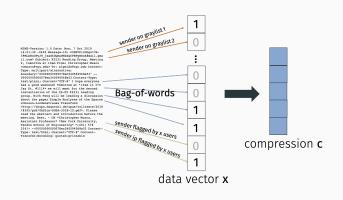
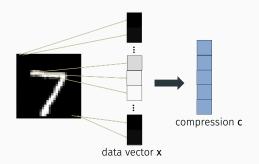
CS-GY 9223 D: Lecture 9 Low-rank approximation and singular value decomposition

NYU Tandon School of Engineering, Prof. Christopher Musco

Return to data compression:

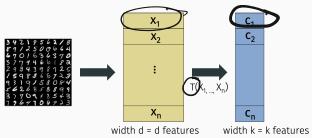


Return to data compression:



Main difference from randomized methods:





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

Advantages of data independent methods:

- less compristional cost
- earl to analyze, clean + Jeneral bounds
- none easily distributed + streams

Advantages of data dependent methods:

- better compression, in practice
- don't ux roud owness
- mon voter patable.

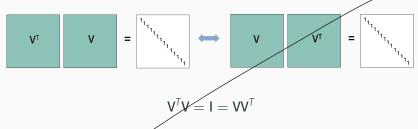
If a square matrix has orthonormal rows, it also have orthonormal columns:



Same thing goes for Frobenius norm: for any matrix \mathbf{X} ,

$$\begin{split} \|VX\|_F^2 &= \|X\|_F^2 \text{ and } \|V^TX\|_F^2 = \|X\|_F^2. \\ &\nearrow \|X_1\|_F^2 + \|X_2\|_F^2 + \dots \|X_N\|_F^2 = \|X\|_F^2. \\ &= \|V_{X_1}\|_F^2 + \|V_{X_2}\|_F^2 + \dots \|V_{X_N}\|_F^2 \quad \text{where} \quad X_1 &\text{ is it column of } 6 \end{split}$$

If a <u>square</u> matrix has orthonormal rows, it also have orthonormal columns:



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

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 X, $\|\mathbf{V}\mathbf{X}\|_F^2 = \|\mathbf{X}\|_F^2$ and $\|\mathbf{V}^T\mathbf{X}\|_F^2 = \|\mathbf{X}\|_F^2$.

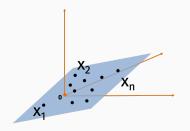
The same is <u>not true</u> for rectangular matrices:

VT V =
$$\begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix}$$
 V VT = $\begin{bmatrix} .5 & -1 & .7 & -2 \\ 1.6 & -.44 & 4.2 & -1.5 \\ 7.8 & .42 & -5. & -67 \\ -2 & 2.0 & 1.1 & 8.0 \\ -1.5 & .55 & 3.2 & .5 \\ .67 & -2.8 & -2.4 & 1.6 \\ 9.0 & 8.7 & -7.7 & 7.8 \end{bmatrix}$

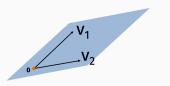
$$\begin{array}{ll} V^TV = I & \text{but} & VV^T \neq I \\ \|V_Y\|_{r}^{1} = ||X^TV^TV_X| = ||X||_2^2 \text{ but} ||V^TX||_2^2 \neq ||X||_2^2 \text{ in general.} \\ \text{Equivalently, } x, ||x^TV^T||_2^2 = ||x||_2^2 \text{ but} ||x^TV||_2^2 \neq ||x||_2^2 \text{ in general.} \\ (V^T \times)^T (V^T \times) = ||X|^T V^T \times ||X^T \times||X^T \times ||X^T \times$$

Multiplying a vector by **V** with orthonormal columns rotates and/or reflects the vector. (Va, Vb) aeB2 VaeB3 V t B3×2 = a 1 v 7 V b = a 1 b = 20, 1> a X

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

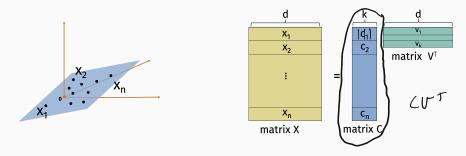


Let $\mathbf{v}_1, \dots, \mathbf{v}_k$ be orthogonal unit vectors spanning S.

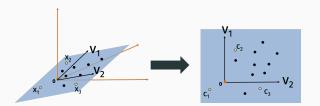


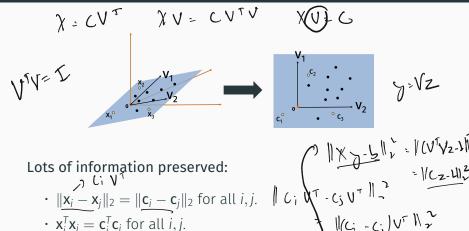
For all *i*, we can write:

$$\underline{\mathbf{x}}_{i} = \underbrace{\mathbf{c}_{i,1}\mathbf{y}_{1}}_{\mathbf{c}_{i,k}} + \dots + \underbrace{\mathbf{c}_{i,k}\mathbf{y}_{k}}_{\mathbf{c}_{i,k}}$$



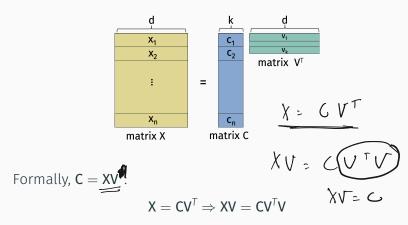
What are $\mathbf{c}_1, \dots, \mathbf{c}_n$?





 $\begin{aligned} & \cdot \|\mathbf{x}_{i} - \mathbf{x}_{j}\|_{2} = \|\mathbf{c}_{i} - \mathbf{c}_{j}\|_{2} \text{ for all } i, j. \\ & \cdot \mathbf{x}_{i}^{\mathsf{T}} \mathbf{x}_{j} = \mathbf{c}_{i}^{\mathsf{T}} \mathbf{c}_{j} \text{ for all } i, j. \\ & \cdot \text{Norms preserved, linear separability preserved, } = \|\mathbf{V}(c_{i} - c_{j})\mathbf{V}^{\mathsf{T}}\|_{2}^{2} \\ & \min \|\mathbf{X}\mathbf{y} - \mathbf{b}\| = \min \|\mathbf{C}\mathbf{z} - \mathbf{b}\|, \text{ etc., etc.} \end{aligned}$

12



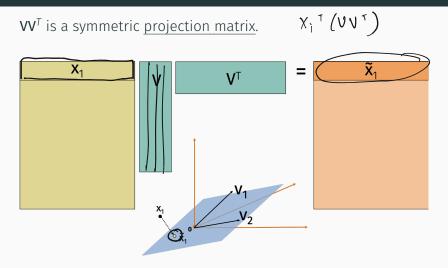
Since V's columns are an orthonormal basis, $V^TV = I$.

$$\chi : CV^{T}$$

$$\chi \times \chi = \chi VV^{T}$$

$$A = \chi VV^{T}$$

PROJECTION MATRICES



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

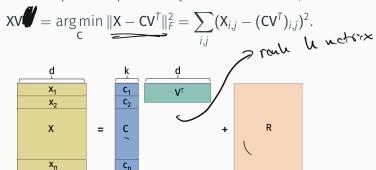
LOW-RANK APPROXIMATION

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

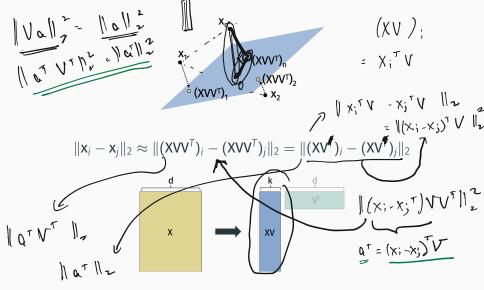
$$X \approx XVV^T$$
.

 XVV^T is a <u>low-rank approximation</u> for X.

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



LOW-RANK APPROXIMATION

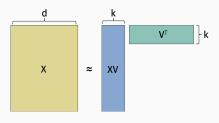


XV can be used as a compressed version of data matrix X.

WHY IS DATA APPROXIMATELY LOW-RANK?

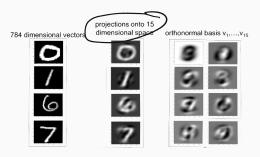
DUAL VIEW

Rows of X (data points) are approximately spanned by k vectors. Columns of X (data features) are approximately spanned by k vectors.



ROW REDUNDANCY

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.

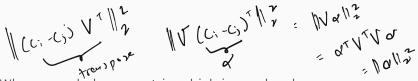


COLUMN REDUNDANCY

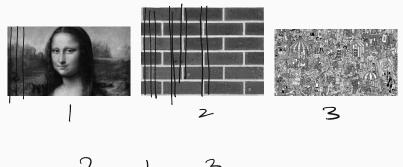
Colinearity/correlation of data features leads to a low-rank data matrix.

	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

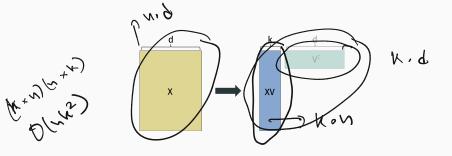
OTHER REASONS FOR LOW-RANK STRUCTURE



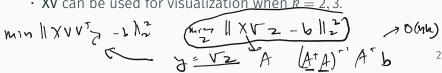
When encoded as a matrix, which image has lower approximate rank?



APPLICATIONS OF LOW-RANK APPROXIMATION

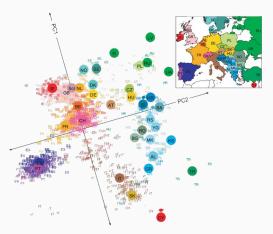


- XV · V^T takes O(k(n+d)) space to store instead of O(nd).
- Regression problems involving $XV \cdot V^T$ can be solved in $O(nk^2)$ instead of $O(nd^2)$ time.
- XV can be used for visualization when k = 2, 3.



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.

COMPUTATIONAL QUESTION

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

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

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

he best
$$\mathbf{V} \in \mathbb{R}^{d \times k}$$
:

$$\min_{\substack{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times k}}} \|\mathbf{X} - \mathbf{X} \mathbf{V} \mathbf{V}^{\mathsf{T}}\|_{\mathbf{F}}^{2} - \|\mathbf{X} \mathbf{V} \mathbf{V}^{\mathsf{T}}\|_{\mathbf{F}}^{2}$$
(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 VV^T is a projection). Equivalent form:

$$\max_{\text{orthonormal } \mathbf{V} \in \mathbb{R}^{d \times h}} \|\mathbf{X} \mathbf{V} \mathbf{V}^{\mathsf{T}} \mathbf{V}\|_F^2 = \|\mathbf{X} \mathbf{V}\|_F^2$$
 (2)

RANK 1 CASE

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

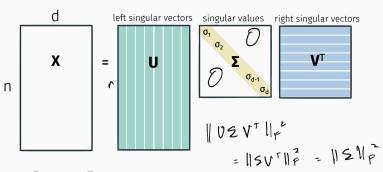
$$\|\underline{Xv_1v_1^T}\|_F^2 = \|\underline{Xv_1}\|_F^2 = \|\underline{Xv_1}\|_2^2 = \underbrace{v_1^TX^TXv_1}.$$

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 $\mathbf{U}^{\mathsf{T}}\mathbf{U} = \mathbf{I}$, $\mathbf{V}^{\mathsf{T}}\mathbf{V} = \mathbf{I}$, 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

- V_{b} 's columns are called the "top right singular vectors of X"
- U_b's columns are called the "top left singular vectors of X"
- $\cdot \sigma_1, \ldots, \sigma_h$ are the "top singular values". $\sigma_1, \ldots, \sigma_d$ are sometimes called the "spectrum of X" (although this is more typically used to refer to eigenvalues).
- U contains the orthonormal eigenvectors of XX^T



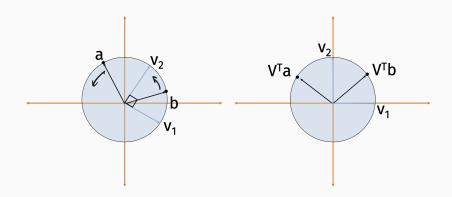
- \cdot V contains the orthonormal eigenvectors of $\underline{X}^{T}\underline{X}$.
- $\sigma_i^2 = \lambda_i(XX^T) = \lambda_i(X^TX)$

Exercise: Check this can be checked directly.

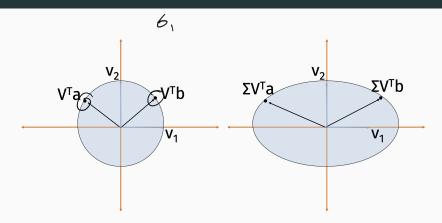
Multiplying any vector **a** by a matrix **X** to form **Xa** can be viewed as a composition of 3 operations:

- 1. Rotate/reflect the vector (multiplication by to V^T).
- 2. Scale the coordinates (multiplication by Σ .
- 3. Rotate/reflect the vector again (multiplication by **U**).

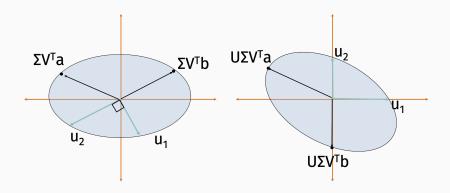
SINGULAR VALUE DECOMPOSITION: ROTATE/REFLECT

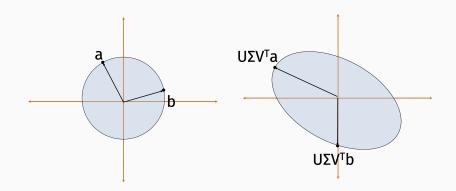


SINGULAR VALUE DECOMPOSITION: STRETCH

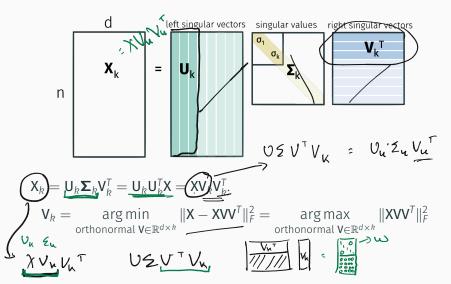


SINGULAR VALUE DECOMPOSITION: ROTATE/REFLECT





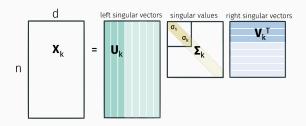
Can read off optimal low-rank approximations from the SVD:



Connection to Principal Component Analysis:

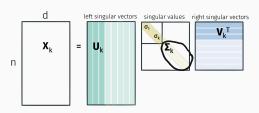
- Let $\bar{\mathbf{X}} = \mathbf{X} \mathbf{1} \boldsymbol{\mu}^T$ where $\boldsymbol{\mu} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i$. I.e. $\bar{\mathbf{X}}$ is obtained by mean centering X's rows.
- Let $\bar{\mathbf{U}}\bar{\mathbf{\Sigma}}\bar{\mathbf{V}}^T$ be the SVD of $\bar{\mathbf{X}}$. $\bar{\mathbf{U}}$'s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

USEFUL OBSERVATIONS



Observation 1: The optimal compression XV_R has orthogonal columns.

USEFUL OBSERVATIONS



Observation 2: The optimal low-rank approximation error

$$E_k = \|\mathbf{X} - \mathbf{X} \mathbf{V}_k \mathbf{V}_k^T\|_F^2 = \|\mathbf{X}\|_F^2 - \|\mathbf{X} \mathbf{V}_k \mathbf{V}_k^T\|_F^2 \text{ can be written:}$$

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

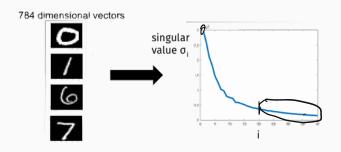
$$\sum_{i=1}^{k} 6_{i}^{2} - \sum_{i=1}^{k} 6_{i}^{2} = \sum_{i=k+1}^{k} 6_{i}^{2}$$

SPECTRAL PLOTS

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:

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

Can immediately get a sense of "how low-rank" a matrix is from it's spectrum:

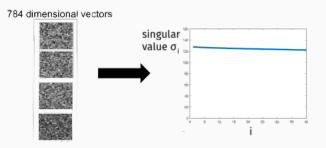


SPECTRAL PLOTS

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:

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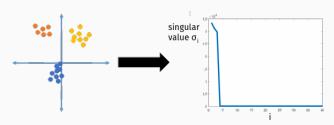


SPECTRAL PLOTS

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:

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

Can immediately get a sense of "how low-rank" a matrix is from it's spectrum:



COMPUTING THE SVD

Suffices to compute right singular vectors **V**:

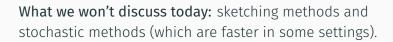
- Compute X^TX . $(V \subseteq V^T)^T V \subseteq V^T \subseteq$
- Find eigendecomposition $V \wedge V^T = (X^T X)$
- Compute L = XV. Set $\sigma_i = ||L_i||_2$ and $U_i = L_i/||L_i||_2$.

Total runtime
$$\approx O(n d^2)$$

† $O(d^3)$

COMPUTING THE SVD (FASTER)

- · Compute <u>approximate</u> solution.
- Only compute $\underline{\text{top } k \text{ singular vectors/values}}$. 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.
 - <u>Power method</u> is the simplest Krylov subspace method, and still works very well.





POWER METHOD

Today: What about when k = 1?

Goal: Find some $\underline{z} \approx v_1$.

Input: $X \in \mathbb{R}^{n \times d}$ with SVD $U \not \Sigma V^T$.

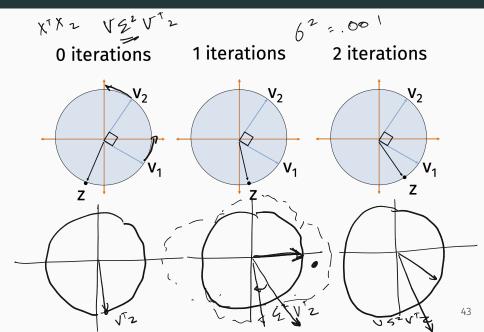
Power method:



- Choose $\mathbf{z}^{(0)}$ randomly. E.g. $\mathbf{z}_0 \sim \mathcal{N}(0,1)$.
- $\cdot z^{(0)} = z^{(0)} / ||z^{(0)}||_2$
- For $i = 1, \ldots, T$
 - $\cdot z^{(i)} = X^T \cdot (X\underline{z^{(i-1)}})$
 - $n_{i} = ||\mathbf{z}^{(i)}||_{2}$
 - $\cdot z^{(i)} = z^{(i)}/n_{\perp}$

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

POWER METHOD INTUITION



POWER METHOD FORMAL CONVERGENCE

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 $T = O\left(\frac{\log d/\epsilon}{\gamma}\right)$ teps, we have either:

$$\|\mathbf{v}_1 + \mathbf{z}^{(T)}\|_2 \le \epsilon$$
 or $\|\mathbf{v}_1 - (-\mathbf{z}^{(T)})\|_2 \le \epsilon$.

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

ONE STEP ANALYSIS OF POWER METHOD

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

$$\underline{\mathbf{z}^{(0)}} = c_1^{(0)} \underline{\mathbf{v}}_1 + c_2^{(0)} \underline{\mathbf{v}}_2 + \dots + c_d^{(0)} \underline{\mathbf{v}}_d
\underline{\mathbf{z}^{(1)}} = c_1^{(1)} \mathbf{v}_1 + c_2^{(1)} \underline{\mathbf{v}}_2 + \dots + c_d^{(1)} \mathbf{v}_d
\vdots
\underline{\mathbf{z}^{(i)}} = c_1^{(i)} \underline{\mathbf{v}}_1 + c_2^{(i)} \underline{\mathbf{v}}_2 + \dots + c_d^{(i)} \underline{\mathbf{v}}_d$$

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

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

ONE STEP ANALYSIS OF POWER METHOD

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

$$= \mathbf{V} \mathbf{Z} \mathbf{U}^{\mathsf{T}} \mathbf{U} \mathbf{S} \mathbf{V}^{\mathsf{T}}$$

$$= \mathbf{V} \mathbf{Z}^{\mathsf{D}} \mathbf{V}^{\mathsf{T}}$$

$$z^{(i)} = \frac{1}{n_1!} \left[c_1^{(i-1)} \frac{\sigma_1^2 \cdot v_1 + c_2^{(i-1)} \frac{\sigma_2^2}{\sigma_2^2} \cdot v_2 + \dots + c_d^{(i-1)} \frac{\sigma_d^2}{\sigma_d^2} \cdot v_d \right]$$

$$\left[c_1^{(i-1)} \cdot \dots \cdot c_d^{(i-1)} \right]$$

$$\left[c_1^{(i-1)} \cdot \dots \cdot c_d^{(i-1)} \right]$$

MULTI-STEP ANALYSIS OF POWER METHOD

Claim: After *T* updates:

$$\mathbf{z}^{(7)} = \frac{1}{\prod_{i=1}^{T} n} \left[c_1^{(0)} \sigma_1^{2T} \cdot \mathbf{v}_1 + c_2^{(0)} \sigma_2^{2T} \cdot \mathbf{v}_2 + \dots + c_d^{(0)} \sigma_d^{2T} \cdot \mathbf{v}_d \right]$$

$$\mathbf{z}^{(1)}$$

POWER METHOD FORMAL CONVERGENCE

Since $\mathbf{z}^{(7)}$ is a unit vector, $\sum_{i=1}^{d} \alpha_i^2 = 1$. So $\alpha_1 \leq 1$. If we can prove that $\frac{\alpha_i}{\alpha_1} \leq \sqrt{\frac{\epsilon}{d}}$ then:

$$\alpha_{1}^{2} \geq 1 - d \cdot \left(\sqrt{\frac{\epsilon}{d}}\right)^{2} \Longrightarrow |\underline{\alpha_{1}}| \geq 1 - \epsilon$$

$$Q_{1}^{2} = |-\sum_{j=2}^{2} \alpha_{j}^{2}| \geqslant |-d \cdot \left(\sqrt{\frac{\epsilon}{d}}\right)^{2}$$

$$||\underline{v_{1}} - \underline{z^{(T)}}||_{2} = 2 - 2(\underline{v_{1}}, \underline{z^{(T)}}) \leq 2\epsilon$$

$$Q_{1}^{2} \bowtie |-\epsilon|$$

$$Q_{2}^{2} \bowtie |-\epsilon|$$

$$Q_{1}^{2} \bowtie |-\epsilon|$$

$$Q_{2}^{2} \bowtie |-\epsilon|$$

$$Q_{3}^{2} \bowtie |-\epsilon|$$

$$Q_{4}^{2} \bowtie |-\epsilon|$$

$$Q_{5}^{2} \bowtie |-\epsilon|$$

$$Q_{7}^{2} \bowtie |-\epsilon|$$

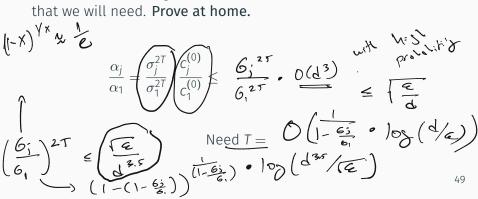
$$Q_{7}^$$

POWER METHOD FORMAL CONVERGENCE

Lets proves that
$$\sqrt{\frac{\alpha_j}{\sigma}} \sqrt{\frac{\epsilon}{d}}$$
 where $\alpha_j = \frac{1}{\prod_{i=1}^T n_i} c_i^{(0)} \sigma_i^{2T}$

First observation: Starting coefficients are all roughly equal.

For all
$$j$$
 $O(1/d^3) \le c_j^{(0)} \le 1$ with probability $1 - \frac{1}{d}$. This is a very loose bound, but it's all that we will need. **Prove at home.**



POWER METHOD - NO GAP DEPENDENCE

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 **z** satisfying:

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

GENERALIZATIONS TO LARGER R

 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.
- $Z_0 = \text{orth}(G)$.
- For $i = 1, \ldots, T$
 - $\cdot Z^{(i)} = X^T \cdot (X^{2(i-1)})$
 - $\cdot Z^{(i)} = \operatorname{orth}(\mathbf{Z}^{(i)})$

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

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

$$\|\mathbf{X} - \mathbf{X}\mathbf{Z}\mathbf{Z}^{\mathsf{T}}\|_F^2 \le (1 + \epsilon)\|\mathbf{X} - \mathbf{X}\mathbf{V}_{\mathsf{k}}\mathbf{V}_{\mathsf{k}}^{\mathsf{T}}\|_F^2.$$