# COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

Cameron Musco University of Massachusetts Amherst. Fall 2019. Lecture 17

#### LOGISTICS

- Problem Set 3 was released on Saturday. Due next Friday 11/15 at 8pm.
- I will hold office hours after class until 12:30pm today.

## Last Class:

- · Finished up spectral clustering and stochastic block model.
- Started discussion of efficient algorithms for SVD/eigendecomposition.

## This Class:

- · Finish efficient algorithms for SVD/eigendecomposition.
- · Iterative methods: power method, Krylov subspace methods.
- · Start optimization unit. Gradient Descent.

## **FASTER ALGORITHMS**

To speed up SVD computation we will take advantage of the fact that we typically only care about computing the top (or bottom) k singular vectors of a matrix  $\mathbf{X} \in \mathbb{R}^{n \times d}$  for  $k \ll d$ .

- Suffices to compute  $\underline{V}_k \in \mathbb{R}^{d \times k}$  and then compute  $U_k \Sigma_k = XV_k$ .
- Use an *iterative algorithm* to compute an *approximation* to the top k singular vectors  $\mathbf{V}_k$ .
- Runtime will be roughly O(ndk) instead of  $O(nd^2)$ .

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Sparse (iterative) vs. Direct Method. svd vs. svds.

**Power Method:** The most fundamental iterative method for approximate SVD. Applies to computing k = 1 singular vectors, but can easily be generalized to larger k.

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**Goal:** Given  $\mathbf{X} \in \mathbb{R}^{n \times d}$ , with SVD  $\mathbf{X} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}$ , find  $\vec{z} \approx \vec{v}_1$ .

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- · Initialize: Choose  $\vec{z}^{(0)}$  randomly. E.g.  $\vec{z}^{(0)}(i) \sim \mathcal{N}(0,1)$ .
- For i = 1, ..., t  $\cdot \vec{z}^{(i)} = (\mathbf{X}^{\mathsf{T}}\mathbf{X}) \cdot \vec{z}^{(i-1)}$   $\cdot n_i = \|\vec{z}^{(i)}\|_2$   $\cdot \vec{z}^{(i)} = \vec{z}^{(i)}/n_i$

Return  $\vec{z}_t$ 

**Power Method:** The most fundamental iterative method for approximate SVD. Applies to computing k = 1 singular vectors, but can easily be generalized to larger k.

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• Initialize: Choose 
$$\vec{z}^{(0)}$$
 randomly. E.g.  $\vec{z}^{(0)}(i) \sim \mathcal{N}(0,1)$ .  
• For  $i = 1, \ldots, t$   $\vec{x} (X \mathbf{z}^{i-i})$  Runtime:  $2 \cdot nd$   $\vec{x}^{(i)} = (X^TX) \cdot \vec{z}^{(i-1)}$  Runtime:  $d$ 

• For 
$$i = 1, \dots, t$$

$$\cdot \ \vec{z}^{(i)} = (\mathbf{X}^T \mathbf{X}) \cdot \vec{z}^{(i-1)}$$

$$\cdot n_i = \|\vec{z}^{(i)}\|_2$$

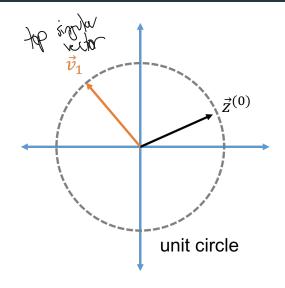
$$\cdot \vec{z}^{(i)} = \vec{z}^{(i)}/n_i$$

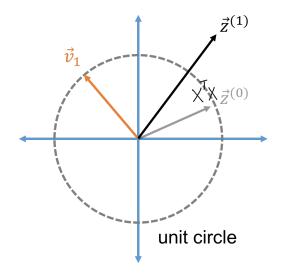
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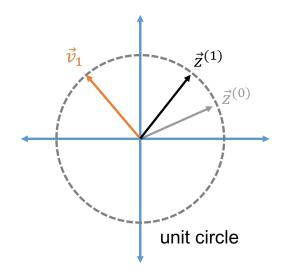
Runtime: d

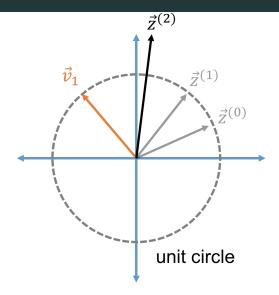
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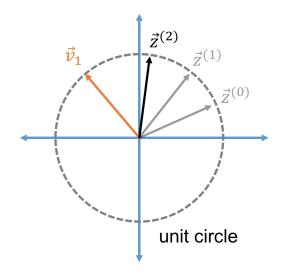
Total Runtime:  $O(ndt) \sim O(nd)$ 

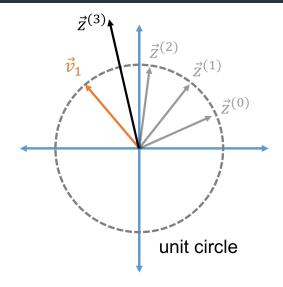


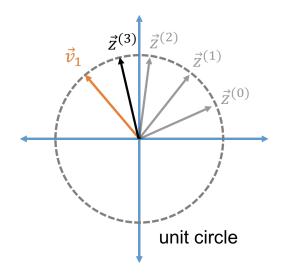


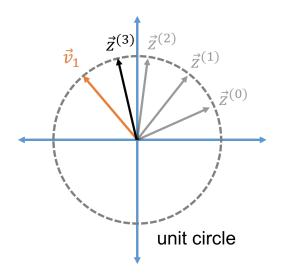












Why is it converging towards  $\vec{v}_1$ ?

Write  $\vec{z}^{(0)}$  in the right singular vector basis:

$$\vec{z}^{(0)} = c_1 \vec{v}_1 + c_2 \vec{v}_2 + \ldots + c_d \vec{v}_d.$$

 $\mathbf{X} \in \mathbb{R}^{n \times d}$ : input matrix with SVD  $\mathbf{X} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^\mathsf{T}$ .  $\vec{v}_1$ : top right singular vector, being computed,  $\vec{z}^{(i)}$ : iterate at step i, converging to  $\vec{v}_1$ .

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$$\times : \mathcal{I} \mathcal{I}^{(0)} = c_1 \vec{v}_1 + c_2 \vec{v}_2 + \ldots + c_d \vec{v}_d.$$

Update step: 
$$\vec{z}^{(i)} = \overset{\uparrow}{XX}^{\emptyset} \cdot \vec{z}^{(i-1)} = V \Sigma^2 V^T \cdot \vec{z}^{(i-1)}$$
 (then normalize)

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Write  $\vec{z}^{(0)}$  in the right singular vector basis:

$$\not x$$
  $\vec{z}^{(0)} = \vec{c_1} \vec{v_1} + \vec{c_1} \vec{v_2} + \dots + c_d \vec{v_d}.$ 

Update step:  $\vec{z}^{(i)} = XX^T \cdot \vec{z}^{(i-1)} = V\Sigma^2 V^T \cdot \vec{z}^{(i-1)}$  (then normalize)

$$\underline{V}^{T}\overline{Z}^{(0)} = \begin{bmatrix} C_{1} \\ C_{2} \\ \vdots \\ c_{d} \end{bmatrix} \qquad V^{T}\overline{Z}^{(0)} = V^{T}(C_{1}V_{1} + C_{2}V_{2} \dots)$$

$$C_{1} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} + C_{2} \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}$$

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$$\mathbf{V}^{\mathsf{T}}\mathbf{z}^{(0)} = \begin{bmatrix} \mathbf{c}_{1} \\ \mathbf{c}_{2} \end{bmatrix}$$

$$\mathbf{\Sigma}^{2}\mathbf{V}^{\mathsf{T}}\mathbf{z}^{(0)} = \begin{bmatrix} \mathbf{c}_{1}^{2} & \mathbf{c}_{1} \\ \mathbf{c}_{2}^{2} & \mathbf{c}_{2} \\ \mathbf{c}_{3}^{2} & \mathbf{c}_{2} \end{bmatrix}$$

 $\mathbf{X} \in \mathbb{R}^{n \times d}$ : input matrix with SVD  $\mathbf{X} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^{\mathsf{T}}$ .  $\vec{\mathbf{v}}_1$ : top right singular vector, being computed,  $\vec{\mathbf{z}}^{(i)}$ : iterate at step i, converging to  $\vec{\mathbf{v}}_1$ .

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Update step:  $\vec{z}^{(i)} = \vec{X} \vec{b} \cdot \vec{z}^{(i-1)} = V \Sigma^2 V^T \cdot \vec{z}^{(i-1)}$  (then normalize)

$$\nabla^{T} \vec{z}^{(0)} =$$

$$\Sigma^{2} V^{T} \vec{z}^{(0)} = \begin{bmatrix} G_{1}^{1} c_{1} \\ \vdots \\ G_{d}^{2} c_{J} \end{bmatrix}$$

$$\vec{z}^{(1)} = V \left(\Sigma^{2} V^{T} \cdot \vec{z}^{(0)}\right) = V \begin{bmatrix} G_{1}^{1} c_{1} \\ G_{1}^{2} c_{J} \end{bmatrix} = G_{1}^{2} c_{1} V_{1} + G_{1}^{2} c_{2} V_{2} + \dots + G_{J}^{2} c_{J} V_{J}$$

 $X \in \mathbb{R}^{n \times d}$ : input matrix with SVD  $X = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T$ .  $\vec{v}_1$ : top right singular vector, being computed,  $\vec{z}^{(i)}$ : iterate at step i, converging to  $\vec{v}_1$ .

Claim 1: Writing 
$$\vec{z}^{(0)} = c_1 \vec{v}_1 + c_2 \vec{v}_2 + \dots + c_d \vec{v}_d$$
, 
$$\vec{z}^{(1)} = c_1 \cdot \sigma_1^2 \vec{v}_1 + c_2 \cdot \sigma_2^2 \vec{v}_2 + \dots + c_d \cdot \sigma_d^2 \vec{v}_d$$
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$$\vec{z}^{(2)} = X^T X \vec{z}^{(1)} = V \mathbf{\Sigma}^2 V^T \vec{z}^{(1)} = c_1 \mathbf{e}_1^{\forall} v_1 + \dots \mathbf{e}_2 \mathbf{e}_3^{\forall} v_4$$

 $\mathbf{X} \in \mathbb{R}^{n \times d}$ : input matrix with SVD  $\mathbf{X} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^\mathsf{T}$ .  $\vec{\mathbf{v}}_1$ : top right singular vector, being computed,  $\vec{\mathbf{z}}^{(i)}$ : iterate at step i, converging to  $\vec{\mathbf{v}}_1$ .

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$$\vec{z}^{(2)} = \mathbf{X}^{\mathsf{T}} \mathbf{X} \vec{z}^{(1)} = \mathbf{V} \mathbf{\Sigma}^{2} \mathbf{V}^{\mathsf{T}} \vec{z}^{(1)} =$$

## Claim 2:

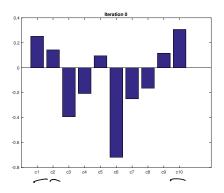
$$\vec{Z}^{(t)} = c_1 \cdot \frac{\sigma_1^{2t} \vec{v}_1 + c_2 \cdot \sigma_2^{2t} \vec{v}_2 + \ldots + c_d \cdot \sigma_d^{2t} \vec{v}_d}{\left\| \vec{z}^{(4)} \right\|}$$

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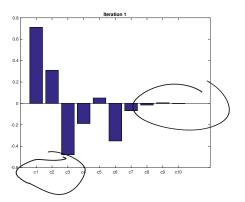
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After t iterations, we have 'powered' up the singular values, making the component in the direction of  $v_1$  much larger, relative to the other components.

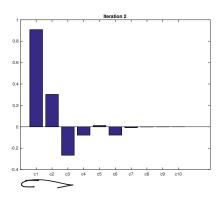
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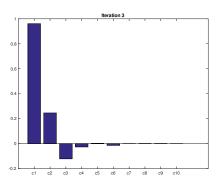
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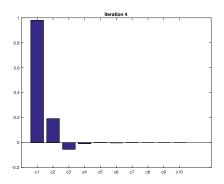
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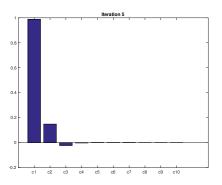
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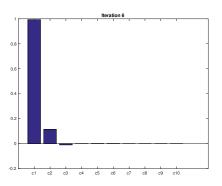
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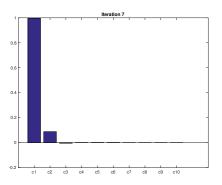
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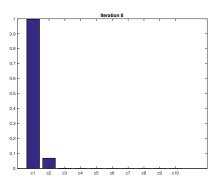
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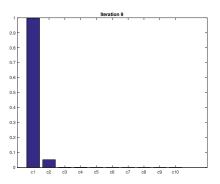
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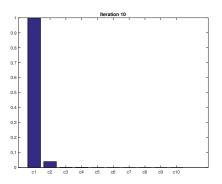


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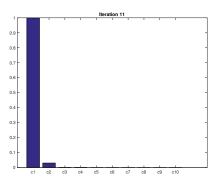
After t iterations, we have 'powered' up the singular values, making the component in the direction of  $v_1$  much larger, relative to the other components.

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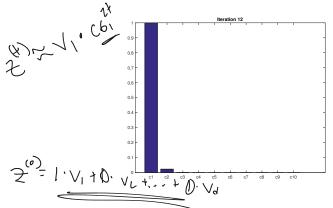
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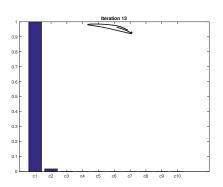
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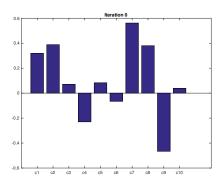
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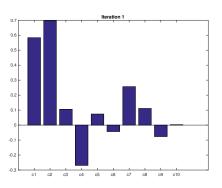
When will convergence be slow?

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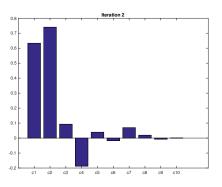
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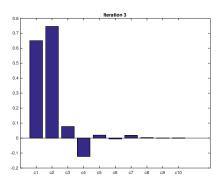
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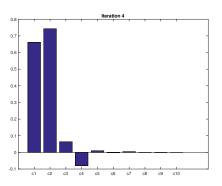
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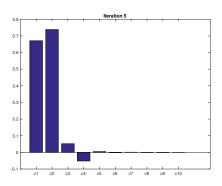
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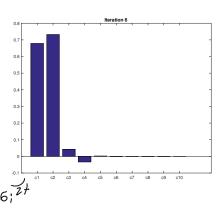
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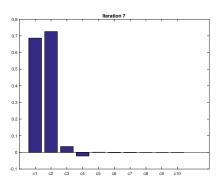
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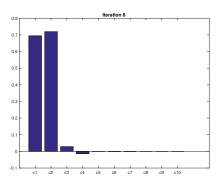
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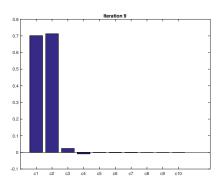
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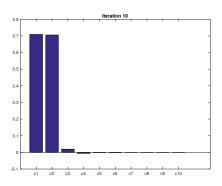
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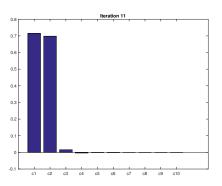
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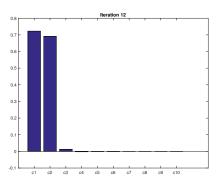
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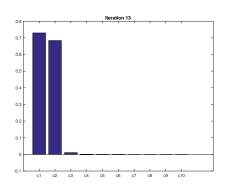


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$$\vec{c}_2^{t} \le \vec{c}_1^{t} \Rightarrow \vec{c}_2^{t} \le \vec{c}_1^{t} \Rightarrow \vec{c}_2^{t} \le \vec{c}_1^{t} \Rightarrow \vec{c}_2^{t} = \vec{c}_1^{t} + \vec{c}_1^{t} + \vec{c}_2^{t} =$$

 $\mathbf{X} \in \mathbb{R}^{n \times d}$ : matrix with SVD  $\mathbf{X} = \mathbf{U} \mathbf{\Sigma} \mathbf{V}^T$ . Singular values  $\sigma_1, \sigma_2, \dots, \sigma_d$ .  $\vec{\mathbf{v}}_1$ : top right singular vector, being computed,  $\vec{\mathbf{z}}^{(i)}$ : iterate at step i, converging to  $\vec{\mathbf{v}}_1$ .

+= D(1/4) -> (1-4)2+ < =

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How many iterations t does it take to have  $\sigma_2^{2t} \leq \delta \cdot \sigma_1^{2t}$ ?  $|o_{S_1-y}| \leq \delta \cdot \sigma_1^{2t}$ ?

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How small must we set  $\delta$  to ensure that  $c_1\sigma_1^{2t}$  dominates all other components and so  $\vec{z}^{(t)}$  is very close to  $\vec{v_1}$ ?

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**Claim:** When  $z^{(0)}$  is chosen with random Gaussian entries, writing  $z^{(0)} = c_1 \mathbf{v}_1 + \mathbf{c}_2 \mathbf{v}_2 + \ldots + c_d \mathbf{v}_d$ , with very high probability, for all i:

$$\frac{\left(O(1/d^2) \leq c_i \leq O(\log d)\right)}{\text{How is ci distributed?}}$$

$$\sqrt{\frac{1}{2}}(0) = \left(\frac{1}{2}\right)$$

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$$\frac{1$$

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$$\max_{j} \left| \frac{c_{j}}{c_{1}} \right| \leq O(d^{2} \log d). \quad \left| \frac{C_{j}}{c_{1}} \right| \leq \sum_{j=1}^{|a_{j}|} \frac{|a_{j}|}{|a_{j}|} \leq \sum_{j=1}^{|a_{j$$

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, after  $t = O\left(\frac{\log(1/\delta)}{\gamma}\right)$  iterations: 
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 If we set  $\delta = O\left(\frac{\epsilon}{d^3 \log d}\right)$  by Claim 1 will have: 
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, after  $t = O\left(\frac{\log(1/\delta)}{\gamma}\right)$  iterations:  $\vec{z}^{(t)} = c_1 \vec{v}_1 + c_2 \vec{v}_2 + \ldots + c_d \vec{\sigma}_d \vec{v}_d \propto c_1 \vec{v}_1 + c_2 \delta \vec{v}_2 + \ldots + c_d \delta \vec{v}_d$ 

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$$\vec{z}^{(t)} \propto \vec{v}_1 + \left(\frac{\epsilon}{d} \left(\vec{v}_2 + \ldots + \vec{v}_d\right)\right)$$

Gives 
$$\|\vec{z}^{(t)} - \vec{v}_1\|_2 \leq O(\epsilon)$$
.

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# Theorem (Basic Power Method Convergence)

Let  $\gamma = \frac{\sigma_1 - \sigma_2}{\sigma_1}$  be the relative gap between the first and second largest singular values. If Power Method is initialized with a random Gaussian vector  $\vec{\mathbf{v}}^{(0)}$  then, with high probability, after  $\mathbf{t} = \mathbf{0}\left(\frac{\log d/\epsilon}{\gamma}\right)$  steps:

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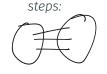
Total runtime: O(t) matrix-vector multiplications.

$$O\left(\frac{\operatorname{nnz}(\mathbf{X})}{\gamma} \cdot \frac{\log(d/\epsilon)}{\gamma}\right) = O\left(nd\left(\frac{\log(d/\epsilon)}{\gamma}\right)\right).$$
  $O\left(nd\left(\frac{\log(d/\epsilon)}{\gamma}\right)\right)$ 

## POWER METHOD THEOREM

# Theorem (Basic Power Method Convergence)

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$$(\|\vec{z}^{(t)} - \vec{v}_1\|_2) \leq \epsilon.$$

**Total runtime:** O(t) matrix-vector multiplications.

ne: 
$$O(t)$$
 matrix-vector multiplications.  $\mathcal{E} \xrightarrow{\mathcal{E}} \mathcal{E}$ 

$$O\left(\operatorname{nnz}(\mathbf{X}) \cdot \frac{\log(d/\epsilon)}{\gamma} \cdot \right) = O\left(nd \cdot \frac{\log(d/\epsilon)}{\gamma}\right) \cdot \log\left(1/\epsilon\right) \cdot \log\left(1/\epsilon\right) \cdot \log\left(1/\epsilon\right)$$

How is  $\epsilon$  dependence? "linewly unvoyent"

How is  $\gamma$  dependence?

#### KRYLOV SUBSPACE METHODS

# Krylov subspace methods (Lanczos method, Arnoldi method.)

• How svds/eigs are actually implemented. Only need  $t = O\left(\frac{\log d/\epsilon}{\sqrt{\gamma}}\right)$  steps for the same guarantee.

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Main Idea: Need to separate  $\sigma_1$  from  $\sigma_i$  for  $i \geq 2$ .  $\rho(x) \stackrel{?}{\sim} x^{\dagger}$ . Power method: power up to  $\sigma_1^{2\cdot t}$  and  $\sigma_i^{2\cdot t}$ .  $\rightarrow \rho(\varsigma_i^{\tau})$   $\nearrow 7P(\varsigma_i^{\tau})$ 

- Krylov methods: apply a better degree t polynomial  $T_t(\sigma_1^2)$ and  $T_t(\sigma_i^2)$ .

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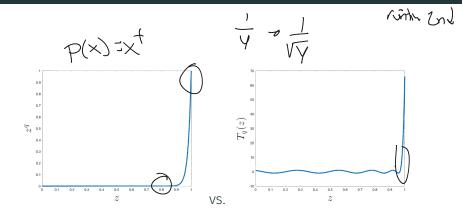
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- Power method: power up to  $\sigma_1^{2\cdot t}$  and  $\sigma_i^{2\cdot t}$ .
- Krylov methods: apply a better degree t polynomial  $T_t(\sigma_1^2)$  and  $T_t(\sigma_i^2)$ .
- Still requires just 2t matrix vector multiplies. Why?  $a_1 \times^{7} \times a_1 \times^{8} \times a_2 \times x^{8}$

$$\times^{T} \times V^{0}$$
  $(\cancel{X} \times) V_{1}$   $(\cancel{X} \times) V_{2}$   $(\cancel{X} \times)^{3} V_{0}$   $(\cancel{X} \times)^{3} V_{0}$ 



### KRYLOV SUBSPACE METHODS



Optimal 'jump' polynomial in general is given by a degree *t* Chebyshev polynomial. Krylov methods find a polynomial tuned to the input matrix that does at least as well.

# GENERALIZATIONS TO LARGER R

- Block Power Method aka Simultaneous Iteration aka Subspace Iteration aka Orthogonal Iteration
- · Block Krylov methods

Runtime: 
$$O\left(nd\underline{k} \cdot \frac{\log d/\epsilon}{\sqrt{\gamma}}\right)$$

$$C \in \mathcal{E}_{k+1}$$

to accurately compute the top k singular vectors.

# GENERALIZATIONS TO LARGER R

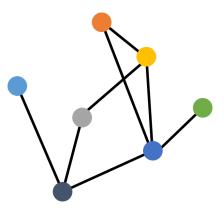
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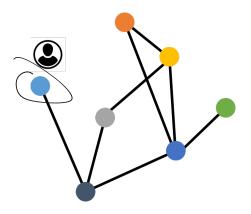
to accurately compute the top *k* singular vectors.

'Gapless' Runtime: 
$$O\left(ndk \cdot \frac{\log d/\epsilon}{\sqrt{\epsilon}}\right)$$

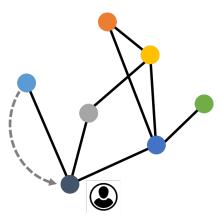
if you just want a set of vectors that gives an  $\epsilon$ -optimal low-rank approximation when you project onto them.

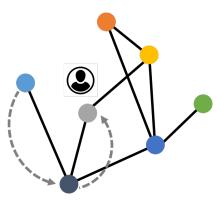


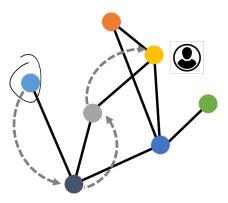
Consider a random walk on a graph G with adjacency matrix A.



At each step, move to a random vertex, chosen uniformly at random from the neighbors of the current vertex.







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2; 
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$$= \vec{z}^T \vec{p}^{(t-1)}$$

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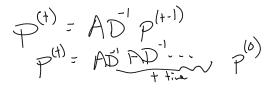
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$$\vec{p}^{(t)} = AD^{-1}\vec{p}^{(t-1)} = \underbrace{AD^{-1}AD^{-1}...AD^{-1}}_{t \text{ times}} \vec{p}^{(0)}$$

**Claim:** After t steps, the probability that a random walk is at node i is given by the  $i^{th}$  entry of

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- Like the power method, the time a random walk takes to converge to its stationary distribution (mixing time) is dependent on the gap between the top two eigenvalues of  $AD^{-1}$ . The spectral gap.