COMPSCI 514: ALGORITHMS FOR DATA SCIENCE

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Lecture 21

LOGISTICS

- I released Problem Set 4 this am. Due Wednesday 12/1.
- At least one group is looking to add a third teammate. if you are working alone and would like to join a group for Problem Set 4, let me know.
- Problem Set 5 will be released right after break and will be optimal extra credit.
- No quiz this week.
- This is the last day of our spectral unit. Then will have 3-4 classes on optimization + a possible review class before the end of the semester.
- I am holding hybrid office hours today at 5-6pm, so feel free to come by in person if you like.

Last Few Classes: Spectral Graph Partitioning

- Focus on separating graphs with small but relatively balanced cuts.
- Connection to second smallest eigenvector of graph Laplacian.
- Provable guarantees for stochastic block model.
- Idealized analysis in class. See slides for full analysis.

This Class: Computing the SVD/eigendecomposition.

- Efficient algorithms for SVD/eigendecomposition.
- Iterative methods: power method, Krylov subspace methods.
- High level: a glimpse into fast methods for linear algebraic computation, which are workhorses behind data science.

Upshot: The second smallest eigenvector of $\mathbb{E}[\mathbf{L}]$ is $\chi_{B,C}$ – the indicator vector for the cut between the communities.

- If the random graph G (equivalently $\mathbf{A}$ and $\mathbf{L}$) were exactly equal to its expectation, partitioning using this eigenvector (i.e., spectral clustering) would exactly recover the two communities B and C.

How do we show that a matrix (e.g., $\mathbf{A}$) is close to its expectation? Matrix concentration inequalities.

- Analogous to scalar concentration inequalities like Markovs, Chebyshevs, Bernsteins.
- Random matrix theory is a very recent and cutting edge subfield of mathematics that is being actively applied in computer science, statistics, and ML.

We have talked about the eigendecomposition and SVD as ways to compress data, to embed entities like words and documents, to compress/cluster non-linearly separable data.

How efficient are these techniques? Can they be run on massive datasets?

Basic Algorithm: To compute the SVD of full-rank $\mathbf{X} \in \mathbb{R}^{n \times d}$, $\mathbf{X} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T$:

- Compute $\mathbf{X}^T\mathbf{X}$ – $O(nd^2)$ runtime.
- Find eigendecomposition $\mathbf{X}^T\mathbf{X} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T$ – $O(d^3)$ runtime.
- Compute $\mathbf{L} = \mathbf{X}\mathbf{V}$ – $O(nd^2)$ runtime. Note that $\mathbf{L} = \mathbf{U}\mathbf{\Sigma}$.
- Set $\sigma_i = \|\mathbf{L}_i\|_2$ and $\mathbf{U}_i = \mathbf{L}_i / \|\mathbf{L}_i\|_2$. – $O(nd)$ runtime.

  Total runtime: $O(nd^2 + d^3) = O(nd^2)$ (assume w.l.o.g. $n \geq d$)

- If we have $n = 10$ million images with $200 \times 200 \times 3 = 120,000$ pixel values each, runtime is 1.5×10^{17} operations!
- The worlds fastest super computers compute at ≈ 100 petaFLOPS = 10^{17} FLOPS (floating point operations per second).
- This is a relatively easy task for them – but no one else.

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 $\mathbf{X} \in \mathbb{R}^{n \times k}$ for $k \ll d$.

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

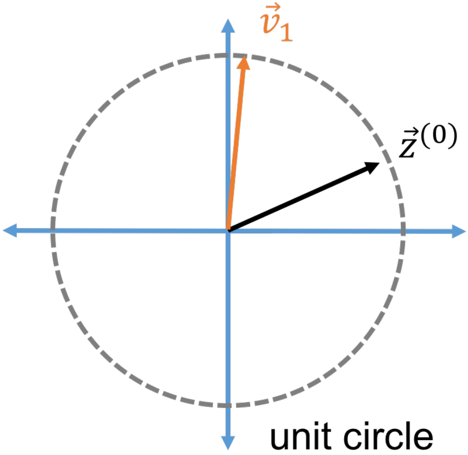
Sparse (iterative) vs. Direct Method. `svd` vs. `svds`.

Power Method: The most fundamental iterative method for approximate SVD/eigendecomposition. Applies to computing $k = 1$ eigenvectors, but can be generalized to larger k.

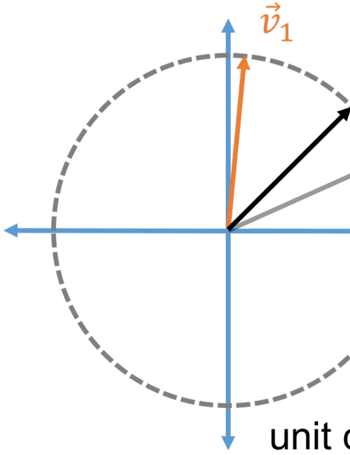
Goal: Given symmetric $\mathbf{A} \in \mathbb{R}^{d \times d}$, with eigendecomposition $\mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T$, find $\vec{z} \approx \vec{v}_1$ – the top eigenvector of $\mathbf{A}$.

- **Initialize:** Choose $\vec{z}^{(0)}$ randomly. E.g. $\vec{z}^{(0)}(i) \sim \mathcal{N}(0, 1)$.
- For $i = 1, \ldots, t$
  - $\vec{z}^{(i)} := \mathbf{A} \cdot \vec{z}^{(i-1)}$
  - $\vec{z}_i := \frac{\vec{z}^{(i)}}{\|\vec{z}^{(i)}\|_2}$

  Return $\vec{z}_t$



$\vec{v}_1$
$\vec{z}^{(0)}$
unit circle



$\vec{v}_1$

Write $\vec{z}^{(0)}$ in A's eigenvector basis:

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

Update step: $\vec{z}^{(i)} = \mathbf{A} \cdot \vec{z}^{(i-1)} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^T \cdot \vec{z}^{(i-1)}$ (then normalize)

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

$$\boldsymbol{\Lambda}\mathbf{V}^T\vec{z}^{(0)} =$$

$$\vec{z}^{(1)} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^T \cdot \vec{z}^{(0)} =$$

$\mathbf{A} \in \mathbb{R}^{d\times d}$: input matrix with eigendecomposition $\mathbf{A} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^T$. $\vec{v}_1$: top eigenvector, being computed, $\vec{z}^{(i)}$: iterate at step i, converging to $\vec{v}_1$.

Claim 1 : Writing $\vec{z}^{(0)} = c_1\vec{v}_1 + c_2\vec{v}_2 + \ldots + c_d\vec{v}_d$,

$$\vec{z}^{(1)} = c_1 \cdot \lambda_1\vec{v}_1 + c_2 \cdot \lambda_2\vec{v}_2 + \ldots + c_d \cdot \lambda_d\vec{v}_d.$$

$$\vec{z}^{(2)} = \mathbf{A}\vec{z}^{(1)} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T\vec{z}^{(1)} =$$

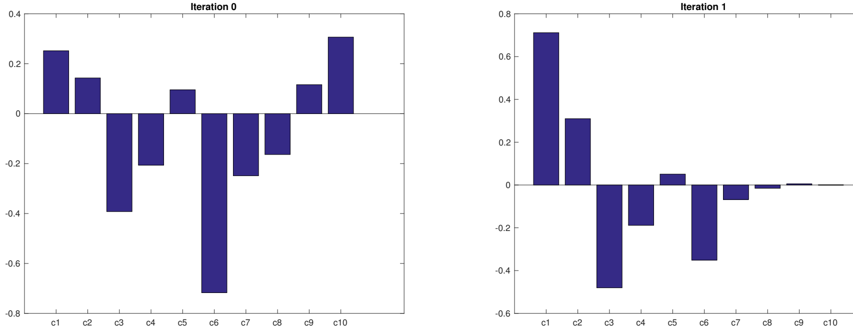
Claim 2:

$$\vec{z}^{(t)} = c_1 \cdot \lambda_1^t\vec{v}_1 + c_2 \cdot \lambda_2^t\vec{v}_2 + \ldots + c_d \cdot \lambda_d^t\vec{v}_d.$$

$\mathbf{A} \in \mathbb{R}^{d\times d}$: input matrix with eigendecomposition $\mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T$. $\vec{v}_1$: top eigenvector, being computed, $\vec{z}^{(i)}$: iterate at step i, converging to $\vec{v}_1$.

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

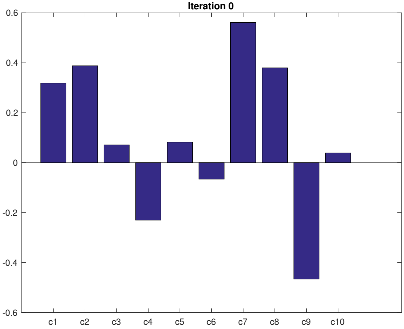
$$\vec{z}^{(0)} = c_1\vec{v}_1 + c_2\vec{v}_2 + \ldots + c_d\vec{v}_d \implies \vec{z}^{(t)} = c_1\lambda_1^t\vec{v}_1 + c_2\lambda_2^t\vec{v}_2 + \ldots + c_d\lambda_d^t\vec{v}_d$$

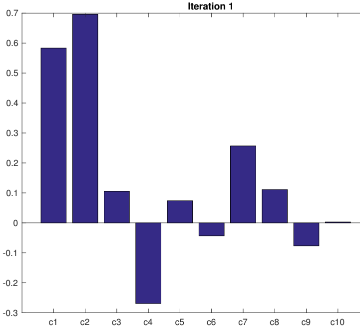


When will convergence be slow?

Slow Case: A has eigenvalues: $\lambda_1 = 1, \lambda_2 = .99, \lambda_3 = .9, \lambda_4 = .8, \ldots$

$$\vec{z}^{(0)} = c_1\vec{v}_1 + c_2\vec{v}_2 + \ldots + c_d\vec{v}_d \implies \vec{z}^{(t)} = c_1\lambda_1^t\vec{v}_1 + c_2\lambda_2^t\vec{v}_2 + \ldots + c_d\lambda_d^t\vec{v}_d$$





$$\vec{z}^{(0)} = c_1\vec{v}_1 + c_2\vec{v}_2 + \ldots + c_d\vec{v}_d \implies \vec{z}^{(t)} = c_1\lambda_1^t\vec{v}_1 + c_2\lambda_2^t\vec{v}_2 + \ldots + c_d\lambda_2^t\vec{v}_d$$

Write $|\lambda_2| = (1-\gamma)|\lambda_1|$ for 'gap' $\gamma = \frac{|\lambda_1|-|\lambda_2|}{|\lambda_1|}$.

How many iterations t does it take to have $|\lambda_2|^t \leq \frac{1}{e} \cdot |\lambda_1|^t$? $1/\gamma$.

How many iterations t does it take to have $|\lambda_2|^t \leq \delta \cdot |\lambda_1|^t$? $\frac{\ln(1/\delta)}{\gamma}$.

Will have for all $i > 1$, $|\lambda_i|^t \leq |\lambda_2|^t \leq \delta \cdot |\lambda_1|^t$.

How small must we set δ to ensure that $c_1\lambda_1^t$ dominates all other components and so $\vec{z}^{(t)}$ is very close to $\vec{v}_1$?

$\mathbf{A} \in \mathbb{R}^{d\times d}$: input matrix with eigendecomposition $\mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T$. $\vec{v}_1$: top eigenvector, being computed, $\vec{z}^{(i)}$: iterate at step i, converging to $\vec{v}_1$.

Claim: When $z^{(0)}$ is chosen with random Gaussian entries, writing $z^{(0)} = c_1\vec{v}_1 + c_2\vec{v}_2 + \ldots + c_d\vec{v}_d$, with very high probability, for all i:

$$O(1/d^2) \leq |c_i| \leq O(\log d)$$

Corollary:

$$\max_j \left|\frac{c_j}{c_1}\right| \leq O(d^2 \log d).$$

$\mathbf{A} \in \mathbb{R}^{d\times d}$: input matrix with eigendecomposition $\mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T$. $\vec{v}_1$: top eigenvector, being computed, $\vec{z}^{(i)}$: iterate at step i, converging to $\vec{v}_1$.

Claim 1: When $z^{(0)}$ is chosen with random Gaussian entries, writing $z^{(0)} = c_1\vec{v}_1 + c_2\vec{v}_2 + \ldots + c_d\vec{v}_d$, with very high probability, $\max_j \left|\frac{c_j}{c_1}\right| \le O(d^2 \log d)$.

Claim 2: For gap $\gamma = \frac{|\lambda_1| - |\lambda_2|}{|\lambda_1|}$, and $t = \frac{\ln(1/\delta)}{\gamma}$, $\left|\frac{\lambda_i^t}{\lambda_1^t}\right| \le \delta$ for all i.

$$\vec{z}^{(t)} := \frac{c_1\lambda_1^t\vec{v}_1 + \ldots + c_d\lambda_d^t\vec{v}_d}{\|c_1\lambda_1^t\vec{v}_1 + \ldots + c_d\lambda_d^t\vec{v}_d\|_2} \implies$$

$$\|\vec{z}^{(t)} - \vec{v}_1\|_2 \le \left\| \frac{c_1\lambda_1^t\vec{v}_1 + \ldots + c_d\lambda_d^t\vec{v}_d}{\|c_1\lambda_1^t\vec{v}_1\|_2} - \vec{v}_1 \right\|_2$$

$$= \left\| \frac{c_2\lambda_2^t}{c_1\lambda_1^t}\vec{v}_2 + \ldots + \frac{c_d\lambda_d^t}{\lambda_1^t}\vec{v}_d \right\|_2 = \left|\frac{c_2\lambda_2^t}{c_1\lambda_1^t}\right| + \ldots + \left|\frac{c_d\lambda_d^t}{\lambda_1^t}\right| \le \delta \cdot O(d^2 \log d) \cdot d.$$

Setting $\delta = O\left(\frac{\epsilon}{d^3 \log d}\right)$ gives $\|\vec{z}^{(t)} - \vec{v}_1\|_2 \le \epsilon$.

$\mathbf{A} \in \mathbb{R}^{d \times d}$: input matrix with eigendecomposition $\mathbf{A} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T$. $\vec{v}_1$: top eigenvector, being computed, $\vec{z}^{(i)}$: iterate at step i, converging to $\vec{v}_1$.

Theorem (Basic Power Method Convergence)

Let $\gamma = \frac{|\lambda_1| - |\lambda_2|}{|\lambda_1|}$ *be the relative gap between the first and second eigenvalues. If Power Method is initialized with a random Gaussian vector* $\vec{v}^{(0)}$ *then, with high probability, after* $t = O\left(\frac{\ln(d/\epsilon)}{\gamma}\right)$ *steps:*

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

Total runtime: $O(t)$ matrix-vector multiplications. If $\mathbf{A} = \mathbf{X}^T\mathbf{X}$:

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

How is ϵ dependence?

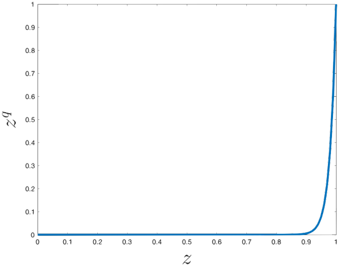
How is γ dependence?

Krylov subspace methods (Lanczos method, Arnoldi method.)

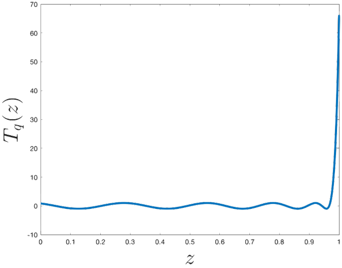
- How `svds`/`eigs` are actually implemented. Only need $t = O\left(\frac{\ln(d/\epsilon)}{\sqrt{\gamma}}\right)$ steps for the same guarantee.

Main Idea: Need to separate λ_1 from λ_i for $i \geq 2$.

- Power method: power up to λ_1^t and λ_i^t.
- Krylov methods: apply a better degree t polynomial $T_t(\cdot)$ to the eigenvalues to separate $T_t(\lambda_1)$ from $T_t(\lambda_i)$.
- Still requires just t matrix vector multiplies. Why?



vs.



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.

- Block Power Method (a.k.a. Simultaneous Iteration, Subspace Iteration, or Orthogonal Iteration)
- Block Krylov methods

$$\text{Runtime: } O\left(ndk \cdot \frac{\ln(d/\epsilon)}{\sqrt{\gamma}}\right)$$

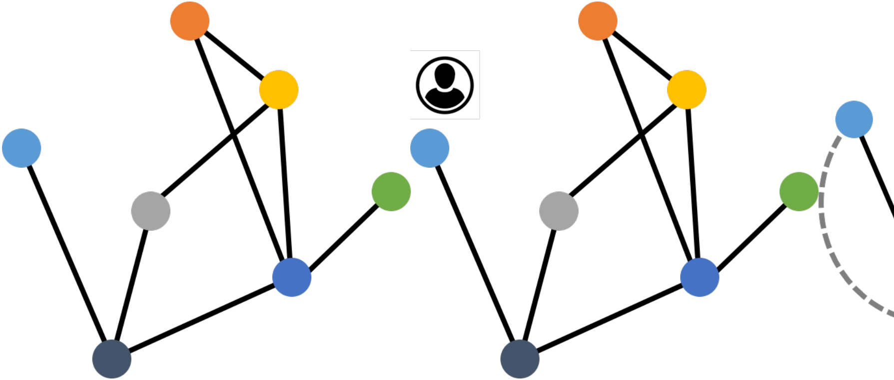
to accurately compute the top k singular vectors.

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

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

Connection Between Random Walks, Eigenvectors, and Power Method (Bonus Material)

Consider a random walk on a graph G with adjacency matrix $\mathbf{A}$.



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

Let $\vec{p}^{(t)} \in \mathbb{R}^n$ have i^{th} entry $\vec{p}_i^{(t)} = \Pr(\text{walk at node i at step t})$.

- **Initialize:** $\vec{p}^{(0)} = [1, 0, 0, \ldots, 0]$.
- **Update:**

$$\begin{aligned}\Pr(\text{walk at i at step t}) &= \sum_{j \in neigh(i)} \Pr(\text{walk at j at step t-1}) \cdot \frac{1}{degree(j)} \\ &= \vec{z}^T \vec{p}^{(t-1)}\end{aligned}$$

where $\vec{z}(j) = \frac{1}{degree(j)}$ for all $j \in neigh(i)$, $\vec{z}(j) = 0$ for all $j \notin neigh(i)$.

- $\vec{z}$ is the i^{th} row of the right normalized adjacency matrix $\mathbf{AD}^{-1}$.
- $\vec{p}^{(t)} = \mathbf{AD}^{-1}\vec{p}^{(t-1)} = \underbrace{\mathbf{AD}^{-1}\mathbf{AD}^{-1}\ldots\mathbf{AD}^{-1}}_{t \text{ times}}\vec{p}^{(0)}$

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

$$\vec{p}^{(t)} = \underbrace{\mathbf{A}\mathbf{D}^{-1}\mathbf{A}\mathbf{D}^{-1}\ldots\mathbf{A}\mathbf{D}^{-1}}_{t \text{ times}}\vec{p}^{(0)}.$$

$$\mathbf{D}^{-1/2}\vec{p}^{(t)} = \underbrace{(\mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2})(\mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2})\ldots(\mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2})}_{t \text{ times}}(\mathbf{D}^{-1/2}\vec{p}^{(0)}).$$

- $\mathbf{D}^{-1/2}\vec{p}^{(t)}$ is exactly what would obtained by applying $t/2$ iterations of power method to $\mathbf{D}^{-1/2}\vec{p}^{(0)}$!
- Will converge to the top eigenvector of the normalized adjacency matrix $\mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}$. Stationary distribution.
- 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 $\mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}$. The spectral gap.