

# Discovery of Latent Factors in High-dimensional Data via Spectral Methods

**Furong Huang**

University of Maryland

Workshop on Quantum Machine Learning

# Machine Learning - Excitements

## Success of Supervised Learning



Image classification



Speech recognition



Text processing

# Machine Learning - Excitements

## Success of Supervised Learning



Image classification



Speech recognition



Text processing

## Key to Success

- Deep composition of nonlinear units
- Enormous labeled data
- Computation power growth

# Machine Learning - Modern Challenges

Automated discovery of features and categories?



Filter bank learning



Feature extraction



Embeddings, Topics

# Machine Learning - Modern Challenges

Automated discovery of features and categories?

Real AI requires **Unsupervised Learning**



Filter bank learning



Feature extraction



Embeddings, Topics

- Summarize key features in data
  - ▶ State-of-the-art: Humans are better than machines
  - ▶ Goal: Intelligent machines that summarize key features in data
- Interpretable modeling and learning of the data
  - ▶ Theoretically guaranteed learning
  - ▶ Extracted features are interpretable

# Unsupervised Learning with Big Data

## Curse of Dimensionality

- **More information** → **more unknowns/variables** → **challenging model learning**



**PubMed**  
[www.pubmed.gov](http://www.pubmed.gov)

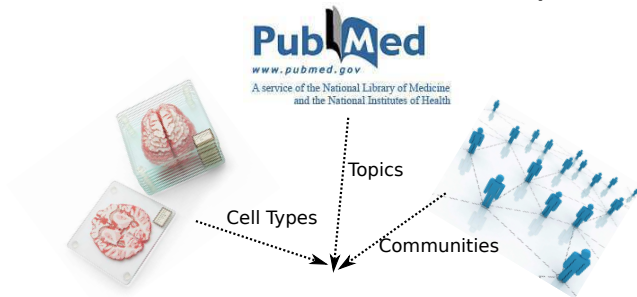
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# Unsupervised Learning with Big Data

## Information Extraction

- **High dimension observation** vs **Low dimension representation**



# Unsupervised Learning with Big Data

## Information Extraction

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Finding Needle In the Haystack Is Challenging



# Unsupervised Learning with Big Data

## Information Extraction

- **High dimension observation** vs **Low dimension representation**



**My Solution: A Unified Tensor Decomposition Framework**

# App 1: Automated Categorization of Documents

SECTIONS

HOME

SEARCH

The New York Times

COLLEGE FOOTBALL

## At Florida State, Football Clouds Justice

Now, an examination by The New York Times of police and court records, along with interviews with crime witnesses, has found that, far from an aberration, the treatment of the Winston complaint was in keeping with the way the police on numerous occasions have soft-pedaled allegations of wrongdoing by Seminoles football players. From criminal mischief and motor-vehicle theft to domestic violence, arrests have been avoided, investigations have stalled and players have escaped serious consequences.

In a community whose self image and economic well-being are so tightly bound to the fortunes of the nation's top-ranked college football team, law enforcement officers are finely attuned to a suspect's football connections. Those ties are cited repeatedly in police reports examined by The Times. What's more, dozens of officers work second jobs directing traffic and providing security at home football games and many express their devotion to the Seminoles on social media.

On Jan. 10, 2013, a female student at Florida State spotted the man she believed had raped her the previous month. After learning his name, Jameis Winston, she reported him to the Tallahassee police.

In the 22 months since, Florida State officials have said little about how they handled the case, which is no different from the way the federal Department aggressively investigated the rape accusation. It did not become public until November, when a Tampa reporter, Matt Baker, acting on a tip, sought records of the police investigation.

Upon learning of Mr. Baker's inquiry, Florida State, having shown little curiosity about the rape accusation, suddenly took a keen interest in the journalist seeking to report it, according to emails obtained by The Times.

"Can you share any details on the requesting source?" David Perry, the university's police chief, asked the Tallahassee police. Several hours later, Mr.

TMZ, the gossip website, also requested the police report and later asked the school's deputy police chief, Jim L. Russell, if the campus police had interviewed Mr. Winston about the rape report. Mr. Russell responded by saying his officers were not investigating the case, omitting any reference to the city police, even though the campus police knew of their involvement. "Thank you for contacting me regarding this rumor — I am glad I can dispel that one!" Mr. Russell told TMZ in an email. The university said Mr. Russell was unaware of any other police investigation at the time of the inquiry. Soon after, the Tallahassee police belatedly sent their files to the news media and to the prosecutor, William N. Meggs. By then critical evidence had been lost and Mr. Meggs, who criticized the police's handling of the case, declined to

loom after the Seminoles' first game, five am's second-leading receiver.

## Document modeling

- **Observed:** words in document corpus: search logs, emails etc
- **Hidden:** (mixed) topics: personal interests, professional area etc

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Topics

Education

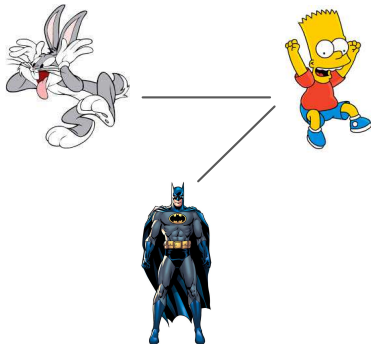
Crime

Sports

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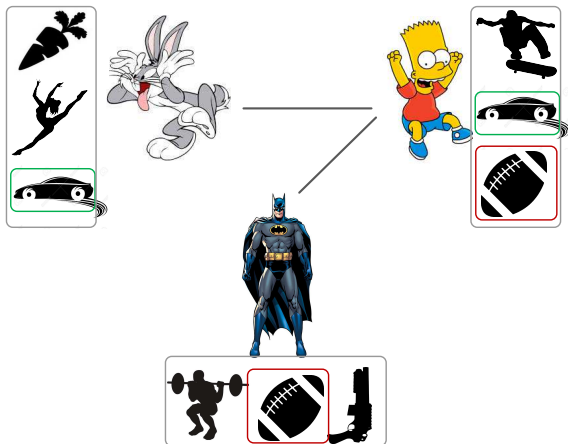
## App 2: Community Extraction From Connectivity Graph



### Social Networks

- **Observed:** network of social ties: friendships, transactions etc
- **Hidden:** (mixed) groups/communities of social actors

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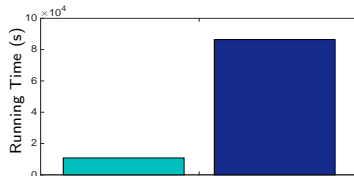
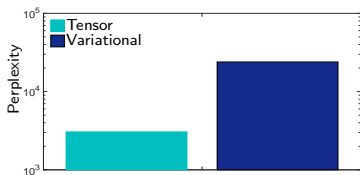


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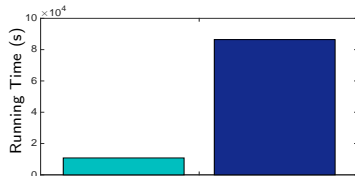
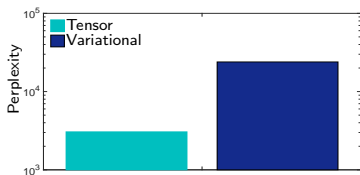
# Tensor Methods Compared with Variational Inference

Learning Topics from PubMed on Spark: 8 million docs



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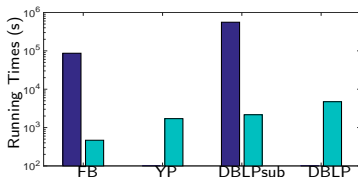
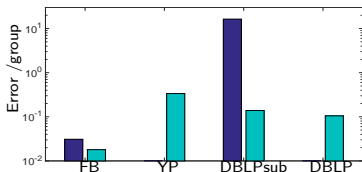


Learning Communities from Graph Connectivity

Facebook:  $n \sim 20k$     Yelp:  $n \sim 40k$

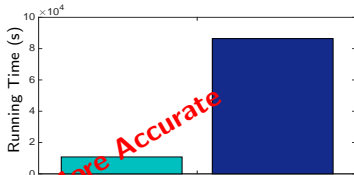
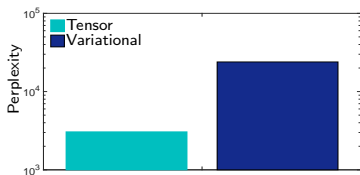
DBLPsub:  $n \sim 0.1m$

DBLP:  $n \sim 1m$



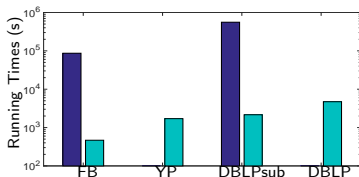
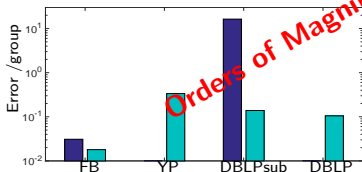
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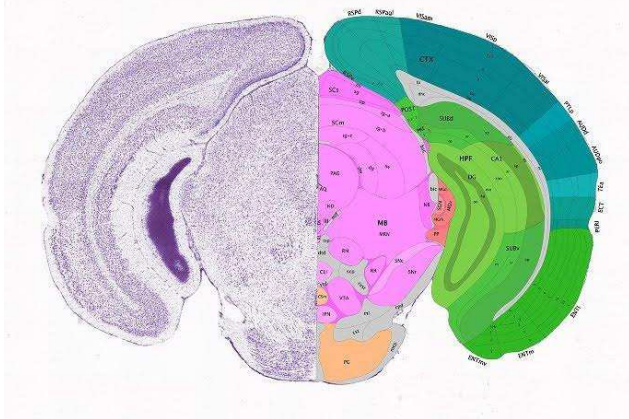


"Online Tensor Methods for Learning Latent Variable Models", F. Huang, U. Niranjan, M. Hakeem, A. Anandkumar, JMLR14.

"Tensor Methods on Apache Spark", F. Huang, A. Anandkumar, Oct. 2015.



# App 3: Cataloging Neuronal Cell Types In the Brain

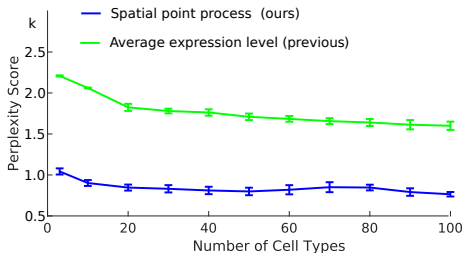


## Neuroscience

- **Observed:** cellular-resolution brain slices
- **Hidden:** neuronal cell types

# App 3: Cataloging Neuronal Cell Types In the Brain

- Our method vs Average expression level [Grange 14']



## Recovered known cell types

1 *Interneurons*

2 *S1Pyramidal*

3 *Astrocytes*

4 *Ependymal*

5 *Microglia*

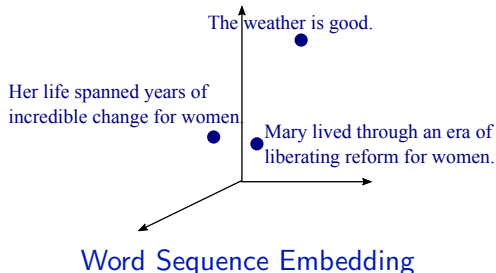
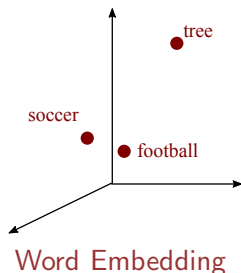
6 *Endothelial*

7 *Mural*

8 *Oligodendrocytes*

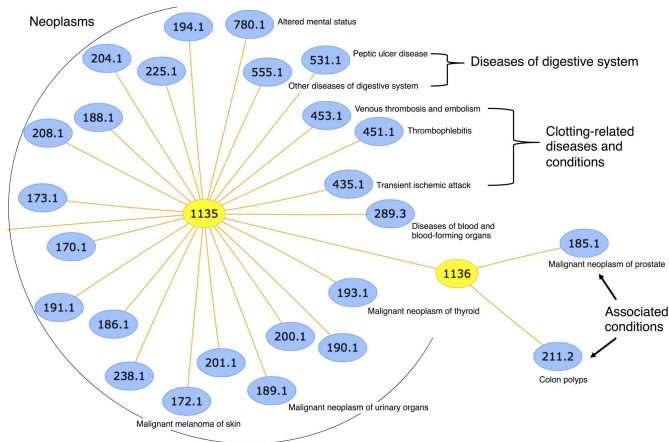
"Discovering Neuronal Cell Types and Their Gene Expression Profiles Using a Spatial Point Process Mixture Model", F. Huang, A. Anandkumar, C. Borgs, J. Chayes, E. Fraenkel, M. Hawrylycz, E. Lein, A. Ingrosso, S. Turaga, NIPS 2015 BigNeuro workshop.

## App 4: Word Sequence Embedding Extraction



# App 5: Human Disease Hierarchy Discovery

CMS: 1.6 million patients, 168 million diagnostic events, 11 k diseases.



- **Observed:** co-occurrence of diseases on patients
- **Hidden:** disease similarity/hierarchy

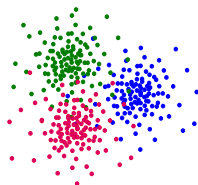
" Scalable Latent TreeModel and its Application to Health Analytics " by F. Huang, N. U.Niranjan, I. Perros, R. Chen, J. Sun, A. Anandkumar, NIPS 2015 MLHC workshop.

Involve discovering the hidden and compact structure  
that is embedded in the high-dimensional complex observed data

# How to model hidden effects?

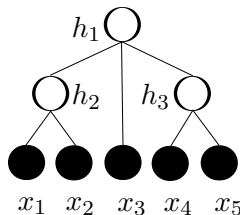
## Basic Approach: mixtures/clusters

- Hidden variable  $h$  is **categorical**.



## Advanced: Probabilistic models

- Hidden variable  $h$  has more general distributions.
- Can model mixed memberships.



This talk: basic mixture model and some advanced models (topic model)

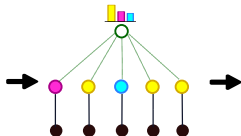
# Challenges in Learning

Basic goal in all mentioned applications

Discover hidden structure in data: **unsupervised** learning.



Unlabeled data



Latent variable model

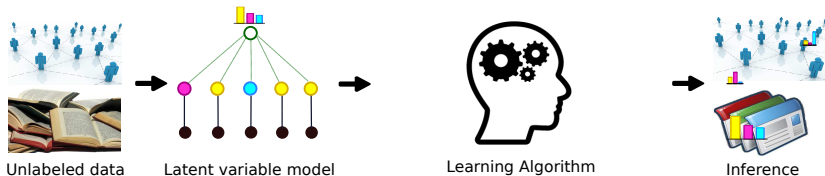


Learning Algorithm



Inference

# Challenges in Learning – find hidden structure in data

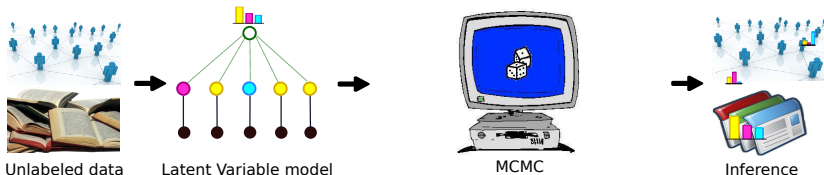


## Challenge: Conditions for Identifiability

- Whether can model be identified given **infinite computation and data**?
- Are there **tractable algorithms** under identifiability?



# Challenges in Learning – find hidden structure in data



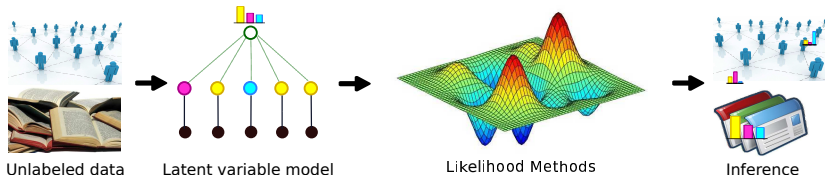
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## Challenge: Efficient Learning of Latent Variable Models

- MCMC: **random sampling**, **slow**  
Exponential mixing time

# Challenges in Learning – find hidden structure in data



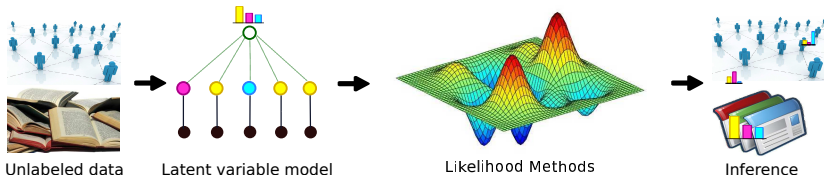
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Exponential critical points

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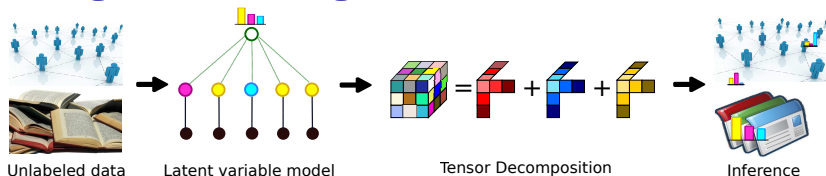
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- Efficient **computational** and **sample complexities**?

# Challenges in Learning – find hidden structure in data



## Challenge: Conditions for Identifiability

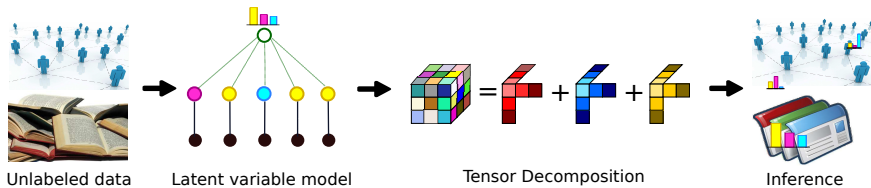
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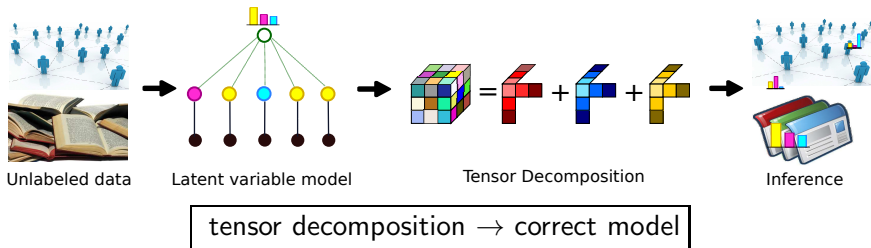
Guaranteed and efficient learning through spectral methods

# Unsupervised Learning via Probabilistic Models



tensor decomposition  $\rightarrow$  correct model

# Unsupervised Learning via Probabilistic Models



## Contributions

- Guaranteed **online** algorithm with **global convergence** guarantee
- Highly **scalable**, highly **parallel**, dimensionality reduction
- Tensor library on **CPU/GPU/Spark**
- **Interdisciplinary** applications
- Extension to model with **group invariance**

# Outline

- 1 Introduction
- 2 Introduction of Method of Moments and Tensor Notations
- 3 LDA and Community Models
  - From Data Aggregates to Model Parameters
  - Guaranteed Online Algorithm
- 4 Quantum Algorithms for Leading Eigenvector Computation
- 5 Conclusion

# Method-of-Moments At A Glance

- 1 Determine **function of model parameters**  $\theta$  estimatable from observable data:

- ▶ **Moments**

$$\mathbb{E}_{\theta}[f(\mathbf{X})]$$

- 2 Form estimates of moments using data (iid samples  $\{x_i\}_{i=1}^n$ ):

- ▶ **Empirical Moments**

$$\hat{\mathbb{E}}[f(\mathbf{X})]$$

- 3 Solve the approximate equations for parameters  $\theta$ :

- ▶ **Moment matching**

$$\mathbb{E}_{\theta}[f(\mathbf{X})] \stackrel{n \rightarrow \infty}{=} \hat{\mathbb{E}}[f(\mathbf{X})]$$

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## Toy Example

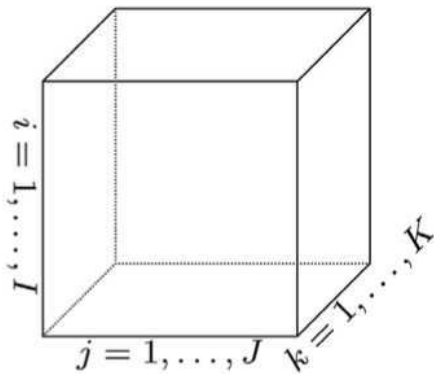
How to estimate Gaussian variable, i.e.,  $(\mu, \Sigma)$ ,  
given iid samples  $\{x_i\}_{i=1}^n \sim \mathcal{N}(\mu, \Sigma^2)$ ?



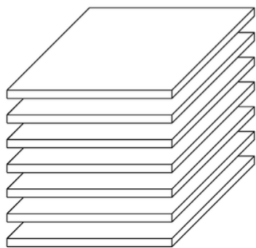
# What is a tensor?

## Multi-dimensional Array

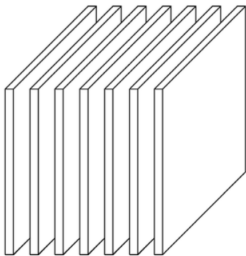
- Tensor - Higher order matrix
- The number of dimensions is called tensor order.



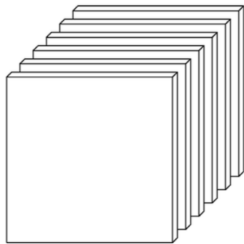
## Slices



- Horizontal slices

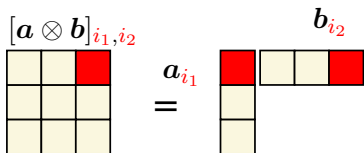


- Lateral slices

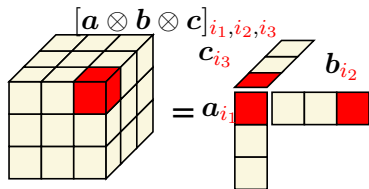


- Frontal slices

# Tensor Product

$$[a \otimes b]_{i_1, i_2} = a_{i_1} b_{i_2}$$


- $[a \otimes b]_{i_1, i_2} = a_{i_1} b_{i_2}$
- Rank-1 matrix

$$[a \otimes b \otimes c]_{i_1, i_2, i_3} = a_{i_1} b_{i_2} c_{i_3}$$


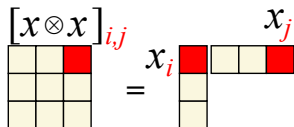
- $[a \otimes b \otimes c]_{i_1, i_2, i_3} = a_{i_1} b_{i_2} c_{i_3}$
- Rank-1 tensor

# Tensors in Method of Moments

## Matrix: Pair-wise relationship

- Signal or data observed  $\mathbf{x} \in \mathbb{R}^d$
- Rank 1 matrix:  $[\mathbf{x} \otimes \mathbf{x}]_{i,j} = x_i x_j$
- Aggregated pair-wise relationship

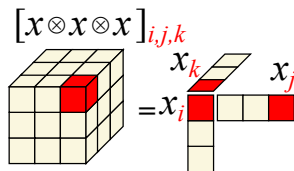
$$\mathbf{M}_2 = \mathbb{E}[\mathbf{x} \otimes \mathbf{x}]$$


$$[\mathbf{x} \otimes \mathbf{x}]_{i,j} = x_i x_j$$

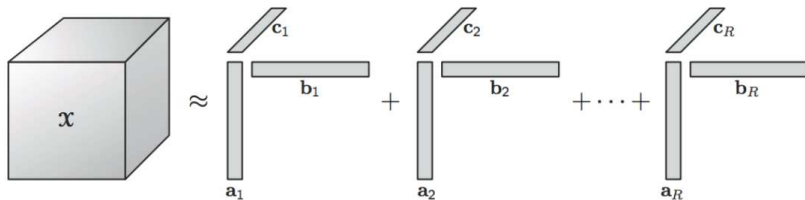
## Tensor: Triple-wise relationship or higher

- Signal or data observed  $\mathbf{x} \in \mathbb{R}^d$
- Rank 1 tensor:  
 $[\mathbf{x} \otimes \mathbf{x} \otimes \mathbf{x}]_{i,j,k} = x_i x_j x_k$
- Aggregated triple-wise relationship

$$\mathcal{M}_3 = \mathbb{E}[\mathbf{x} \otimes \mathbf{x} \otimes \mathbf{x}] = \mathbb{E}[\mathbf{x} \otimes^3]$$


$$[\mathbf{x} \otimes \mathbf{x} \otimes \mathbf{x}]_{i,j,k} = x_i x_j x_k$$

# CP decomposition



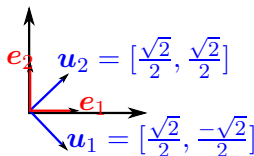
- $\mathcal{X} = \sum_{h=1}^R \mathbf{a}_h \otimes \mathbf{b}_h \otimes \mathbf{c}_h$
- Summation of rank-1 tensors

# Why are tensors powerful?

## Matrix Orthogonal Decomposition

- **Not unique** without eigenvalue gap

$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \mathbf{e}_1 \mathbf{e}_1^\top + \mathbf{e}_2 \mathbf{e}_2^\top = \mathbf{u}_1 \mathbf{u}_1^\top + \mathbf{u}_2 \mathbf{u}_2^\top$$



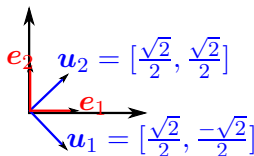
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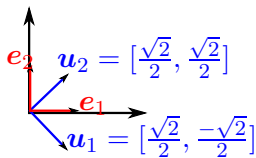
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- **Unique** with eigenvalue gap



## Tensor Orthogonal Decomposition (Harshman, 1970)

- **Unique**: eigenvalue gap not needed

$$\text{Tensor} = \mathbf{u}_1 \otimes \mathbf{u}_1 \otimes \mathbf{u}_1 + \mathbf{u}_2 \otimes \mathbf{u}_2 \otimes \mathbf{u}_2$$



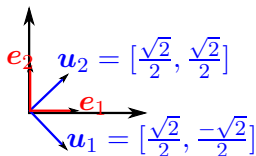
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- **Unique** with eigenvalue gap



## Tensor Orthogonal Decomposition (Harshman, 1970)

- **Unique**: eigenvalue gap not needed
- Slice of tensor has eigenvalue gap

$$\text{Slice}_i = u_1(i) u_1 \otimes u_1 + u_2(i) u_2 \otimes u_2$$

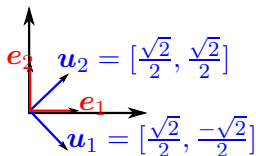
# Why are tensors powerful?

## Matrix Orthogonal Decomposition

- **Not unique** without eigenvalue gap

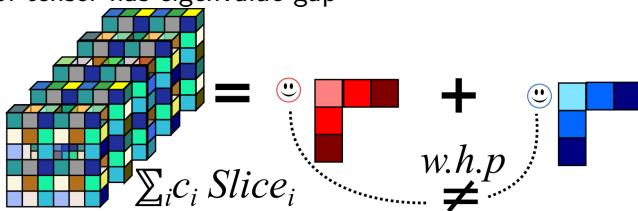
$$\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \mathbf{e}_1 \mathbf{e}_1^\top + \mathbf{e}_2 \mathbf{e}_2^\top = \mathbf{u}_1 \mathbf{u}_1^\top + \mathbf{u}_2 \mathbf{u}_2^\top$$

- **Unique** with eigenvalue gap



## Tensor Orthogonal Decomposition (Harshman, 1970)

- **Unique**: eigenvalue gap not needed
- Slice of tensor has eigenvalue gap



# Outline

- 1 Introduction
- 2 Introduction of Method of Moments and Tensor Notations
- 3 LDA and Community Models
  - From Data Aggregates to Model Parameters
  - Guaranteed Online Algorithm
- 4 Quantum Algorithms for Leading Eigenvector Computation
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# Probabilistic Topic Models - LDA

## Bag of words

## Generative model

- Infer topics of documents
- Learn hidden process drives the obs.
- Topic proportion  $\sim \text{Dir}(\alpha)$  for a doc
- Draw a topic, then a word for a token

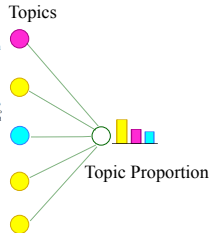
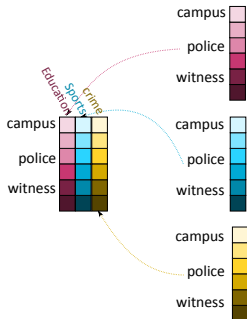


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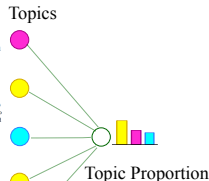
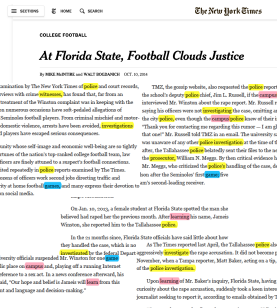
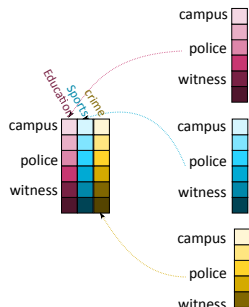


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## Goal



- Topic-word matrix

$$\mathbb{P}[\text{word} = e_i | \text{topic} = j]$$

# Moments Matching

Goal: Linearly independent topic-word table



campus

police

witness

$$\mathbb{E}[\text{word} | \text{topic} = j] = \sum_i \mathbb{P}[\text{word} = e_i | \text{topic} = j] e_i = \text{column } j$$



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No unique decomposition of vectors

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$$\mathbb{E}[\text{word}|\text{topic} = j] = \sum_i \mathbb{P}[\text{word} = e_i|\text{topic} = j]e_i = \text{column } j$$

$M_2$ : Modified Co-occurrence Frequency of Word Pairs

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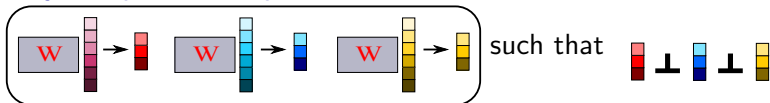


Matrix decomposition recovers subspace, not actual model

# Moments Matching

Goal: Linearly independent topic-word table

Find a  $W$



$M_2$ : Modified Co-occurrence Frequency of Word Pairs

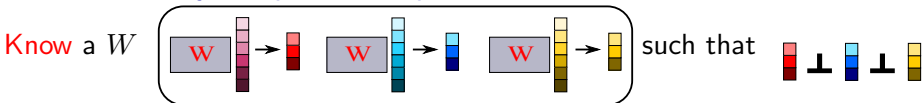
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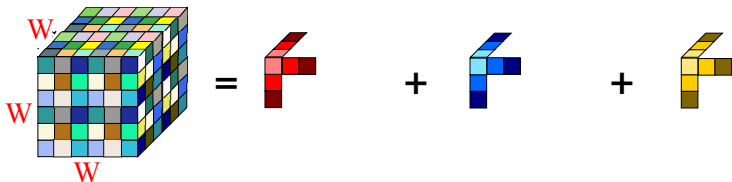
Many such  $W$ 's, find one, project data with  $W$

# Moments Matching

Goal: Linearly independent topic-word table



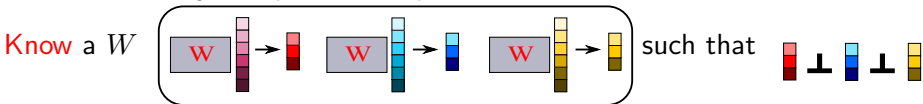
$M_3$ : Modified Co-occurrence Frequency of Word Triplets



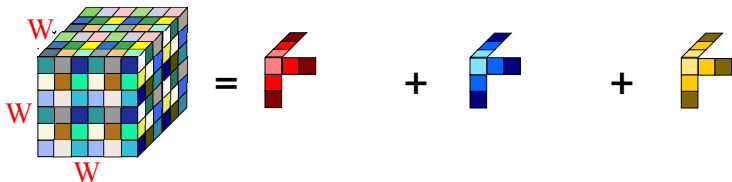
Unique orthogonal tensor decomposition, project result with  $W^\dagger$

# Moments Matching

Goal: Linearly independent topic-word table



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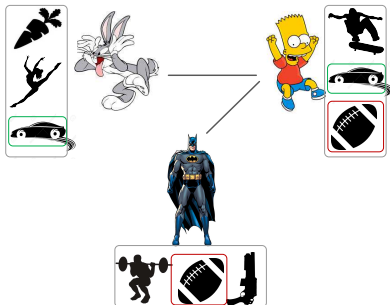


Tensor decomposition uniquely discovers the correct model

Learning Topic Models through Matrix/Tensor Decomposition

# Mixed Membership Community Models

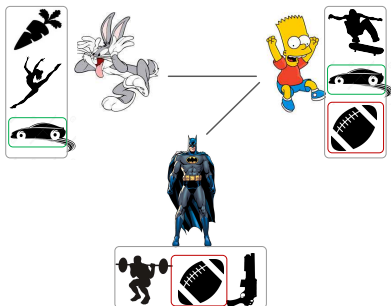
## Mixed memberships



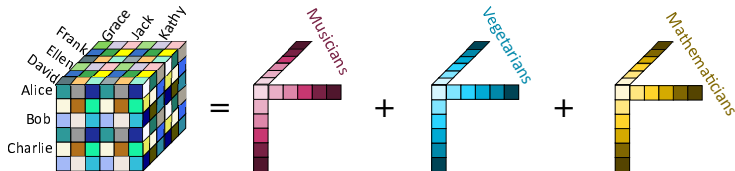


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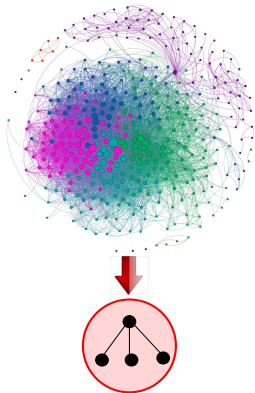
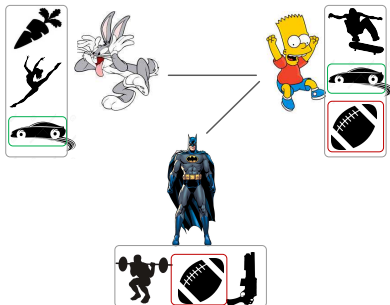


## What ensures guaranteed learning?

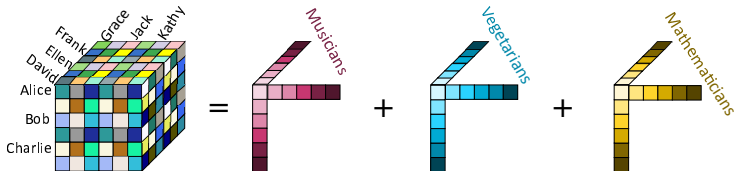


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**Theorem:** The proposed objective function has **equivalent local optima**.

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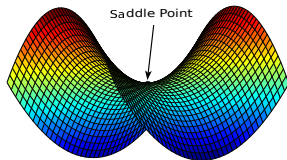
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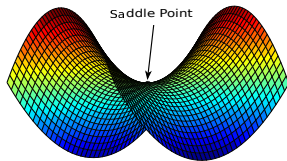
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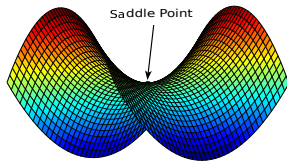
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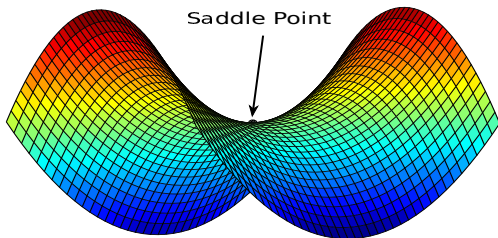


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Global Convergence Guarantee For Online Tensor Decomposition

# Why could we escape from saddle points?

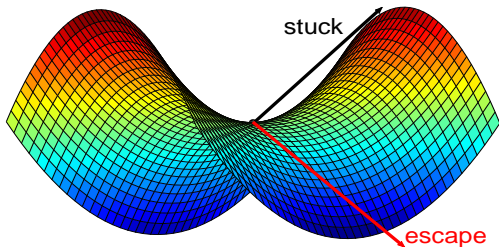
Stochastic Gradient Descent with Noise



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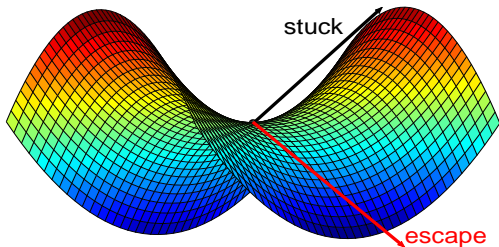
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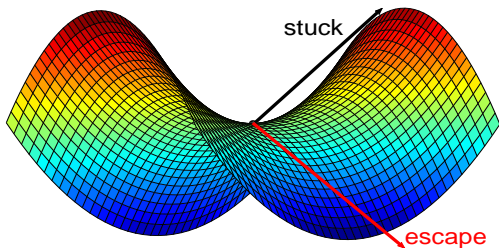
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Noise could help!

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# First PCA

## PCA problem

- Sample  $S = \{\mathbf{x}_i\}_{i=1}^m$ , where  $\mathbf{x}_i \in \mathbb{R}^d$
- Q: Identifies the direction of the largest variance in the data?

## Problem Formulation

Solving

$$\max_{\mathbf{u} \in \mathbb{R}^d, \|\mathbf{u}\|_2=1} \mathbf{u}^\top \mathbf{A} \mathbf{u},$$

where covariance matrix  $\mathbf{A} = \frac{1}{m} \sum_{i=1}^m \mathbf{x}_i \mathbf{x}_i^\top$

## Problem Regime

- Assume  $0 \preceq \mathbf{A} \preceq \mathbf{I}$  and  $s$ -sparse (i.e.,  $\text{nnz}(\text{each row or column}) \leq s$ )



# Classical Algorithm

## Spectral Gap

- Spectral gap  $\Delta = \lambda_1 - \lambda_2$ 
  - ▶ ordered eigenvalues  $1 \geq \lambda_1 \geq \dots \lambda_d \geq 0$
  - ▶ and corresponding eigenvectors  $\mathbf{u}_1, \dots, \mathbf{u}_d$ .

## Methods under Warm Start

- Warm start: Initialization  $\mathbf{v}_0$  such that  $|\langle \mathbf{v}_0, \mathbf{u}_1 \rangle| > \phi > 0$
- Iteration methods achieve  $\epsilon$  precision:  $\langle \mathbf{v}_k, \mathbf{u}_1 \rangle \geq 1 - \epsilon$ 
  - ▶ Power method  $\frac{\mathbf{A}^k \mathbf{v}_0}{\|\mathbf{A}^k \mathbf{v}_0\|}$  takes  $O(\frac{sd}{\Delta} \log(\frac{1}{\phi\epsilon}))$
  - ▶ Lanczos method or accelerated power method takes  $O(\frac{sd}{\sqrt{\Delta}} \log(\frac{1}{\phi\epsilon}))$
  - ★ Replacing the monomial  $\mathbf{A}^k$  by its Chebyshev polynomial approximation

---

Question: Speedup from  $O(d)$  to  $\text{poly}(\log d)$ ?

# Quantum Speedup

## Motivation

Quantum effects can achieve significant speedup.

## Examples

- Shor's algorithm
  - ▶ exponential speed-up for factoring integers
- Grover's algorithm
  - ▶ quadratic speed-up for searching in unstructured database
- (Harrow, Hassidim, Lloyd '09) & (Childs, Kothari, Somma '17)
  - ▶  $\Omega(d) \rightarrow \text{poly}(\log d)$  for solving  $d$ -dimensional linear equation systems.
  - ▶ weaker output requirement
    - ★ a quantum state whose vector representation is roughly the solution to the linear equation system.

# Quantum Leading PCA

## Input model

- Quantum oracle which generates a quantum state whose vector representation is  $\mathbf{v}_0$  and  $\mathbf{A}$ .

## Output model

- A quantum state whose vector representation is  $\mathbf{v}_k$

## Main Result

Under warm start  $|\langle \mathbf{v}_0, \mathbf{u}_1 \rangle| = \phi > 0$ , there is a quantum algorithm which prepares a quantum state with vector representation  $\mathbf{v}_k$  such that  $\langle \mathbf{v}_k, \mathbf{u}_1 \rangle \geq 1 - \epsilon$  with probability at least  $2/3$

- using  $O(s \log(s/\phi\epsilon)/\phi\sqrt{\Delta})$  queries to quantum oracle  $U_{A,s}, U_{A,e}$
- $O(1/\phi)$  queries to  $U_{\mathbf{v}_0}$

w.  $O(s(\log d \log(\frac{s}{\phi\epsilon}) + \log^{3.5}(\frac{s}{\phi\epsilon}))/\phi\sqrt{\Delta})$  2-qubit quantum gates in total.

Joint work with Tongyang Li and Xiaodi Wu.

# Intuition for Speedup

Chebyshev polynomials can be significantly accelerated  
in quantum computation

- Matrix power  $A^k \mathbf{b}$  is the key
  - ▶ Quantum-walk
    - ★ effectively constructs a degree- $m$  Chebyshev polynomial of  $A/s$ .
  - ▶ Quantum primitive: the linear combination of unitaries (LCU)
    - ★ effectively linearly combines these Chebyshev polynomials to derive the desired approximation polynomial.

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Quantum Computation for Linear Algebraic Problems

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# Summary

## Spectral methods reveal hidden structure

- Text/Image processing
- Social networks
- Neuroscience, healthcare ...



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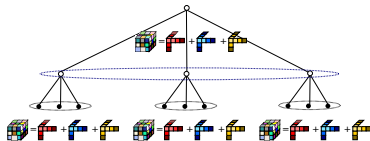
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## Versatile for latent variable models

- Flat model  $\rightarrow$  hierarchical model
- Sparse coding  $\rightarrow$  convolutional model
- Efficient, convergence guarantee



# Thank You

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