## CSCI B609:

## "Foundations of Data Science"

## Lecture 8/9: Faster Power Method

and Applications of SVD

Slides at http://grigory.us/data-science-class.html

## Grigory Yaroslavtsev <br> http://grigory.us

## Faster Power Method

- PM drawback: $A^{T} A$ is dense even for sparse $A$
- Pick random Gaussian $\boldsymbol{x}$ and compute $B^{k} \boldsymbol{x}$
- $\boldsymbol{x}=\sum_{i=1}^{d} c_{i} \boldsymbol{v}_{i}$ (augment $\boldsymbol{v}_{\boldsymbol{i}}$ 's to o.n.b. if $r<\boldsymbol{d}$ )
- $B^{k} \boldsymbol{x} \approx\left(\sigma_{1}^{2 k} \boldsymbol{v}_{1} \boldsymbol{v}_{1}^{T}\right)\left(\sum_{i=1}^{d} c_{i} \boldsymbol{v}_{i}\right)=\sigma_{1}^{2 k} c_{1} \boldsymbol{v}_{1}$

$$
B^{k} \boldsymbol{x}=\left(A^{T} A\right)\left(A^{T} A\right) \ldots\left(A^{T} A\right) \boldsymbol{x}
$$

- Theorem: If $\boldsymbol{x}$ is unit $\mathbb{R}^{d}$-vector, $\left|\boldsymbol{x}^{T} \boldsymbol{v}_{1}\right| \geq \delta$ :
$-V=$ subspace spanned by $\boldsymbol{v}_{i}^{\prime} s$ for $\sigma_{j} \geq(1-\epsilon) \sigma_{1}$
$-\boldsymbol{w}=$ unit vector after $k=\frac{1}{2 \epsilon} \ln \left(\frac{1}{\epsilon \delta}\right)$ iterations of PM
$\Rightarrow \boldsymbol{w}$ has a component at most $\epsilon$ orthogonal to $V$


## Faster Power Method: Analysis

- $A=\sum_{i=1}^{r} \sigma_{i} \boldsymbol{u}_{i} \boldsymbol{v}_{i}^{T}$ and $\boldsymbol{x}=\sum_{i=1}^{d} c_{i} \boldsymbol{v}_{i}$
- $B^{k} \boldsymbol{x}=\sum_{i=1}^{d} \sigma_{i}^{2 k} \boldsymbol{v}_{i} \boldsymbol{v}_{i}^{T} \sum_{j=1}^{d} c_{j} \boldsymbol{v}_{j}=\sum_{i=1}^{d} \sigma_{i}^{2 k} c_{i} \boldsymbol{v}_{i}$

$$
\left\|B^{k} \boldsymbol{x}\right\|_{2}^{2}=\left\|\sum_{i=1}^{d} \sigma_{i}^{2 k} c_{i} \boldsymbol{v}_{i}\right\|_{2}^{2}=\sum_{i=1}^{d} \sigma_{i}^{4 k} c_{i}^{2} \geq \sigma_{1}^{4 k} c_{1}^{2} \geq \sigma_{i}^{4 k} \delta^{2}
$$

- (Squared) component orthogonal to $V$ is

$$
\sum_{i=m+1}^{d} \sigma_{i}^{4 k} c_{i}^{2} \leq(1-\epsilon)^{4 k} \sigma_{1}^{4 k} \sum_{i=m+1}^{d} c_{i}^{2} \leq(1-\epsilon)^{4 k} \sigma_{1}^{4 k}
$$

- Component of $\boldsymbol{w} \perp V \leq(1-\epsilon)^{2 k} / \delta \leq \epsilon$


## Choice of $\boldsymbol{x}$

- $y$ random spherical Gaussian with unit variance
- $\boldsymbol{x}=\frac{y}{\|y\|_{2}}$ :

$$
\operatorname{Pr}\left[\left|x^{T} v\right| \leq \frac{1}{20 \sqrt{d}}\right] \leq \frac{1}{10}+3 e^{-d / 64}
$$

- $\operatorname{Pr}\left[||y||_{2} \geq 2 \sqrt{d}\right] \leq 3 e^{-d / 64}$ (Gaussian Annulus)
- $\boldsymbol{y}^{\boldsymbol{T}} \boldsymbol{v} \sim N(0,1) \Rightarrow \operatorname{Pr}\left[| | \boldsymbol{y}^{\boldsymbol{T}} \boldsymbol{v} \|_{2} \leq \frac{1}{10}\right] \leq \frac{1}{10}$
- Can set $\delta=\frac{1}{20 \sqrt{d}}$ in the "faster power method"


## Singular Vectors and Eigenvectors

- Right singular vectors are eigenvectors of $A^{T} A$
- $\sigma_{i}^{2}$ are eigenvalues of $A^{T} A$
- Left singular vectors are eigenvectors of $A A^{T}$
- $A^{T} A$ satisfies $\forall \boldsymbol{x}: \boldsymbol{x}^{T} B \boldsymbol{x} \geq 0$
$-B=\sum_{i} \sigma_{i}^{2} \boldsymbol{v}_{i} \boldsymbol{v}_{i}^{T}$
$-\forall \boldsymbol{x}: \boldsymbol{x}^{T} \boldsymbol{v}_{i} \boldsymbol{v}_{i}^{T} \boldsymbol{x}=\left(\boldsymbol{x}^{T} \boldsymbol{v}_{i}\right)^{2} \geq 0$
- Such matrices are called positive semi-definite
- Any p.s.d matrix can be decomposed as $A^{T} A$


## Application of SVD: Centering Data

- Minimize sum of squared distances from $\boldsymbol{A}_{\boldsymbol{i}}$ to $S_{k}$
- SVD: best fitting $S_{k}$ if data is centered
- What if not?
- Thm. $S_{k}$ that minimizes squared distance goes through centroid of the point set:

$$
\frac{1}{n} \sum \boldsymbol{A}_{\boldsymbol{i}}
$$

- Will only prove for $k=1$, analogous proof for arbitrary $k$ (see textbook)


## Application of SVD: Centering Data

- Thm. Line that minimizes squared distance goes through the centroid
- Line: $\ell=\boldsymbol{a}+\lambda \boldsymbol{v}$; distance $\operatorname{dist}\left(\boldsymbol{A}_{\boldsymbol{i}}, \ell\right)$
- $\left\|\boldsymbol{A}_{\boldsymbol{i}}-\boldsymbol{a}\right\|_{2}^{2}=\operatorname{dist}\left(\boldsymbol{A}_{\boldsymbol{i}}, \boldsymbol{\ell}\right)^{2}+\left\langle\boldsymbol{v}, \boldsymbol{A}_{\boldsymbol{i}}\right\rangle^{2}$
- Center so that $\sum_{i=1}^{n} \boldsymbol{A}_{\boldsymbol{i}}=\mathbf{0}$ by subtracting the centroid
- $\sum_{i}^{n} \operatorname{dist}\left(\boldsymbol{A}_{\boldsymbol{i}}, \ell\right)^{2}=\sum_{i=1}^{n}\left(| | \boldsymbol{A}_{\boldsymbol{i}}-\boldsymbol{a} \|_{2}^{2}-\left\langle\boldsymbol{v}, \boldsymbol{A}_{\boldsymbol{i}}\right\rangle^{2}\right)$

$$
\begin{gathered}
=\sum_{i=1}^{n}\left(| | \boldsymbol{A}_{\boldsymbol{i}}\left\|_{2}^{2}+\right\| \boldsymbol{a} \|_{2}^{2}-2\left\langle\boldsymbol{A}_{\boldsymbol{i}}, \boldsymbol{a}\right\rangle-\left\langle\boldsymbol{v}, \boldsymbol{A}_{\boldsymbol{i}}\right\rangle^{2}\right) \\
=\sum_{i=1}^{n}| | \boldsymbol{A}_{\boldsymbol{i}}\left\|_{2}^{2}+n| | \boldsymbol{a}\right\|_{2}^{2}-2\left\langle\sum_{i=1}^{n} \boldsymbol{A}_{\boldsymbol{i}}, \boldsymbol{a}\right\rangle-\sum_{i=1}^{n}\left\langle\boldsymbol{v}, \boldsymbol{A}_{\boldsymbol{i}}\right\rangle^{2} \\
=\sum_{i=1}^{n}| | \boldsymbol{A}_{\boldsymbol{i}}\left\|_{2}^{2}+n| | \boldsymbol{a}\right\|_{2}^{2}-\sum_{i=1}^{n}\left\langle\boldsymbol{v}, \boldsymbol{A}_{\boldsymbol{i}}\right\rangle^{2}
\end{gathered}
$$

- Minimized when $\boldsymbol{a}=\mathbf{0}$


## Principal Component Analysis

- $\boldsymbol{n} \times d$ matrix: customers $\times$ movies preference
- $\boldsymbol{n}=$ \#customers, $\boldsymbol{d}=$ \#movies
- $A_{i j}=$ how much customer $i$ likes movie $j$
- Assumption: $A_{i j}$ can be described with $k$ factors
- Customers and movies: vectors in $\boldsymbol{u}_{\boldsymbol{i}}$ and $\boldsymbol{v}_{\boldsymbol{i}} \in \mathbb{R}^{k}$
$-A_{i j}=\left\langle\boldsymbol{u}_{\boldsymbol{i}}, \boldsymbol{v}_{\boldsymbol{j}}\right\rangle$
- Solution: $A_{k}$



## Class Project

- Survey of 3-5 research papers
- Closely related to the topics of the class
- Algorithms for high-dimensional data
- Fast algorithms for numerical linear algebra
- Algorithms for machine learning and/or clustering
- Algorithms for streaming and massive data
- Office hours if you need suggestions
- Individual (not a group) project
- 1-page Proposal Due: October 31, 2016 at 23:59 EST
- Final Deadline: December 09, 2016 at 23:59 EST
- Submission by e-mail to Lisul Islam (IU id: islammdl)
- Submission Email Title: Project + Space + "Your Name"
- Submission format: PDF from LaTeX


## Separating mixture of $k$ Gaussians

- Sample origin problem:
- Given samples from $k$ well-separated spherical Gaussians
- Q: Did they come from the same Gaussian?
- $\delta=$ distance between centers
- For two Gaussians naïve separation requires

$$
\delta>\omega\left(d^{1 / 4}\right)
$$

- Thm. $\delta=\Omega\left(k^{\frac{1}{4}}\right)$ suffices
- Idea:
- Project on a $\boldsymbol{k}$-dimensional subspace through centers
- Key fact: This subspace can be found via SVD
- Apply naïve algorithm


## Separating mixture of $k$ Gaussians

- Easy fact: Projection preserves the property of being a unit-variance spherical Gaussian
- Def. If $p$ is a probability distribution, best fit line $\{c \boldsymbol{v}, c \in \mathbb{R}\}$ is:

$$
\boldsymbol{v}=\operatorname{argmax}_{|\boldsymbol{v}|=1} \mathbb{E}_{\boldsymbol{x} \sim p}\left[\left(\boldsymbol{v}^{\boldsymbol{T}} \boldsymbol{x}\right)^{2}\right]
$$

- Thm: Best fit line for a Gaussian centered at $\boldsymbol{\mu}$ passes through $\boldsymbol{\mu}$ and the origin


## Best fit line for a Gaussian

- Thm: Best fit line for a Gaussian centered at $\boldsymbol{\mu}$ passes through $\boldsymbol{\mu}$ and the origin

$$
\begin{aligned}
& \mathbb{E}_{\boldsymbol{x} \sim p}\left[\left(\boldsymbol{v}^{\boldsymbol{T}} \boldsymbol{x}\right)^{2}\right]=\mathbb{E}_{\boldsymbol{x} \sim p}\left[\left(\boldsymbol{v}^{\boldsymbol{T}}(\boldsymbol{x}-\boldsymbol{\mu})+\boldsymbol{v}^{\boldsymbol{T}} \boldsymbol{\mu}\right)^{2}\right] \\
& =\mathbb{E}_{\boldsymbol{x} \sim p}\left[\boldsymbol{v}^{\boldsymbol{T}}(\boldsymbol{x}-\boldsymbol{\mu})^{2}+2\left(\boldsymbol{v}^{\boldsymbol{T}} \boldsymbol{\mu}\right) \boldsymbol{v}^{\boldsymbol{T}}(\boldsymbol{x}-\boldsymbol{\mu})+\left(\boldsymbol{v}^{\boldsymbol{T}} \boldsymbol{\mu}\right)^{2}\right] \\
& =\mathbb{E}_{\boldsymbol{x} \sim p}\left[\boldsymbol{v}^{\boldsymbol{T}}(\boldsymbol{x}-\boldsymbol{\mu})^{2}\right]+2\left(\boldsymbol{v}^{\boldsymbol{T}} \boldsymbol{\mu}\right) \mathbb{E}_{\boldsymbol{x} \sim p}\left[\boldsymbol{v}^{\boldsymbol{T}}(\boldsymbol{x}-\boldsymbol{\mu})\right]+\left(\boldsymbol{v}^{\boldsymbol{T}} \boldsymbol{\mu}\right)^{2} \\
& =\mathbb{E}_{\boldsymbol{x} \sim p}\left[\boldsymbol{v}^{\boldsymbol{T}}(\boldsymbol{x}-\boldsymbol{\mu})^{2}\right]+\left(\boldsymbol{v}^{\boldsymbol{T}} \boldsymbol{\mu}\right)^{2} \\
& =\sigma^{2}+\left(\boldsymbol{v}^{\boldsymbol{T}} \boldsymbol{\mu}\right)^{2}
\end{aligned}
$$

- Where we used:

$$
\begin{aligned}
& -\mathbb{E}_{x \sim p}\left[\boldsymbol{v}^{T}(\boldsymbol{x}-\boldsymbol{\mu})\right]=\mathbf{0} \\
& -\mathbb{E}_{\boldsymbol{x \sim p}}\left[\boldsymbol{v}^{T}(\boldsymbol{x}-\boldsymbol{\mu})^{2}\right]=\sigma^{2}
\end{aligned}
$$

- Best fit line maximizes $\left(\boldsymbol{v}^{\boldsymbol{T}} \boldsymbol{\mu}\right)^{2}$


## Best fit subspace for one Gaussian

- Best fit $k$-dimensional subspace $\boldsymbol{V}_{k}$ :

$$
\boldsymbol{V}_{k}=\underset{\boldsymbol{V}: \operatorname{dim}(\boldsymbol{V})=k}{\operatorname{argmax}} \mathbb{E}_{\boldsymbol{x} \sim p}\left[| | \operatorname{proj}(\boldsymbol{x}, \boldsymbol{V}) \|_{2}^{2}\right]
$$

- For a spherical Gaussian $\boldsymbol{V}$ is a best-fit $k$ dimensional subspace iff it contains $\boldsymbol{\mu}$
- If $\boldsymbol{\mu}=0$ then any $k$-dim. subspace is best fit
- If $\boldsymbol{\mu} \neq 0$ then best fit line $\boldsymbol{v}$ goes through $\boldsymbol{\mu}$
- Same greedy process as SVD projects on $v$
- After projection we have Gaussian with $\boldsymbol{\mu}=0$
- Any ( $k-1$ )-dimensional subspace would do


## Best fit subspace for $k$ Gaussians

- Thm. $\boldsymbol{p}$ is a mixture of $k$ spherical Gaussians $\Rightarrow$ best fit $k$-dim. subspace contains their centers
- $p=w_{1} \boldsymbol{p}_{1}+w_{2} \boldsymbol{p}_{2}+\cdots+w_{k} \boldsymbol{p}_{k}$
- Let $\boldsymbol{V}$ be a subspace of dimension $\leq k$

$$
\mathbb{E}_{\boldsymbol{x} \sim \boldsymbol{p}}\left[| | \operatorname{proj}(\boldsymbol{x}, \boldsymbol{V}) \|_{2}^{2}\right]=\sum_{i=1}^{k} w_{i} \mathbb{E}_{\boldsymbol{x} \sim p_{i}}\left[| | \operatorname{proj}(\boldsymbol{x}, \boldsymbol{V}) \|_{2}^{2}\right]
$$

- Each term is maximized if $\boldsymbol{V}$ contains all $\boldsymbol{\mu}_{i}^{\prime} s$
- If we only have a finite number of samples then accuracy has to be analyzed carefully


## HITS Algorithm for Hubs and Authorities

- Document ranking: project on $1^{\text {st }}$ singular vector
- WWW: directed graph with links = edges
- $\boldsymbol{n}$ Authorities: pages containing original info
- $d$ Hubs: collections of links to authorities
- Authority depends on importance of pointing hubs
- Hub quality depends on how authoritative links are
- Authority vector: $\boldsymbol{v}_{\boldsymbol{j}}, j=1, \ldots, \boldsymbol{n}: \boldsymbol{v}_{\boldsymbol{j}} \sim \sum_{i=1}^{d} \boldsymbol{u}_{i} \boldsymbol{A}_{i j}$
- Hub vector: $u_{i}, i=1, \ldots, d: u_{i} \sim \sum_{j=1}^{n} v_{j} A_{i j}$
- Use power method: $\boldsymbol{u}=\boldsymbol{A} \boldsymbol{v}, \boldsymbol{v}=\boldsymbol{A}^{\boldsymbol{T}} \boldsymbol{u}$
- Converges to first left/right singular vectors


## Exercises

- Ex. 1: $A$ is $n \times n$ matrix with orthonormal rows - Show that it has orthonormal columns
- Ex. 2: Interpret the left and right singular vectors of the document $x$ term matrix
- Ex. 3. Use power method to compute singular values of the matrix:

$$
\left(\begin{array}{ll}
1 & 2 \\
3 & 4
\end{array}\right)
$$

