmatrix} v_1 \cdots v_k\end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \\ 0 & \end{bmatrix} \quad = U\begin{bmatrix}\Sigma_k \\ \cdots \\ 0\end{bmatrix} V_k^T$$

— first k-columns of Σ

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$$\mathbf{X}_k = \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T = \mathbf{U}_k\mathbf{U}_k^T\mathbf{X} = \mathbf{U}_k\mathbf{\Sigma}_k\mathbf{V}_k^T$$

$$XV_kV_k^T = \begin{bmatrix} | & & & | \\ U & & & \\ u_1 & \cdots & u_k & u_r \\ | & & & | \end{bmatrix} \overset{\Sigma_k}{\begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_k \\ & \ddots & \\ & 0 & \end{bmatrix}} \begin{bmatrix} V_k^T \end{bmatrix}$$

$$= U_k \Sigma_k V_k^T$$

$\mathbf{X} \in \mathbb{R}^{n\times d}$: data matrix, $\mathbf{U} \in \mathbb{R}^{n\times \text{rank}(\mathbf{X})}$: matrix with orthonormal columns $\vec{u}_1, \vec{u}_2, \ldots$ (left singular vectors), $\mathbf{V} \in \mathbb{R}^{d\times \text{rank}(\mathbf{X})}$: matrix with orthonormal columns $\vec{v}_1, \vec{v}_2, \ldots$ (right singular vectors), $\mathbf{\Sigma} \in \mathbb{R}^{\text{rank}(\mathbf{X})\times\text{rank}(\mathbf{X})}$: positive diagonal matrix containing singular values of $\mathbf{X}$.

SVD Review

- Every $\mathbf{X} \in \mathbb{R}^{n \times d}$ can be written in its SVD as $\mathbf{U}\boldsymbol{\Sigma}\mathbf{V}^T$.
- $\mathbf{U} \in \mathbb{R}^{n \times r}$ (orthonormal) contains the eigenvectors of $\mathbf{X}\mathbf{X}^T$.
  $\mathbf{V} \in \mathbb{R}^{d \times r}$ (orthonormal) contains the eigenvectors of $\mathbf{X}^{\mathsf{T}}\mathbf{X}$.
  $\boldsymbol{\Sigma} \in \mathbb{R}^{r \times r}$ (diagonal) contains square roots of their eigenvalues. = singular values of X
- $\mathbf{U}_k\mathbf{U}_k^T\mathbf{X} = \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T = \mathbf{U}_k\boldsymbol{\Sigma}_k\mathbf{V}_k^T = \underset{\mathbf{B} \text{ s.t. } \operatorname{rank}(\mathbf{B}) \leq k}{\arg\min} \|\mathbf{X} - \mathbf{B}\|_F$.