COMPSCI 514: Algorithms for Data Science

Cameron Musco

University of Massachusetts Amherst. Fall 2024.

Lecture 20

Logistics

- Problem Set 4 is due 11/25.
- See Piazza for some updates/clarifications on Problem 1.
- No class or quiz next week.
- Additional office hours Friday 10am.

Summary

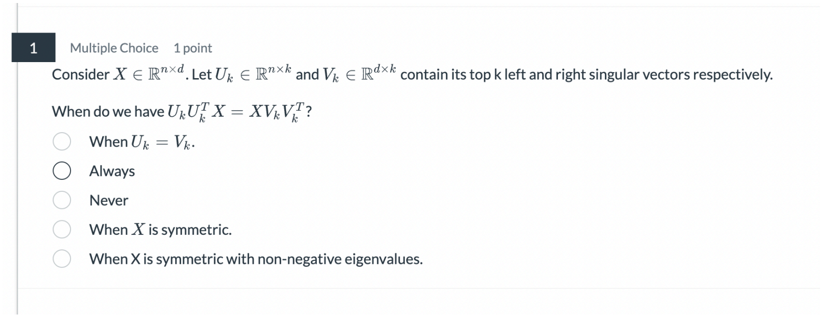
Last Few Classes: Spectral Graph Partitioning

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

Quiz Review



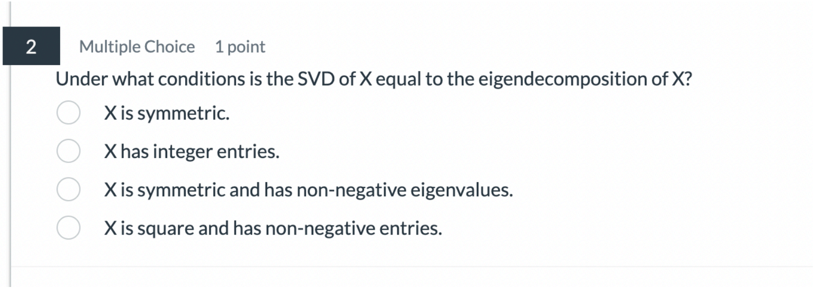
1 Multiple Choice 1 point

Consider $X \in \mathbb{R}^{n \times d}$. Let $U_k \in \mathbb{R}^{n \times k}$ and $V_k \in \mathbb{R}^{d \times k}$ contain its top k left and right singular vectors respectively.

When do we have $U_k U_k^T X = X V_k V_k^T$?

- When $U_k = V_k$.
- Always
- Never
- When X is symmetric.
- When X is symmetric with non-negative eigenvalues.

Quiz Review

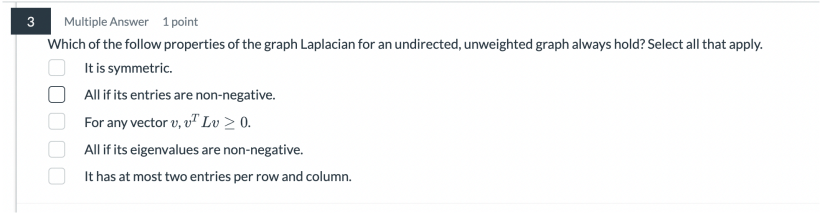


2 Multiple Choice 1 point

Under what conditions is the SVD of X equal to the eigendecomposition of X?

- ◯ X is symmetric.
- ◯ X has integer entries.
- ◯ X is symmetric and has non-negative eigenvalues.
- ◯ X is square and has non-negative entries.

Quiz Review



3 Multiple Answer 1 point

Which of the follow properties of the graph Laplacian for an undirected, unweighted graph always hold? Select all that apply.

- ☐ It is symmetric.
- ☐ All if its entries are non-negative.
- ☐ For any vector v, $v^T Lv \geq 0$.
- ☐ All if its eigenvalues are non-negative.
- ☐ It has at most two entries per row and column.

Efficient Eigendecomposition and SVD

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 large datasets?

Computing the SVD

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.

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 $\mathbf{V}_k \in \mathbb{R}^{d \times k}$ and then compute $\mathbf{U}_k \mathbf{\Sigma}_k = \mathbf{X}\mathbf{V}_k$.
- 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`.

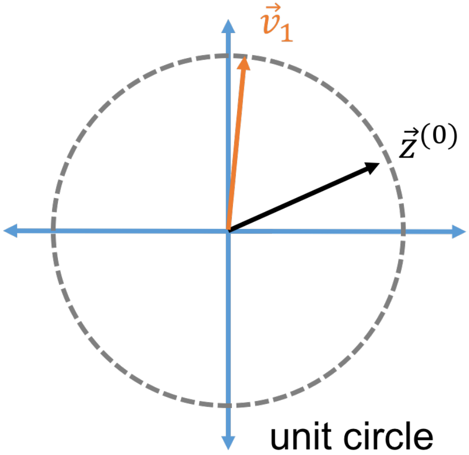
Power Method

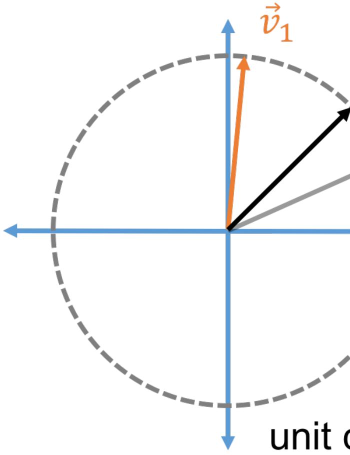
Power Method: The most fundamental iterative method for approximate SVD/eigendecomposition. Applies to computing $k = 1$ eigenvectors, but can be generalized to larger k.

Goal: Given symmetric $\mathbf{A} \in \mathbb{R}^{d \times d}$, with eigendecomposition $\mathbf{A} = \mathbf{V}\boldsymbol{\Lambda}\mathbf{V}^T$, find $\vec{z} \approx \vec{v}_1$. I.e., 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 $\vec{z}_t$

Power Method





Power Method Analysis

Power method:

```
• **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 $\vec{z}_t$.
```

Theoretically equivalent to:

```
• 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 $\vec{z}_t$.
```

Power Method Analysis

Write $\vec{z}^{(0)}$ in $\mathbf{A}$'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 $\vec{v}_1$.

Power Method Analysis

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

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

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

Claim 2:

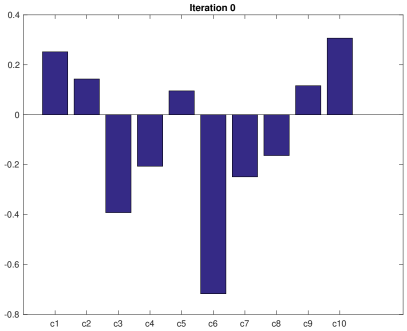
$$\vec{z}^{(t)} = c_1 \cdot \lambda_1^t\vec{v}_1 + c_2 \cdot \lambda_2^t\vec{v}_2 + \ldots + c_d \cdot \lambda_d^t\vec{v}_d.$$

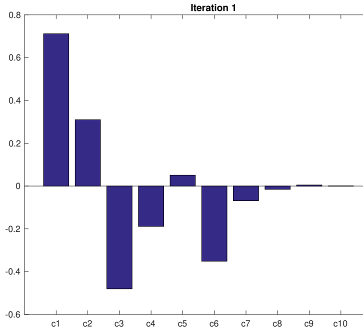
$\mathbf{A} \in \mathbb{R}^{d\times d}$: input matrix with eigendecomposition $\mathbf{A} = \mathbf{V\Lambda V}^T$. $\vec{v}_1$: top eigenvector, being computed, $\vec{z}^{(i)}$: iterate at step i, converging to $\vec{v}_1$.

Power Method Convergence

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.

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



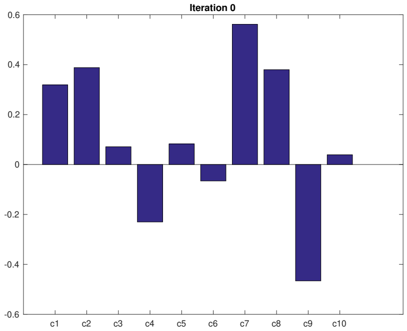


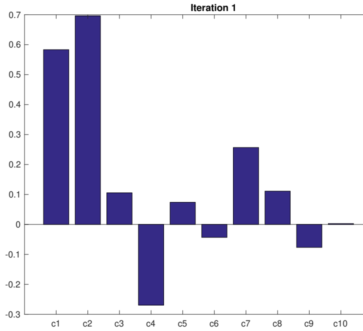
When will convergence be slow?

Power Method Slow Convergence

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

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





Power Method Convergence Rate

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

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 $|\lambda_2|^t \leq \delta \cdot |\lambda_1|^t$ for $\delta > 0$?

$$\begin{aligned} |\lambda_2|^t &= (1-\gamma)^t \cdot |\lambda_1|^t \\ &= (1-\gamma)^{1/\gamma \cdot \gamma t} \cdot |\lambda_1|^t \\ &\leq e^{-\gamma t} \cdot |\lambda_1|^t \end{aligned}$$

So it suffices to set $\gamma t = \ln(1/\delta)$. Or $t = \frac{\ln(1/\delta)}{\gamma}$.

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 $\vec{v}_1$?

$\vec{v}_1$: top eigenvector, being computed, $\vec{z}^{(i)}$: iterate at step i, converging to $\vec{v}_1$. $\lambda_1, \lambda_2, \ldots \lambda_n$: eigenvalues of $\mathbf{A}$, $\gamma = \frac{|\lambda_1|-|\lambda_2|}{|\lambda_1|}$: eigengap controlling convergence rate