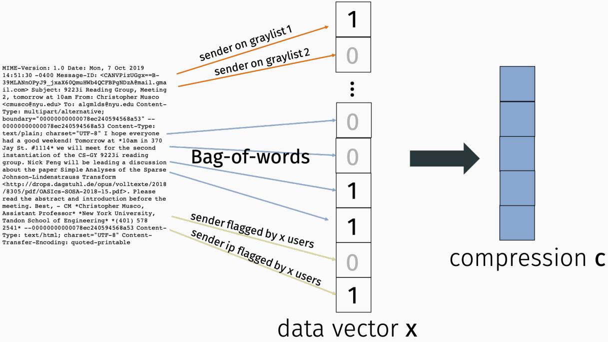
CS-GY 9223 D: Lecture 9
Low-rank approximation and singular value decomposition

NYU Tandon School of Engineering, Prof. Christopher Musco

Return to data compression:



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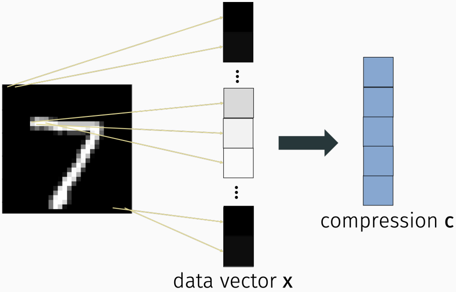
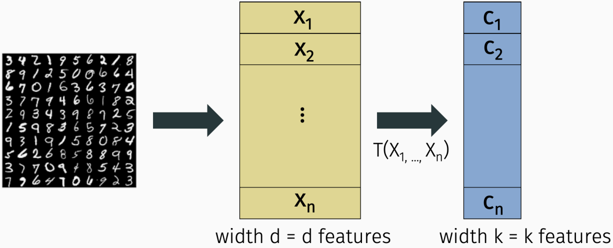


Main difference from randomized methods:

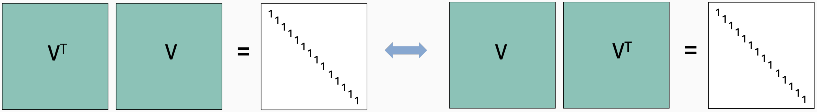


In this section, we will discuss data dependent transformations. Johnson-Lindenstrauss, MinHash, SimHash were all data oblivious.

Advantages of data independent methods:

Advantages of data dependent methods:

If a square matrix has orthonormal rows, it also have orthonormal columns:



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

Implies that for any vector $\mathbf{x}$, $\|\mathbf{V}\mathbf{x}\|_2^2 = \|\mathbf{x}\|_2^2$ and $\|\mathbf{V}^T\mathbf{x}\|_2^2$.

Equivalently, any vector $\mathbf{x}$, $\|\mathbf{x}^T\mathbf{V}^T\|_2^2 = \|\mathbf{x}\|_2^2$ and $\|\mathbf{x}^T\mathbf{V}\|_2^2 = \|\mathbf{x}\|_2^2$.

Same thing goes for Frobenius norm: for any matrix $\mathbf{X}$, $\|\mathbf{V}\mathbf{X}\|_F^2 = \|\mathbf{X}\|_F^2$ and $\|\mathbf{V}^T\mathbf{X}\|_F^2 = \|\mathbf{X}\|_F^2$.

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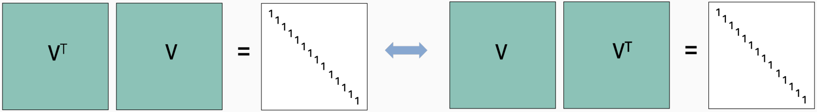

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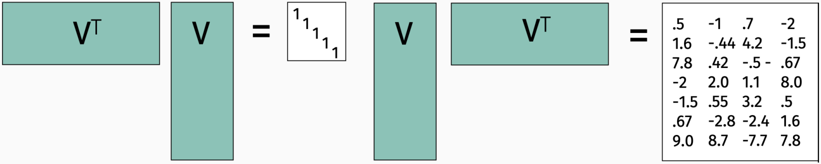
The same is not true for rectangular matrices:

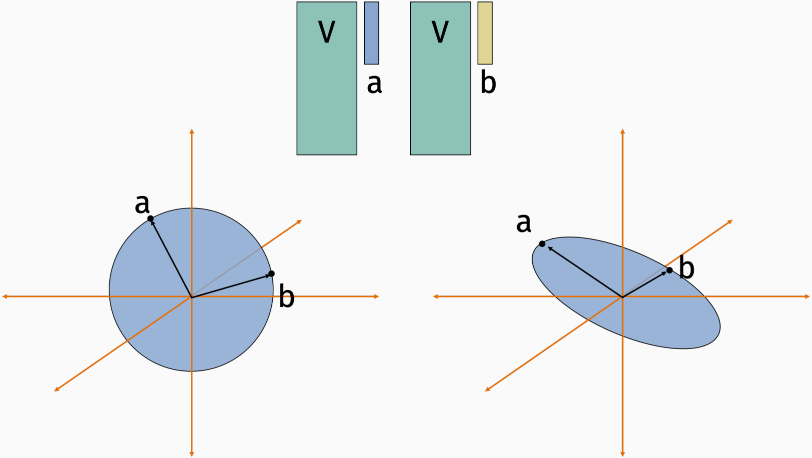


$\mathbf{V}^T\mathbf{V} = \mathbf{I}$ but $\mathbf{V}\mathbf{V}^T \neq \mathbf{I}$

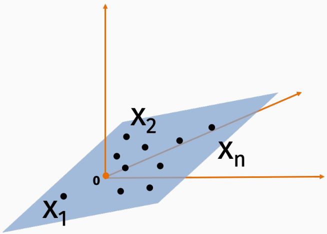
For any $\mathbf{x}$, $\|\mathbf{V}\mathbf{x}\|_2^2 = \|\mathbf{x}\|_2^2$ but $\|\mathbf{V}^T\mathbf{x}\|_2^2 \neq \|\mathbf{x}\|_2^2$ in general.

Equivalently, $\mathbf{x}$, $\|\mathbf{x}^T\mathbf{V}^T\|_2^2 = \|\mathbf{x}\|_2^2$ but $\|\mathbf{x}^T\mathbf{V}\|_2^2 \neq \|\mathbf{x}\|_2^2$ in general.

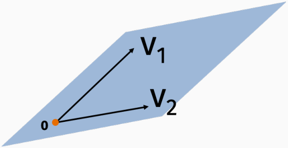
Multiplying a vector by **V** with orthonormal columns rotates and/or reflects the vector.



Suppose $\mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^d$ lie on a low-dimensional subspace S through the origin. I.e. our data set is rank k for $k < d$.



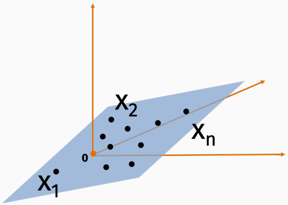
Let $\mathbf{v}_1, \ldots, \mathbf{v}_k$ be orthogonal unit vectors spanning S.

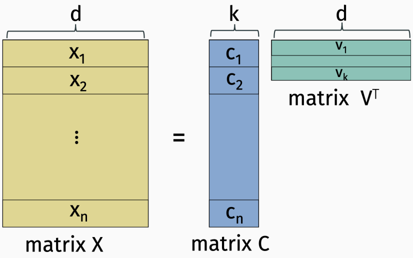


For all i, we can write:

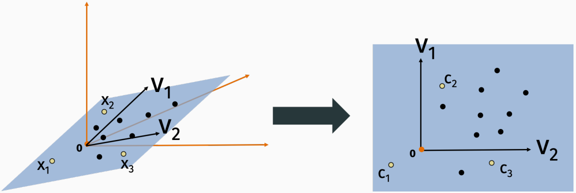
$$\mathbf{x}_i = c_{i,1}\mathbf{v}_1 + \ldots + c_{i,k}\mathbf{v}_k.$$

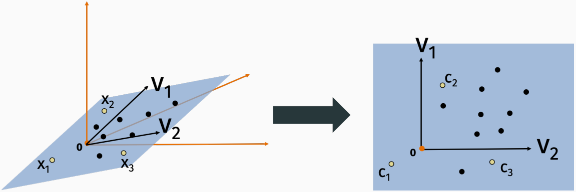
LOW-RANK DATA





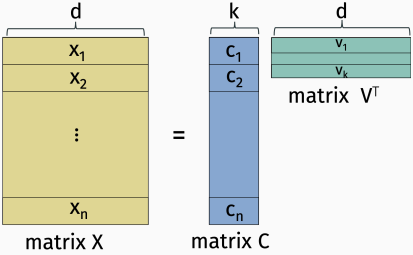
What are $\mathbf{c}_1, \ldots, \mathbf{c}_n$?





Lots of information preserved:

- $\|\mathbf{x}_i - \mathbf{x}_j\|_2 = \|\mathbf{c}_i - \mathbf{c}_j\|_2$ for all i, j.
- $\mathbf{x}_i^T \mathbf{x}_j = \mathbf{c}_i^T \mathbf{c}_j$ for all i, j.
- Norms preserved, linear separability preserved, $\min \|\mathbf{X}\mathbf{y} - \mathbf{b}\| = \min \|\mathbf{C}\mathbf{z} - \mathbf{b}\|$, etc., etc.



Formally, $C = XV^T$:

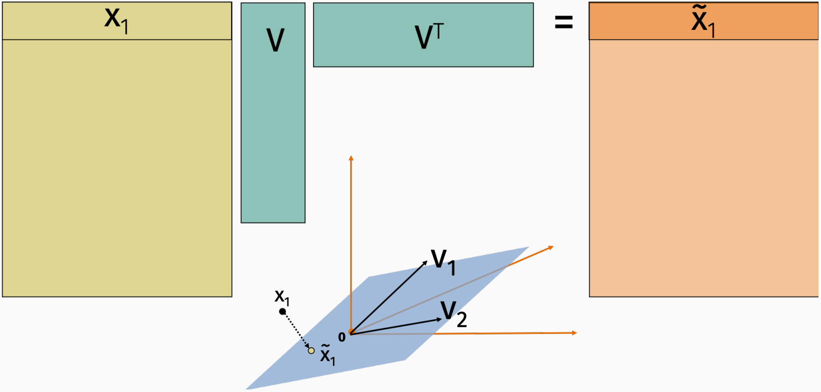
$$X = CV^T \Rightarrow XV = CV^T V$$

Since V's columns are an orthonormal basis, $V^T V = I$.

So $X = XVV^T$.

PROJECTION MATRICES

VV^T is a symmetric projection matrix.



When all data points already lie in the subspace spanned by V's columns, projection doesn't do anything. So $X = XVV^T$.

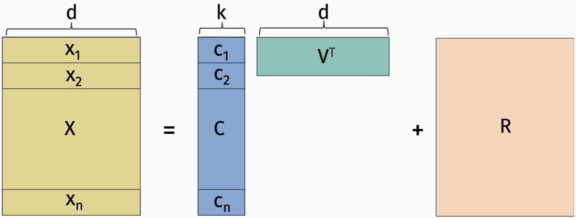
When X's rows lie close to a k dimensional subspace, we can still approximate

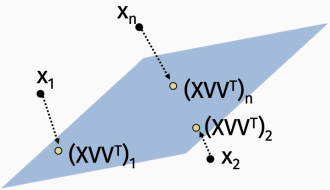
$$\mathbf{X} \approx \mathbf{X}\mathbf{V}\mathbf{V}^T.$$

$\mathbf{X}\mathbf{V}\mathbf{V}^T$ is a low-rank approximation for $\mathbf{X}$.

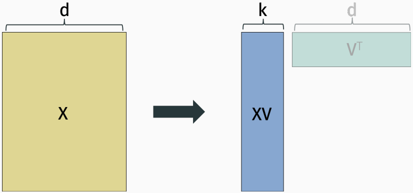
For a given subspace $\mathcal{V}$ spanned by the columns in $\mathbf{V}$,

$$\mathbf{X}\mathbf{V}\mathbf{V}^T = \arg\min_{\mathbf{C}} \|\mathbf{X} - \mathbf{C}\mathbf{V}^T\|_F^2 = \sum_{i,j} (\mathbf{X}_{i,j} - (\mathbf{C}\mathbf{V}^T)_{i,j})^2.$$





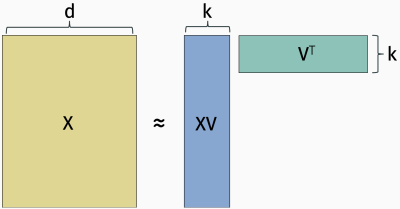
$$\|\mathbf{x}_i - \mathbf{x}_j\|_2 \approx \|(\mathbf{X}\mathbf{V}\mathbf{V}^T)_i - (\mathbf{X}\mathbf{V}\mathbf{V}^T)_j\|_2 = \|(\mathbf{X}\mathbf{V}^T)_i - (\mathbf{X}\mathbf{V}^T)_j\|_2$$



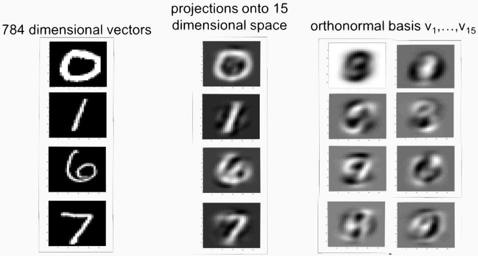
$\mathbf{XV}$ can be used as a compressed version of data matrix $\mathbf{X}$.

WHY IS DATA APPROXIMATELY LOW-RANK?

Rows of $\mathbf{X}$ (data points) are approximately spanned by k vectors. Columns of $\mathbf{X}$ (data features) are approximately spanned by k vectors.



If a data set only had k unique data points, it would be exactly rank k. If it has k "clusters" of data points (e.g. the 10 digits) it's often very close to rank k.

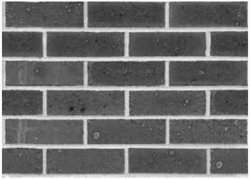


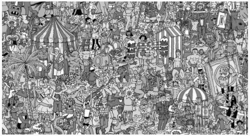
Colinearity/correlation of data features leads to a low-rank data matrix.

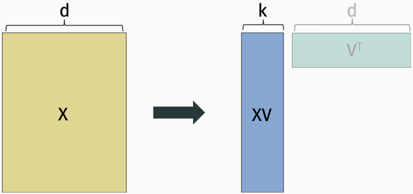
	bedrooms	bathrooms	sq.ft.	floors	list price	sale price
home 1	2	2	1800	2	200,000	195,000
home 2	4	2.5	2700	1	300,000	310,000
⋮	⋮	⋮	⋮	⋮	⋮	⋮
home n	5	3.5	3600	3	450,000	450,000

OTHER REASONS FOR LOW-RANK STRUCTURE

When encoded as a matrix, which image has lower approximate rank?



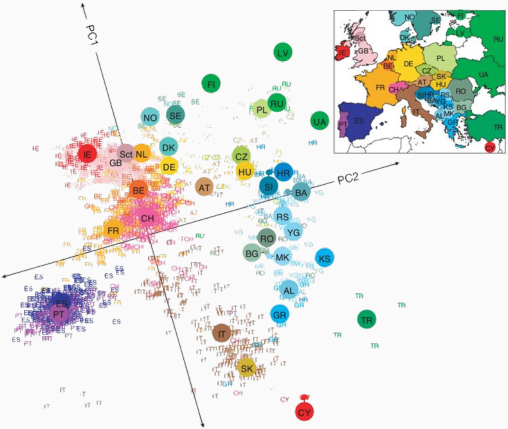




- $\mathbf{XV} \cdot \mathbf{V}^T$ takes $O(k(n+d))$ space to store instead of $O(nd)$.
- Regression problems involving $\mathbf{XV} \cdot \mathbf{V}^T$ can be solved in $O(nk^2)$ instead of $O(nd^2)$ time.
- $\mathbf{XV}$ can be used for visualization when $k = 2, 3$.

APPLICATIONS OF LOW-RANK APPROXIMATION

"Genes Mirror Geography Within Europe" – Nature, 2008.



Each data vector $\mathbf{x}_i$ contains genetic information for one person in Europe. Set $k = 2$ and plot $(XV)_i$ for each i on a 2-d plane. Color points by what country they are from.

Given a subspace $\mathcal{V}$ spanned by the k columns in $\mathbf{V}$,

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

We want to find the best $\mathbf{V} \in \mathbb{R}^{d \times k}$:

$$\min_{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}} \|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2 \tag{1}$$

Note that $\|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2 = \|\mathbf{X}\|_F^2 - \|\mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2$ for all orthonormal $\mathbf{V}$ (since $\mathbf{V}\mathbf{V}^T$ is a projection). Equivalent form:

$$\max_{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}} \|\mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2 = \|\mathbf{X}\mathbf{V}\|_F^2 \tag{2}$$

If $k = 1$, want to find a single vector $\mathbf{v}_1$ which maximizes:

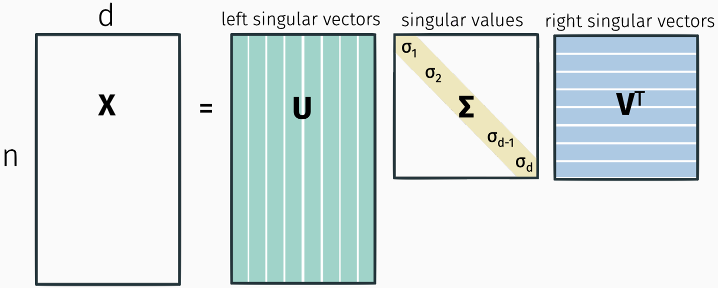
$$\|\mathbf{X}\mathbf{v}_1\mathbf{v}_1^T\|_F^2 = \|\mathbf{X}\mathbf{v}_1\|_F^2 = \|\mathbf{X}\mathbf{v}_1\|_2^2 = \mathbf{v}_1^T\mathbf{X}^T\mathbf{X}\mathbf{v}_1.$$

Choose $\mathbf{v}_1$ to be the top eigenvector of $\mathbf{X}^T\mathbf{X}$.

What about higher k?

One-stop shop for computing optimal low-rank approximations.

Any matrix X can be written:



Where $\mathbf{U}^T\mathbf{U} = \mathbf{I}$, $\mathbf{V}^T\mathbf{V} = \mathbf{I}$, and $\sigma_1 \geq \sigma_2 \geq \ldots \sigma_d \geq 0$.

Note that $\sum_{i=1}^{d} \sigma_i^2 = \|\mathbf{X}\|_F^2$.

CONNECTION TO EIGENDECOMPOSITION

- $\mathbf{V}_k$'s columns are called the "top right singular vectors of $\mathbf{X}$"
- $\mathbf{U}_k$'s columns are called the "top left singular vectors of $\mathbf{X}$"
- $\sigma_1, \ldots, \sigma_k$ are the "top singular values". $\sigma_1, \ldots, \sigma_d$ are sometimes called the "spectrum of $\mathbf{X}$" (although this is more typically used to refer to eigenvalues).

- $\mathbf{U}$ contains the orthonormal eigenvectors of $\mathbf{X}\mathbf{X}^T$.
- $\mathbf{V}$ contains the orthonormal eigenvectors of $\mathbf{X}^T\mathbf{X}$.
- $\sigma_i^2 = \lambda_i(\mathbf{X}\mathbf{X}^T) = \lambda_i(\mathbf{X}^T\mathbf{X})$

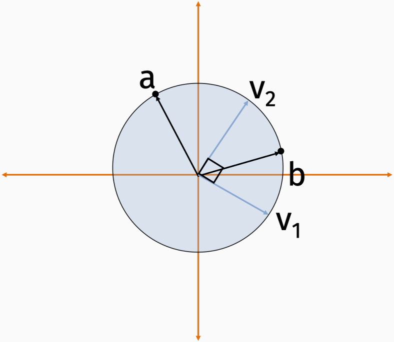
Exercise: Check this can be checked directly.

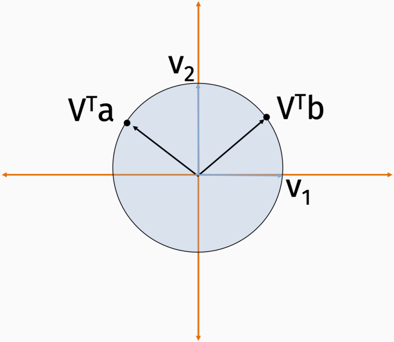
Important take away from singular value decomposition.

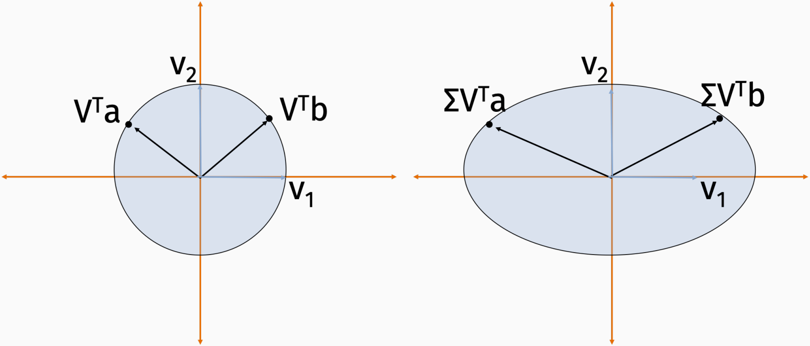
Multiplying any vector $\mathbf{a}$ by a matrix $\mathbf{X}$ to form $\mathbf{X}\mathbf{a}$ can be viewed as a composition of 3 operations:

1. Rotate/reflect the vector (multiplication by to $\mathbf{V}^T$).
2. Scale the coordinates (multiplication by $\mathbf{\Sigma}$.
3. Rotate/reflect the vector again (multiplication by $\mathbf{U}$).

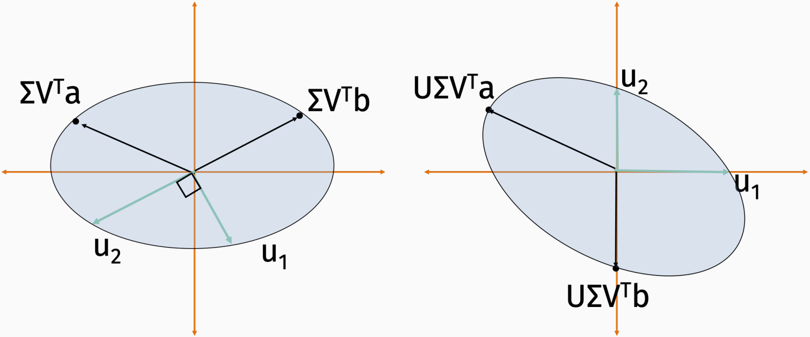
SINGULAR VALUE DECOMPOSITION: ROTATE/REFLECT

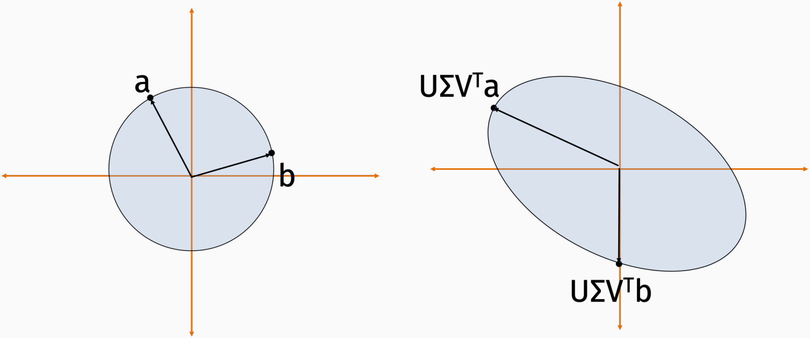




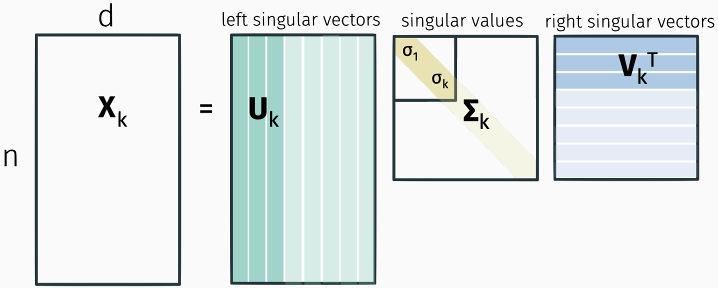

V2
VTa
VTb
V1
V2
ΣVTa
ΣVTb
V1

SINGULAR VALUE DECOMPOSITION: ROTATE/REFLECT




a
b
UΣV^Ta
UΣV^Tb

Can read off optimal low-rank approximations from the SVD:

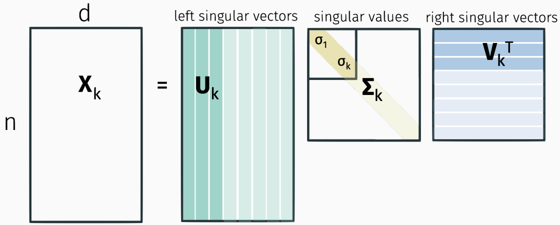


$$\mathbf{X}_k = \mathbf{U}_k \mathbf{\Sigma}_k \mathbf{V}_k^T = \mathbf{U}_k \mathbf{U}_k^T \mathbf{X} = \mathbf{X} \mathbf{V}_k \mathbf{V}_k^T.$$

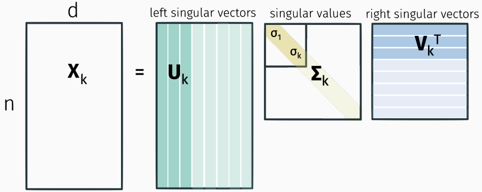
$$\mathbf{V}_k = \underset{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}}{\arg\min} \|\mathbf{X} - \mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2 = \underset{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}}{\arg\max} \|\mathbf{X}\mathbf{V}\mathbf{V}^T\|_F^2$$

Connection to Principal Component Analysis:

- Let $\bar{\mathbf{X}} = \mathbf{X} - \mathbf{1}\boldsymbol{\mu}^T$ where $\boldsymbol{\mu} = \frac{1}{n}\sum_{i=1}^{n}\mathbf{x}_i$. I.e. $\bar{\mathbf{X}}$ is obtained by mean centering $\mathbf{X}$'s rows.
- Let $\bar{\mathbf{U}}\bar{\boldsymbol{\Sigma}}\bar{\mathbf{V}}^T$ be the SVD of $\bar{\mathbf{X}}$. $\bar{\mathbf{U}}$'s first columns are the "top principal components" of $\mathbf{X}$. $\mathbf{V}$'s first columns are the "weight vectors" for these principal components.



Observation 1: The optimal compression XV_k has orthogonal columns.



Observation 2: The optimal low-rank approximation error $E_k = \|\mathbf{X} - \mathbf{X}\mathbf{V}_k\mathbf{V}_k^T\|_F^2 = \|\mathbf{X}\|_F^2 - \|\mathbf{X}\mathbf{V}_k\mathbf{V}_k^T\|_F^2$ can be written:

$$E_k = \sum_{i=k+1}^{d} \sigma_i^2.$$

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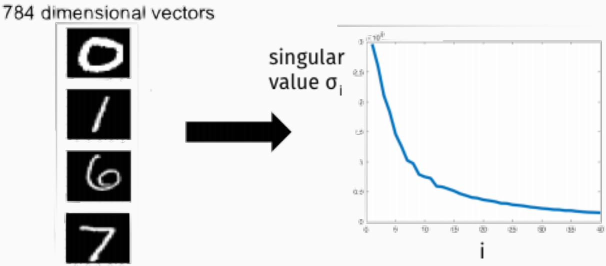
Can immediately get a sense of “how low-rank” a matrix is from it’s spectrum:



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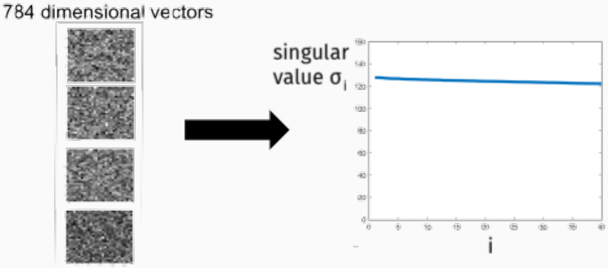

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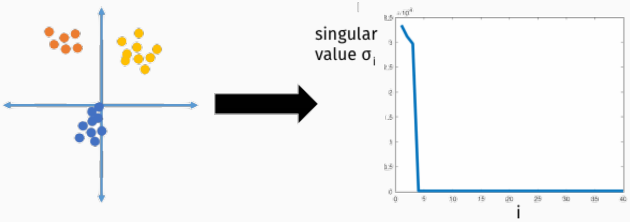


Suffices to compute right singular vectors $\mathbf{V}$:

- Compute $\mathbf{X}^T\mathbf{X}$.
- Find eigendecomposition $\mathbf{V}\mathbf{\Lambda}\mathbf{V}^T = \mathbf{X}^T\mathbf{X}$.
- Compute $\mathbf{L} = \mathbf{X}\mathbf{V}$. Set $\sigma_i = \|\mathbf{L}_i\|_2$ and $\mathbf{U}_i = \mathbf{L}_i / \|\mathbf{L}_i\|_2$.

Total runtime $\approx$

- Compute approximate solution.
- Only compute top k singular vectors/values. Runtime will depend on k. When $k = d$ we can't do any better than classical algorithms based on eigendecomposition.
- Iterative algorithms achieve runtime $\approx O(ndk)$ vs. $O(nd^2)$ time.
  - **Krylov subspace methods** like the Lanczos method are most commonly used in practice.
  - **Power method** is the simplest Krylov subspace method, and still works very well.

What we won't discuss today: sketching methods and stochastic methods (which are faster in some settings).

Today: What about when $k = 1$?

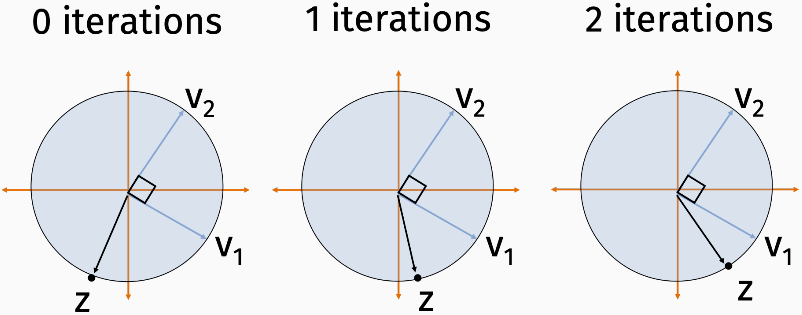
Goal: Find some $\mathbf{z} \approx \mathbf{v}_1$.

Input: $\mathbf{X} \in \mathbb{R}^{n \times d}$ with SVD $\mathbf{U\Sigma V}^T$.

Power method:

- Choose $\mathbf{z}^{(0)}$ randomly. E.g. $\mathbf{z}_0 \sim \mathcal{N}(0, 1)$.
- $\mathbf{z}^{(0)} = \mathbf{z}^{(0)}/\|\mathbf{z}^{(0)}\|_2$
- For $i = 1, \ldots, T$
    - $\mathbf{z}^{(i)} = \mathbf{X}^T \cdot (\mathbf{X}\mathbf{z}^{(i-1)})$
    - $n_i = \|\mathbf{z}^{(i)}\|_2$
    - $\mathbf{z}^{(i)} = \mathbf{z}^{(i)}/n_i$

  Return $\mathbf{z}^{(T)}$


0 iterations
1 iterations
2 iterations
v_2
v_1
z

Theorem (Basic Power Method Convergence)

Let $\gamma = \frac{\sigma_1 - \sigma_2}{\sigma_1}$ be parameter capturing the "gap" between the first and second largest singular values. If Power Method is initialized with a random Gaussian vector then, with high probability, after $T = O\left(\frac{\log d/\epsilon}{\gamma}\right)$ steps, we have either:

$$\|\mathbf{v}_1 - \mathbf{z}^{(T)}\|_2 \leq \epsilon \qquad \text{or} \qquad \|\mathbf{v}_1 - (-\mathbf{z}^{(T)})\|_2 \leq \epsilon.$$

Total runtime: $O\left(nd \cdot \frac{\log d/\epsilon}{\gamma}\right)$

Write $\mathbf{z}^{(i)}$ in the right singular vector basis:

$$
\begin{aligned}
\mathbf{z}^{(0)} &= c_1^{(0)}\mathbf{v}_1 + c_2^{(0)}\mathbf{v}_2 + \ldots + c_d^{(0)}\mathbf{v}_d \\
\mathbf{z}^{(1)} &= c_1^{(1)}\mathbf{v}_1 + c_2^{(1)}\mathbf{v}_2 + \ldots + c_d^{(1)}\mathbf{v}_d \\
&\vdots \\
\mathbf{z}^{(i)} &= c_1^{(i)}\mathbf{v}_1 + c_2^{(i)}\mathbf{v}_2 + \ldots + c_d^{(i)}\mathbf{v}_d
\end{aligned}
$$

Note: $[c_1^{(i)}, \ldots, c_d^{(i)}] = \mathbf{c}^{(i)} = \mathbf{V}^T\mathbf{z}^{(i)}$.

Also: $\sum_{j=1}^{d} \left(c_j^{(i)}\right)^2 = 1$.

Claim: After update $\mathbf{z}^{(i)} = \mathbf{X}^T\mathbf{X}\mathbf{z}^{(i-1)}$,

$$c_j^{(i)} = \sigma_j^2 c_j^{(i-1)}$$

$$\mathbf{z}^{(i)} = \frac{1}{n_1}\left[c_1^{(i-1)}\sigma_1^2 \cdot \mathbf{v}_1 + c_2^{(i-1)}\sigma_2^2 \cdot \mathbf{v}_2 + \ldots + c_d^{(i-1)}\sigma_d^2 \cdot \mathbf{v}_d\right]$$

Claim: After T updates:

$$\mathbf{z}^{(T)} = \frac{1}{\prod_{i=1}^{T} n_i}\left[c_1^{(0)}\sigma_1^{2T}\cdot\mathbf{v}_1 + c_2^{(0)}\sigma_2^{2T}\cdot\mathbf{v}_2 + \ldots + c_d^{(0)}\sigma_d^{2T}\cdot\mathbf{v}_d\right]$$

Let $\alpha_j = \frac{1}{\prod_{i=1}^{T} n_i} c_j^{(0)}\sigma_j^{2T}$. **Goal:** Show that $\alpha_j \ll \alpha_1$ for all $j \neq 1$.

Since $\mathbf{z}^{(T)}$ is a unit vector, $\sum_{i=1}^{d} \alpha_i^2 = 1$. So $\alpha_1 \leq 1$.

If we can prove that $\frac{\alpha_j}{\alpha_1} \leq \sqrt{\frac{\epsilon}{d}}$ then:

$$\alpha_1^2 \geq 1 - d \cdot \left(\sqrt{\frac{\epsilon}{d}}\right)^2 \implies |\alpha_1| \geq 1 - \epsilon$$

$$\|\mathbf{v}_1 - \mathbf{z}^{(T)}\|_2 = 2 - 2\langle \mathbf{v}_1, \mathbf{z}^{(T)} \rangle \leq 2\epsilon$$

Lets proves that $\frac{\alpha_j}{\alpha_1} \leq \sqrt{\frac{\epsilon}{d}}$ where $\alpha_j = \frac{1}{\prod_{i=1}^{T} n_i} c_j^{(0)} \sigma_j^{2T}$

First observation: Starting coefficients are all roughly equal.

For all j $$O(1/d^3) \leq c_j^{(0)} \leq 1$$

with probability $1 - \frac{1}{d}$. This is a very loose bound, but it's all that we will need. **Prove at home.**

$$\frac{\alpha_j}{\alpha_1} = \frac{\sigma_j^{2T}}{\sigma_1^{2T}} \cdot \frac{c_j^{(0)}}{c_1^{(0)}} \leq$$

Need $T =$

Theorem (Gapless Power Method Convergence)

If Power Method is initialized with a random Gaussian vector then, with high probability, after $T = O\left(\frac{\log d/\epsilon}{\epsilon}\right)$ *steps, we obtain a* $\mathbf{z}$ *satisfying:*

$$\|\mathbf{X} - \mathbf{X}\mathbf{z}\mathbf{z}^T\|_F^2 \leq (1+\epsilon)\|\mathbf{X} - \mathbf{X}\mathbf{v}_1\mathbf{v}_1^T\|_F^2$$

- Block Power Method aka Simultaneous Iteration aka Subspace Iteration aka Orthogonal Iteration

Power method:

- Choose $\mathbf{G} \in \mathbb{R}^{d \times k}$ be a random Gaussian matrix.
- $\mathbf{Z}_0 = \text{orth}(\mathbf{G})$.
- For $i = 1, \ldots, T$
    - $\mathbf{Z}^{(i)} = \mathbf{X}^T \cdot (\mathbf{X}\mathbf{z}^{(i-1)})$
    - $\mathbf{Z}^{(i)} = \text{orth}(\mathbf{z}^{(i)})$

  Return $\mathbf{Z}^{(T)}$

Runtime: $O\left(\frac{\log d/\epsilon}{\epsilon}\right)$ iterations to obtain a nearly optimal low-rank approximation:

$$\|\mathbf{A} - \mathbf{A}\mathbf{Z}\mathbf{Z}^T\|_F^2 \leq (1+\epsilon)\|\mathbf{A} - \mathbf{A}\mathbf{V_k}\mathbf{V_k}^T\|_F^2.$$