Learning latent variable models using tensor decompositions

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El tema (subject matter)

Learning algorithms

for **latent variable models**

based on **decompositions of moment tensors**.

El tema (subject matter)

Learning algorithms **(parameter estimation)**

for **latent variable models**

based on **decompositions of moment tensors**.

“Method-of-moments” **(Pearson, 1894)**

Example #1: summarizing a corpus of documents

Observation: **documents express one or more thematic topics.**

Politics Ensnare Mohamed Salah and Switzerland at the World Cup

By Rory Smith, James Montague and Tariq Panja

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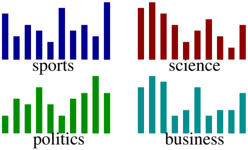
- What topics are expressed in a corpus of documents?
- How prevalent is each topic in the corpus?

Topic model (e.g., latent Dirichlet allocation)



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Document $\equiv$ mixture of topics.

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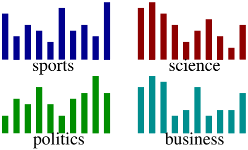

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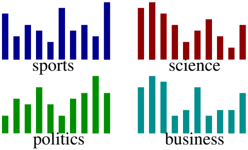

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Given corpus of documents (and "hyper-parameters", e.g., K), produce estimates of **model parameters**, e.g.:

- Distribution $\boldsymbol{P}_t$ over vocab words, for each $t \in [K]$.
- Weight w_t of topic t in document corpus, for each $t \in [K]$.

Labels / annotations

- Suppose each word token x in document is *annotated* with source topic $t_x \in \{1, 2, \ldots, K\}$.

Politics	Ensnare	Mohamed_Salah	and	Switzerland	at
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- Unfortunately, we often don't have such annotations (i.e., data are *unlabeled* / topics are *hidden*).

  "Direct" approach to estimation unavailable.

Example #2: subpopulations in data

Data studied by Pearson (1894):

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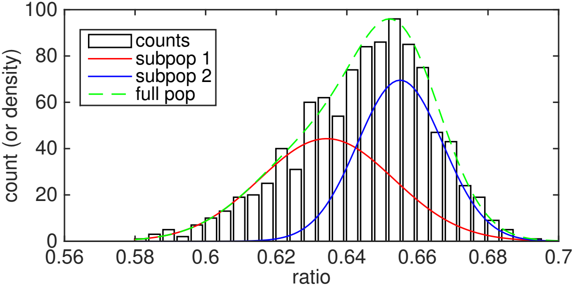
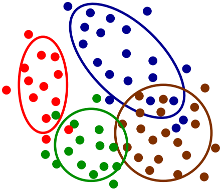
Sample may be comprised of different sub-species of crabs.



Gaussian mixture model

$$\begin{aligned} H &\sim \text{Categorical}(\pi_1, \pi_2, \ldots, \pi_K)\,; \\ \boldsymbol{X} \mid H = t &\sim \text{Normal}(\boldsymbol{\mu}_t, \boldsymbol{\Sigma}_t)\,, \quad t \in [K]\,. \end{aligned}$$



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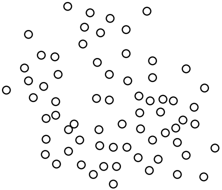

Estimate **mean vector**, **covariance matrix**, and **mixing weight** of each subpopulation from *unlabeled data*.

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  - **Note**: log-likelihood is not necessarily concave function of $\boldsymbol{\theta}$.
  - For latent variable models, often use local optimization, most notably via Expectation-Maximization (EM) (Dempster, Laird, & Rubin, 1977).

MLE for Gaussian mixture models

Given data $\{\boldsymbol{x}_i\}_{i=1}^{n}$, find $\{(\boldsymbol{\mu}_t, \boldsymbol{\Sigma}_t, \pi_t)\}_{t=1}^{K}$ to maximize

$$\sum_{i=1}^{n} \log \left(\sum_{t=1}^{K} \pi_t \cdot \frac{1}{\det(\boldsymbol{\Sigma}_t)^{1/2}} \exp \left\{ -\frac{1}{2} (\boldsymbol{x}_i - \boldsymbol{\mu}_t)^{\top} \boldsymbol{\Sigma}_t^{-1} (\boldsymbol{x}_i - \boldsymbol{\mu}_t) \right\} \right) .$$

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- Sensible with restrictions on $\boldsymbol{\Sigma}_t$ (e.g., $\boldsymbol{\Sigma}_t \succeq \sigma^2 \boldsymbol{I}$).
- But NP-hard to maximize (Tosh and Dasgupta, 2018):
  Can't expect efficient algorithms to work for all data sets.

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$$\Pr\left(\|\hat{\boldsymbol{\theta}} - \boldsymbol{\theta}\| \leq \epsilon\right) \ \geq \ 1 - \delta$$

with $\operatorname{poly}(p, 1/\epsilon, 1/\delta, \dots)$ sample size and running time.

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Barriers

Hard to learn model parameters,
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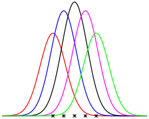
Cryptographic hardness
(e.g., Mossel & Roch, 2006)



Information-theoretic hardness
(e.g., Moitra & Valiant, 2010)

May require $2^{\Omega(K)}$ running time or $2^{\Omega(K)}$ sample size.

Ways around the barriers

- **Separation conditions**.

  E.g., assume mixture component distributions are far apart.
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This lecture: learning algorithms for non-degenerate instances via *method-of-moments*.

Method-of-moments at a glance

1. Determine function of model parameters $\boldsymbol{\theta}$ estimatable from observable data:

$$\mathbb{E}_{\boldsymbol{\theta}}[f(\boldsymbol{X})] \qquad (\text{“moments”})\,.$$

2. Form estimates of moments using data (e.g., iid sample):

$$\widehat{\mathbb{E}}[f(\boldsymbol{X})] \qquad (\text{“empirical moments”})\,.$$

3. Approximately solve equations for parameters $\boldsymbol{\theta}$:

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Which moments? Often low-order moments suffice.

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How? Algorithms for tensor decomposition.

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- Form *estimates* of $\mathbb{E}[X]$ and $\mathbb{E}[X^2]$ from iid sample $\{x_i\}_{i=1}^n$: e.g.,

$$\widehat{\mathbb{E}}[X] \;:=\; \frac{1}{n}\sum_{i=1}^n x_i\,, \qquad \widehat{\mathbb{E}}[X^2] \;:=\; \frac{1}{n}\sum_{i=1}^n x_i^2\,.$$

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We'll follow this same basic recipe for much richer models!

Outline

1. Topic model for single-topic documents.
    - Identifiability.
    - Parameter recovery via orthogonal tensor decomposition.
2. Moment decompositions for other models.
    - Mixtures of Gaussians and linear regressions.
    - Multi-view models (e.g., HMMs).
    - Other models (e.g., single-index models).
3. Error analysis.

Other models amenable to moment tensor decomposition

- Models for independent components analysis (Comon, 1994; Frieze, Jerrum, & Kannan, 1996; Arora, Ge, Moitra & Sachdeva, 2012; Anandkumar, Foster, H., Kakade, & Liu, 2012, 2015; Belkin, Rademacher, & Voss, 2013; etc.)
- Latent Dirichlet Allocation (Anandkumar, Foster, H., Kakade, & Liu, 2012, 2015; Anderson, Goyal, & Rademacher, 2013)
- Mixed-membership stochastic blockmodels (Anandkumar, Ge, H., & Kakade, 2013, 2014)
- Simple probabilistic grammars (H., Kakade, & Liang, 2012)
- Noisy-or networks (Halpern & Sontag, 2013; Jernite, Halpern & Sontag, 2013; Arora, Ge, Ma, & Risteski, 2016)
- Indian buffet process (Tung & Smola, 2014)
- Mixed multinomial logit model (Oh & Shah, 2014)
- Dawid-Skene model (Zhang, Chen, Zhou, & Jordan, 2014)
- Multi-task bandits (Azar, Lazaric, & Brunskill, 2013)
- Partially obs. MDPs (Azizzadenesheli, Lazaric, & Anandkumar, 2016)
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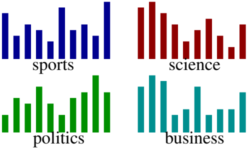
1. Topic model for single-topic documents

Topic model

General topic model (e.g., Latent Dirichlet Allocation)



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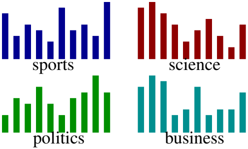

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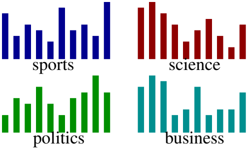

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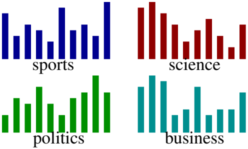

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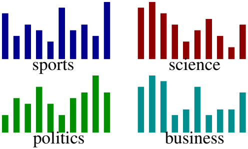

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(Answering this question leads to efficient algorithms for estimating parameters!)

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- $L = 1$: random document (single word) $\sim \sum_{t=1}^{K} w_t \boldsymbol{P}_t$.

  Are parameters $\{(\boldsymbol{P}_t, w_t)\}_{t=1}^{K}$ identifiable from single-word documents?

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  Are parameters $\{(\boldsymbol{P}_t, w_t)\}_{t=1}^{K}$ identifiable from single-word documents?

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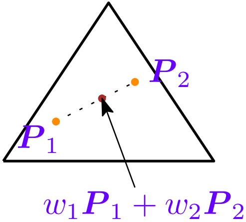

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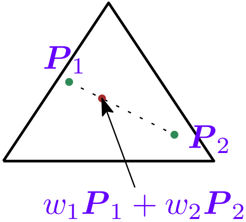

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  Regard $\boldsymbol{P}_t$ as probability vector (ith entry of $\boldsymbol{P}_t$ is $\Pr[\text{word } i]$).
  Joint distribution of word pairs (for topic t) is given by matrix:

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  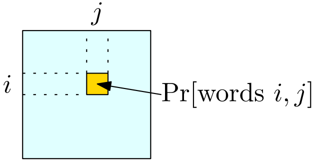

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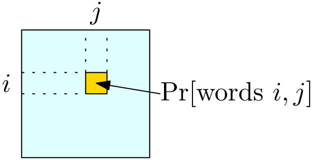

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Are parameters $\{(\boldsymbol{P}_t, w_t)\}_{t=1}^{K}$ identifiable from word pairs?

Simple observation

Suppose distribution of word pairs (as a matrix) can be written as

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Suppose distribution of word pairs (as a matrix) can be written as

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Then it can also be written as

$$\boldsymbol{M} \;=\; (\boldsymbol{A}\boldsymbol{R})(\boldsymbol{A}\boldsymbol{R})^{\top}$$

for any orthogonal matrix $\boldsymbol{R}$ (because $\boldsymbol{R}^{\top}\boldsymbol{R} = \boldsymbol{I}$).

Identifiability: $L = 2$ counterexample

Parameters $\{(\boldsymbol{P}_1, w_1), (\boldsymbol{P}_2, w_2)\}$ and $\{(\widetilde{\boldsymbol{P}}_1, \tilde{w}_1), (\widetilde{\boldsymbol{P}}_2, \tilde{w}_2)\}$

$$\begin{aligned}
(\boldsymbol{P}_1, w_1) &= \left(\begin{bmatrix}0.40\\0.60\end{bmatrix}, 0.5\right), \quad (\boldsymbol{P}_2, w_2) = \left(\begin{bmatrix}0.60\\0.40\end{bmatrix}, 0.5\right); \\
(\widetilde{\boldsymbol{P}}_1, \tilde{w}_1) &= \left(\begin{bmatrix}0.55\\0.45\end{bmatrix}, 0.8\right), \quad (\widetilde{\boldsymbol{P}}_2, \tilde{w}_2) = \left(\begin{bmatrix}0.30\\0.70\end{bmatrix}, 0.2\right)
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$$w_1 \boldsymbol{P}_1 \boldsymbol{P}_1^\top + w_2 \boldsymbol{P}_2 \boldsymbol{P}_2^\top \;=\; \tilde{w}_1 \widetilde{\boldsymbol{P}}_1 \widetilde{\boldsymbol{P}}_1^\top + \tilde{w}_2 \widetilde{\boldsymbol{P}}_2 \widetilde{\boldsymbol{P}}_2^\top \;=\; \begin{bmatrix}0.26 & 0.24\\0.24 & 0.26\end{bmatrix}.$$

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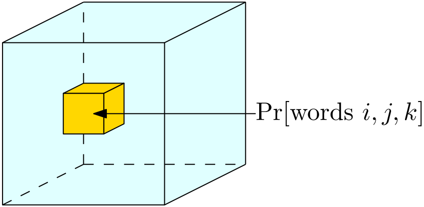
Cannot identify parameters from length-two documents.

Identifiability: $L = 3$

Documents of length $L = 3$

Joint distribution of word triple (for topic t) is given by *tensor*:

$\boldsymbol{P}_t \otimes \boldsymbol{P}_t \otimes \boldsymbol{P}_t =$



Random document $\sim \sum_{t=1}^{K} w_t \boldsymbol{P}_t \otimes \boldsymbol{P}_t \otimes \boldsymbol{P}_t$.

Identifiability from documents of length three

Claim: If $\{\boldsymbol{P}_t\}_{t=1}^K$ are linearly independent & all $w_t > 0$, then parameters $\{(\boldsymbol{P}_t, w_t)\}_{t=1}^K$ are identifiable from word triples.

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Next: Brief overview of tensors.

Tensors of order two

Matrices (tensors of order two): $\boldsymbol{M} \in \mathbb{R}^{d \times d}$.

- Regard as *bi-linear function* $\boldsymbol{M} \colon \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$:

$$\begin{aligned} \boldsymbol{M}(a\boldsymbol{x} + \boldsymbol{x}', \boldsymbol{y}) &= a\boldsymbol{M}(\boldsymbol{x}, \boldsymbol{y}) + \boldsymbol{M}(\boldsymbol{x}', \boldsymbol{y}) \,; \\ \boldsymbol{M}(\boldsymbol{x}, a\boldsymbol{y} + \boldsymbol{y}') &= a\boldsymbol{M}(\boldsymbol{x}, \boldsymbol{y}) + \boldsymbol{M}(\boldsymbol{x}, \boldsymbol{y}') \,. \end{aligned}$$

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Tensors are *multi-linear* generalization.

Tensors of order p

p-**linear functions**: $\boldsymbol{T} \colon \mathbb{R}^d \times \mathbb{R}^d \times \cdots \times \mathbb{R}^d \to \mathbb{R}$.

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  Symmetric rank-1 *tensor*: $\boldsymbol{T} = \boldsymbol{v}^{\otimes p} = \boldsymbol{v} \otimes \boldsymbol{v} \otimes \cdots \otimes \boldsymbol{v}$,

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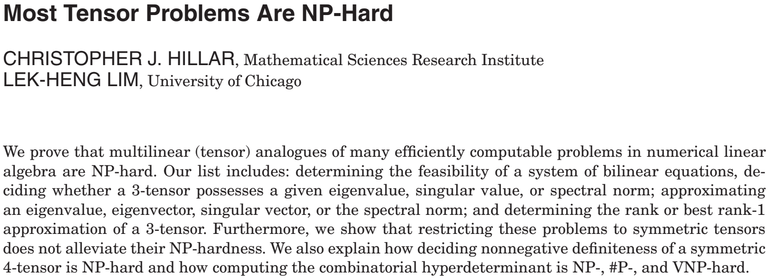
Usual caveat

(Hillar & Lim, 2013)



Most Tensor Problems Are NP-Hard

CHRISTOPHER J. HILLAR, Mathematical Sciences Research Institute
LEK-HENG LIM, University of Chicago

We prove that multilinear (tensor) analogues of many efficiently computable problems in numerical linear algebra are NP-hard. Our list includes: determining the feasibility of a system of bilinear equations, deciding whether a 3-tensor possesses a given eigenvalue, singular value, or spectral norm; approximating an eigenvalue, eigenvector, singular vector, or the spectral norm; and determining the rank or best rank-1 approximation of a 3-tensor. Furthermore, we show that restricting these problems to symmetric tensors does not alleviate their NP-hardness. We also explain how deciding nonnegative definiteness of a symmetric 4-tensor is NP-hard and how computing the combinatorial hyperdeterminant is NP-, #P-, and VNP-hard.

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- Rank is not same as border rank!

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  $$\boldsymbol{T} \;:=\; \boldsymbol{x}\otimes\boldsymbol{x}\otimes\boldsymbol{y}+\boldsymbol{x}\otimes\boldsymbol{y}\otimes\boldsymbol{x}+\boldsymbol{y}\otimes\boldsymbol{x}\otimes\boldsymbol{x}\,,$$

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  Define

  $$\boldsymbol{T}_{1/\epsilon} \;:=\; \frac{1}{\epsilon}(\boldsymbol{x}+\epsilon\boldsymbol{y})\otimes(\boldsymbol{x}+\epsilon\boldsymbol{y})\otimes(\boldsymbol{x}+\epsilon\boldsymbol{y}) - \frac{1}{\epsilon}\boldsymbol{x}\otimes\boldsymbol{x}\otimes\boldsymbol{x}\,,$$

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  which have rank 2.

  For $\epsilon = 1/k$, have $\lim_{k\to\infty} \boldsymbol{T}_k = \boldsymbol{T}$.

Aside: eigenvalue decomposition

Recall: every symmetric matrix $\boldsymbol{M} \in \mathbb{R}^{d \times d}$ of rank K has an *eigen-decomposition* (which can be efficiently computed):

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For (symmetric) tensors of order $p \geq 3$:
an analogous decomposition is **not** guaranteed to exist.

Reduction to orthonormal case

Suppose we have (estimates of) moments of the form

$$\boldsymbol{M} = \sum_{t=1}^{K} \boldsymbol{v}_t \otimes \boldsymbol{v}_t \,, \qquad \text{(e.g., word pairs)}$$

and

$$\boldsymbol{T} = \sum_{t=1}^{K} \lambda_t \cdot \boldsymbol{v}_t \otimes \boldsymbol{v}_t \otimes \boldsymbol{v}_t \,. \qquad \text{(e.g., word triples)}$$

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- $\boldsymbol{M}$ is positive semidefinite of rank K.
- $\boldsymbol{M}$ determines inner product system on $\operatorname{span}\{\boldsymbol{v}_t\}_{t=1}^{K}$ s.t. $\{\boldsymbol{v}_t\}_{t=1}^{K}$ are **orthonormal**:

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle_{\boldsymbol{M}} \;:=\; \boldsymbol{x}^{\top} \boldsymbol{M}^{\dagger} \boldsymbol{y} \,.$$

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$$\boldsymbol{M} \;=\; \sum_{t=1}^{K} \boldsymbol{v}_t \otimes \boldsymbol{v}_t \,, \qquad \text{(e.g., word pairs)}$$

and

$$\boldsymbol{T} \;=\; \sum_{t=1}^{K} \lambda_t \cdot \boldsymbol{v}_t \otimes \boldsymbol{v}_t \otimes \boldsymbol{v}_t \,. \qquad \text{(e.g., word triples)}$$

Here, we assume $\{\boldsymbol{v}_t\}_{t=1}^{K}$ are linearly independent, and $\{\lambda_t\}_{t=1}^{K}$ are positive.

- $\boldsymbol{M}$ is positive semidefinite of rank K.
- $\boldsymbol{M}$ determines inner product system on $\operatorname{span}\{\boldsymbol{v}_t\}_{t=1}^{K}$ s.t. $\{\boldsymbol{v}_t\}_{t=1}^{K}$ are **orthonormal**:

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle_{M} \;:=\; \boldsymbol{x}^\top \boldsymbol{M}^\dagger \boldsymbol{y} \,.$$

- $\therefore$ Can assume $d = K$ and $\{\boldsymbol{v}_t\}_{t=1}^{d}$ are orthonormal.
  (Similar to PCA; called "whitening" in signal processing context.)

Orthogonally decomposable tensors $(d = K)$

Goal: Given tensor $\boldsymbol{T} = \sum_{t=1}^{d} \lambda_t \cdot \boldsymbol{v}_t \otimes \boldsymbol{v}_t \otimes \boldsymbol{v}_t \in \mathbb{R}^{d \times d \times d}$ where:

- $\{\boldsymbol{v}_t\}_{t=1}^{d}$ are orthonormal;
- all $\lambda_t > 0$;

approximately recover $\{(\boldsymbol{v}_t, \lambda_t)\}_{t=1}^{d}$.

Exact orthogonally decomposable tensor

(Zhang & Golub, 2001)

Matching moments:

$$\{(\hat{\boldsymbol{v}}_t, \hat{\lambda}_t)\}_{t=1}^{d} \;:=\; \operatorname*{arg\,min}_{\{(\boldsymbol{x}_t, \sigma_t)\}_{t=1}^{d}} \left\| \boldsymbol{T} - \sum_{t=1}^{d} \sigma_t \cdot \boldsymbol{x}_t \otimes \boldsymbol{x}_t \otimes \boldsymbol{x}_t \right\|_F^2 .$$

(Here, $\| \cdot \|_F$ is "Frobenius norm", just like for matrices.)

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- Greedy approach:
  - Find best rank-1 approximation:

$$(\hat{\boldsymbol{v}}, \hat{\lambda}) \;:=\; \operatorname*{arg\,min}_{\|\boldsymbol{x}\|=1, \sigma \geq 0} \|\boldsymbol{T} - \sigma \cdot \boldsymbol{x} \otimes \boldsymbol{x} \otimes \boldsymbol{x}\|_F^2 .$$

  - "Deflate" $\boldsymbol{T} := \boldsymbol{T} - \hat{\lambda} \cdot \hat{\boldsymbol{v}} \otimes \hat{\boldsymbol{v}} \otimes \hat{\boldsymbol{v}}$ and repeat.

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Rank-1 approximation problem

Claim: Local maximizers of the function

$$\boldsymbol{x} \;\mapsto\; \boldsymbol{T}(\boldsymbol{x},\boldsymbol{x},\boldsymbol{x}) \;=\; \sum_{i,j,k} T_{i,j,k} \cdot x_i x_j x_k$$

(over the unit ball) are $\{\boldsymbol{v}_t\}_{t=1}^{d}$, and

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Corollary: decomposition of $\boldsymbol{T}$ as $\sum_{t=1}^{K} \lambda_t \cdot \boldsymbol{v}_t^{\otimes 3}$ is *unique*!

Proof

By linearity and orthogonality:

$$\boldsymbol{T}(\boldsymbol{v}_t, \boldsymbol{v}_t, \boldsymbol{v}_t) \;=\; \sum_{s=1}^{d} (\lambda_s \cdot \boldsymbol{v}_s^{\otimes 3})(\boldsymbol{v}_t, \boldsymbol{v}_t, \boldsymbol{v}_t)$$

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Uniqueness of orthogonal decompositions

What we have seen so far:

1. When components $\{\boldsymbol{v}_t\}_{t=1}^{d}$ are linearly independent:
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Algorithm: use gradient ascent to find all of the local maximizers, which are exactly $\boldsymbol{v}_t$.

(Can use "deflation" to remove components from $\boldsymbol{T}$ that you've already found.)

Application to topic model parameters

Probabilities of word triples as third-order tensor:

$$\boldsymbol{T} \;=\; \sum_{t=1}^{K} w_t \boldsymbol{P}_t \otimes \boldsymbol{P}_t \otimes \boldsymbol{P}_t \;=\; \sum_{t=1}^{K} \boldsymbol{v}_t \otimes \boldsymbol{v}_t \otimes \boldsymbol{v}_t$$

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- Parameters of topic model for single-topic documents (satisfying linear independence condition) can be efficiently recovered from distribution of three-word documents.

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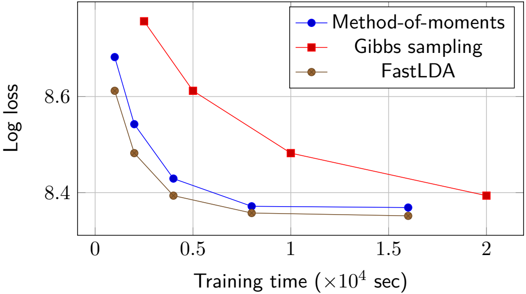
- Two-word documents not sufficient (without further assumptions).
- Variational characterization of orthogonally decomposable tensors leads to simple and efficient algorithms!

Illustrative empirical results

- Corpus: $300,000$ New York Times articles.
- Vocabulary size: $102,660$ words.
- Set number of topics $K := 50$.

Model predictive performance:
≈ 4–$8\times$ speed-up over Gibbs sampling for LDA;
comparable to "FastLDA" (Porteous, Newman, Ihler, Asuncion, Smyth, & Welling, 2008).



Illustrative empirical results

Sample topics: (showing top 10 words for each topic)

Econ.	**Baseball**	**Edu.**	**Health care**	**Golf**
sales	run	school	drug	player
economic	inning	student	patient	tiger_wood
consumer	hit	teacher	million	won
major	game	program	company	shot
home	season	official	doctor	play
indicator	home	public	companies	round
weekly	right	children	percent	win
order	games	high	cost	tournament
claim	dodger	education	program	tour
scheduled	left	district	health	right

Illustrative empirical results

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Invest.	**Election**	**auto race**	**Child's Lit.**	**Afghan War**
percent	al_gore	car	book	taliban
stock	campaign	race	children	attack
market	president	driver	ages	afghanistan
fund	george_bush	team	author	official
investor	bush	won	read	military
companies	clinton	win	newspaper	u_s
analyst	vice	racing	web	united_states
money	presidential	track	writer	terrorist
investment	million	season	written	war
economy	democratic	lap	sales	bin

Illustrative empirical results

Sample topics: (showing top 10 words for each topic)

Web	**Antitrust**	**TV**	**Movies**	**Music**
com	court	show	film	music
www	case	network	movie	song
site	law	season	director	group
web	lawyer	nbc	play	part
sites	federal	cb	character	new_york
information	government	program	actor	company
online	decision	television	show	million
mail	trial	series	movies	band
internet	microsoft	night	million	show
telegram	right	new_york	part	album

etc.

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Learning algorithms

- Estimation via **method-of-moments**:
  1. *Estimate* distribution of three-word documents $\rightarrow$ $\widehat{\boldsymbol{T}}$ (*empirical moment tensor*).
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     In some sense, more stable than matrix eigen-decomposition (Mu, H., & Goldfarb, 2015)!
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Next: Moment decompositions for other models.

2. Moment decompositions for other models

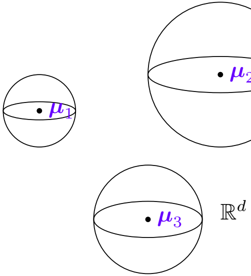
Moment decompositions

Some examples of usable moment decompositions.

1. Two classical mixture models.
2. Models with multi-view structure.
3. Single-index models.

Mixture model #1: Mixtures of spherical Gaussians

$$\begin{aligned} H &\sim \text{Categorical}(\pi_1, \pi_2, \ldots, \pi_K) \quad \text{(hidden)}\,; \\ \boldsymbol{X} \mid H = t &\sim \text{Normal}(\boldsymbol{\mu}_t, \sigma_t^2 \boldsymbol{I}_d)\,, \quad t \in [K]\,. \end{aligned}$$



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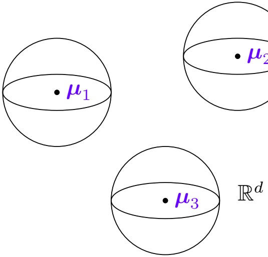

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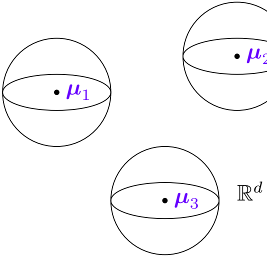
$$\begin{aligned} H &\sim \mathrm{Categorical}(\pi_1, \pi_2, \dots, \pi_K) \quad \text{(hidden)}\,; \\ \boldsymbol{X} \mid H = t &\sim \mathrm{Normal}(\boldsymbol{\mu}_t, \sigma^2 \boldsymbol{I}_d)\,, \quad t \in [K]\,. \end{aligned}$$

(For simplicity, restrict $\sigma_1 = \sigma_2 = \cdots = \sigma_K = \sigma$.)



Generative process:

$$\boldsymbol{X} = \boldsymbol{Y} + \sigma \boldsymbol{Z}$$

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Using moments for spherical Gaussian mixtures

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First- and second-order moments:

$$\mathbb{E}(\boldsymbol{X}) \ \in \ \mathbb{R}^d \qquad \text{and} \qquad \mathbb{E}(\boldsymbol{X} \otimes \boldsymbol{X}) \ \in \ \mathbb{R}^{d \times d}.$$

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Claim (Vempala & Wang, 2002):
Span of top K eigenvectors of $\mathbb{E}(\boldsymbol{X} \otimes \boldsymbol{X})$ contains $\{\boldsymbol{\mu}_t\}_{t=1}^K$.
(K-dimensional Principal Component Analysis (PCA) subspace.)

Proof

Key fact: k-dimensional PCA subspace (based on $\mathbb{E}(\boldsymbol{X} \otimes \boldsymbol{X})$) captures as much of overall variance as any other k-dim. subspace.

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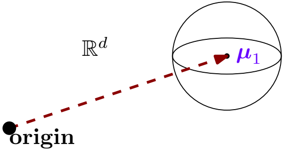

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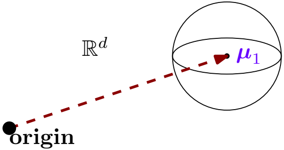

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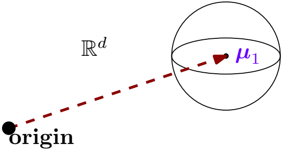

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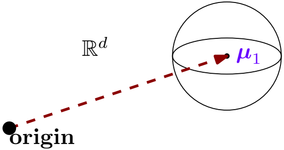

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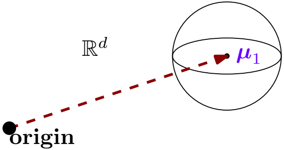

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Best direction (1-dim. PCA subspace): $\boldsymbol{v} = \pm \boldsymbol{\mu}_1 / \|\boldsymbol{\mu}_1\|$.

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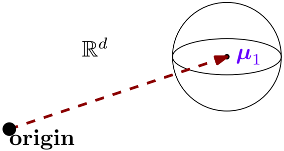

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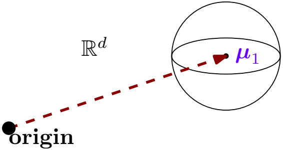

Answer: any k-dim. subspace containing $\boldsymbol{\mu}_1$.

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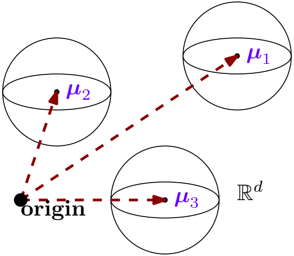

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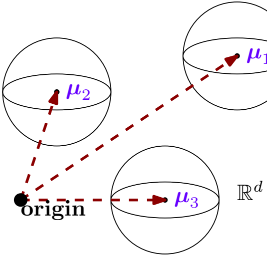

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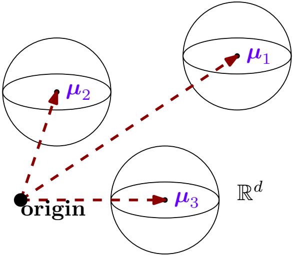

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How does this help with learning mixtures of Gaussians?

Use of moments for mixtures of spherical Gaussians

Separation (Dasgupta, 1999):

$\#$ standard deviations between component means

$$\text{sep} \ := \ \min_{i \neq j} \frac{\|\boldsymbol{\mu}_i - \boldsymbol{\mu}_j\|}{\sigma} \, .$$

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(Belkin & Sinha, 2010; Moitra & Valiant, 2010):

General Gaussians & no minimum sep, but Kth-order moments.

Third-order moments of spherical Gaussian mixtures

Generative process:

$$\boldsymbol{X} \; = \; \boldsymbol{Y} + \sigma \boldsymbol{Z}$$

where $\Pr(\boldsymbol{Y} = \boldsymbol{\mu}_t) = \pi_t$, and $\boldsymbol{Z} \sim \mathrm{Normal}(\mathbf{0}, \boldsymbol{I}_d)$, $\boldsymbol{Y} \perp\!\!\!\perp \boldsymbol{Z}$.

Third-order moment tensor:

$$\mathbb{E}\left(\boldsymbol{X}^{\otimes 3}\right) \; = \; \mathbb{E}\left(\{\boldsymbol{Y} + \sigma \boldsymbol{Z}\}^{\otimes 3}\right)$$

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(Above, $\boldsymbol{\mu} = \mathbb{E}(\boldsymbol{X})$ and $\tau(\boldsymbol{\mu})$ is a third-order tensor involving only $\boldsymbol{\mu}$.)

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Exercise: find explicit formula for $\tau(\boldsymbol{\mu})$.

Tensor decomposition for spherical Gaussian mixtures

(H. & Kakade, 2013)

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Claim: If $\{\boldsymbol{\mu}_t\}_{t=1}^{K}$ are linearly independent and all $\pi_t > 0$, then $\{(\boldsymbol{\mu}_t, \pi_t)\}_{t=1}^{K}$ are identifiable from

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Can use tensor decomposition to recover $\{(\boldsymbol{\mu}_t, \pi_t)\}_{t=1}^K$ from $\boldsymbol{T}$.

Even more Gaussian mixtures

Note: Linear independence condition on $\{\boldsymbol{\mu}_t\}_{t=1}^{K}$ requires $K \leq d$.

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  Mixtures of $d^{O(1)}$ Gaussians (w/ simple or known covariance) via **smoothed analysis** and $O(1)$-order moments.

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  Mixtures of $d^{O(1)}$ Gaussians (w/ simple or known covariance) via **smoothed analysis** and $O(1)$-order moments.
- (Ge, Huang, & Kakade, 2015)
  Also with **unknown covariances of arbitrary shape**.

Mixture model #2: Mixtures of linear regressions

$$\begin{aligned} H &\sim \mathrm{Categorical}(\pi_1, \pi_2, \ldots, \pi_K) \quad \textsf{(hidden)}\,; \\ \boldsymbol{X} &\sim \mathrm{Normal}(\boldsymbol{\mu}, \boldsymbol{\Sigma})\,; \\ Y \mid H = t, \boldsymbol{X} = \boldsymbol{x} &\sim \mathrm{Normal}(\langle \boldsymbol{\beta}_t, \boldsymbol{x} \rangle, \sigma^2)\,. \end{aligned}$$

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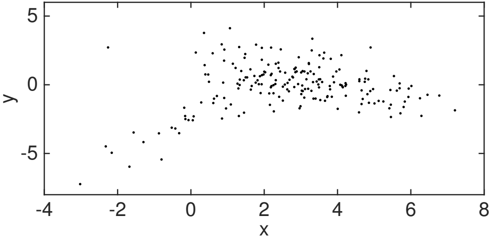

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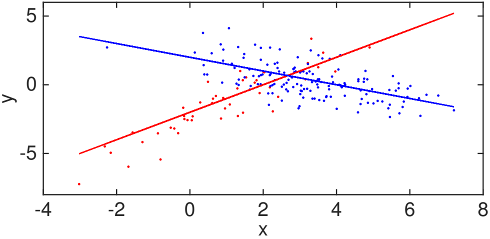

Use of moments for mixtures of linear regressions

Second-order moments (assume $\boldsymbol{X} \sim \mathrm{Normal}(\mathbf{0}, \boldsymbol{I}_d)$):

$$\mathbb{E}(Y^2 \boldsymbol{X} \boldsymbol{X}^\top) \;=\; 2 \sum_{t=1}^{K} \pi_t \cdot \boldsymbol{\beta}_t \boldsymbol{\beta}_t^\top + \left(\sigma^2 + \sum_{t=1}^{K} \pi_t \cdot \|\boldsymbol{\beta}_t\|^2 \right) \boldsymbol{I}_d \, .$$

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Tensor decomposition approach:
Can recover parameters $\{(\boldsymbol{\beta}_t, \pi_t)\}_{t=1}^{K}$ with higher-order moments (Chaganty & Liang, 2013; Yi, Caramanis, & Sanghavi, 2014, 2016).

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- Using Stein's identity (1973), similar approach works for GLMs (Sun, Ioannidis, & Montanari, 2013).

Tensor decomposition approach:

Can recover parameters $\{(\boldsymbol{\beta}_t, \pi_t)\}_{t=1}^{K}$ with higher-order moments (Chaganty & Liang, 2013; Yi, Caramanis, & Sanghavi, 2014, 2016).

Also for GLMs, via Stein's identity (Sedghi & Anandkumar, 2014).

Recap: mixtures of Gaussians and linear regressions

- Parameters of Gaussian mixture models and related models (satisfying linear independence condition) can be efficiently recovered from $O(1)$-order moments.

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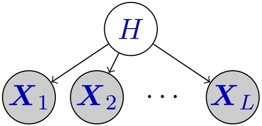
Next: Multi-view approach to finding usable moments.

Multi-view interpretation of topic model

Recall: Topic model for single-topic documents



K topics (dists. over words) $\{\boldsymbol{P}_t\}_{t=1}^{K}$.

Pick topic $H = t$ with prob. w_t (**hidden**).

Word tokens $\boldsymbol{X}_1, \boldsymbol{X}_2, \ldots, \boldsymbol{X}_L \overset{\text{iid}}{\sim} \boldsymbol{P}_H$.

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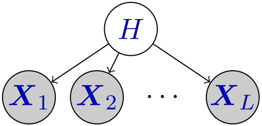

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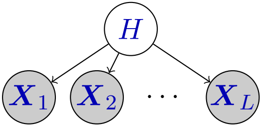

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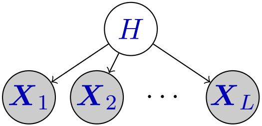

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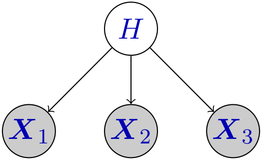
Some previous analyses:

- (Blum & Mitchell, 1998)
  Co-training in semi-supervised learning.
- (Chaudhuri, Kakade, Livescu, & Sridharan, 2009)
  Multi-view Gaussian mixture models.

Multi-view mixture model



View 1: $\boldsymbol{X}_1$

View 2: $\boldsymbol{X}_2$

View 3: $\boldsymbol{X}_3$

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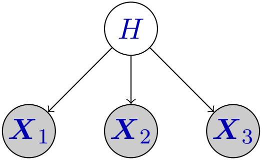

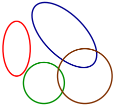
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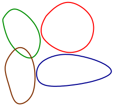
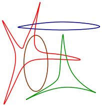

View 2: $\boldsymbol{X}_2$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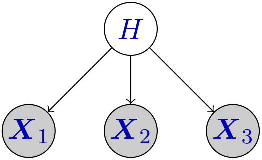

$$\mathbb{E}\left(\boldsymbol{X}_1 \otimes \boldsymbol{X}_2 \otimes \boldsymbol{X}_3\right) = \sum_{t=1}^{K} \pi_t \cdot \boldsymbol{\mu}_t^{(1)} \otimes \boldsymbol{\mu}_t^{(2)} \otimes \boldsymbol{\mu}_t^{(3)}$$

$$\text{where } \boldsymbol{\mu}_t^{(i)} = \mathbb{E}[\boldsymbol{X}_i \mid H = t],$$

$$\pi_t = \Pr(H = t).$$

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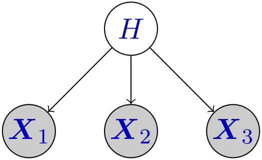

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Tensor decomposition approach works in this asymmetric case as long as $\{\boldsymbol{\mu}_t^{(j)}\}_{t=1}^{K}$ are lin. indpt. for each j, and all $\pi_t > 0$.

Examples of multi-view mixture models

(Mossel & Roch, 2006; Anandkumar, H., & Kakade, 2012)

1. Mixtures of high-dimensional product distributions.
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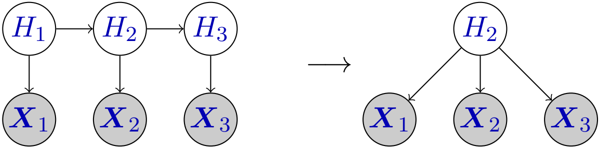

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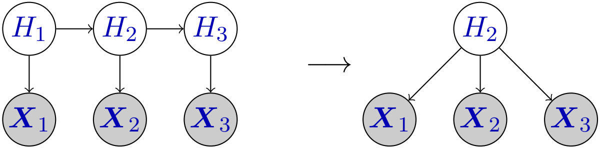

3. Phylogenetic trees.
   - $\boldsymbol{X}_1, \boldsymbol{X}_2, \boldsymbol{X}_3$: genes of three extant species.
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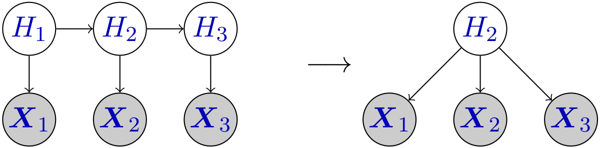

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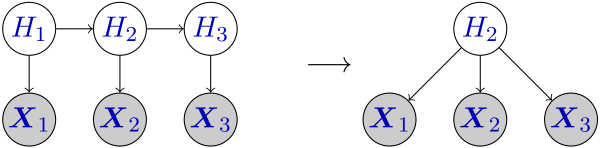

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Next: Single index models.

Single-index models

$$\begin{aligned} \boldsymbol{X} &\sim \mathrm{Normal}(\mathbf{0}, \boldsymbol{I})\,; \\ Y \mid \boldsymbol{X} = \boldsymbol{x} &\sim \mathrm{Normal}(g(\langle \boldsymbol{\beta}, \boldsymbol{x} \rangle), \sigma^2)\,. \end{aligned}$$

Here, $g\colon \mathbb{R} \to \mathbb{R}$ is the *link function*.

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- **Phase retrieval** (real signals): assume $g(z) = z^2$.
- **1-bit compressed sensing**: assume $g(z) = \mathrm{sign}(z)$.
- **Isotonic regression**: assume g is monotone (e.g., $g' \geq 0$).
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Semi-parametric estimation: regard g as nuisance parameter; focus on estimating $\boldsymbol{\beta}$.

Aside: symmetric tensors and homogeneous polynomials

Recall formula for tensor function value:

$$\boldsymbol{T}(\boldsymbol{x}^{(1)}, \ldots, \boldsymbol{x}^{(p)}) \;=\; \sum_{i_1,\ldots,i_p} T_{i_1,\ldots,i_p} \cdot x^{(1)}_{i_1} \cdots x^{(p)}_{i_p} \,.$$

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If $\boldsymbol{T}$ is symmetric (i.e., $T_{i_1,\dots,i_p} = T_{\pi(i_1),\dots,\pi(i_p)}$ for any permutation π), then evaluating at $\boldsymbol{x}^{(1)} = \cdots = \boldsymbol{x}^{(p)} = \boldsymbol{x}$ gives

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p-th order symmetric tensors $\simeq$ degree-p homogeneous polynomials.

Using orthogonal polynomials

(Dudeja & H., 2018)

Let $H_p \colon \mathbb{R} \to \mathbb{R}$ denote the degree-p Hermite polynomial.

Assume (for $Z \sim \mathrm{Normal}(0,1)$):

- $\mathbb{E}[g(Z)^2] = 1$ (normalization—this is WLOG);
- $\mathbb{E}[g'(Z)^2] \geq \epsilon$ (necessary for identifiability);
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There exists $p = O(1/\epsilon)$ such that

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$\Rightarrow$ Get efficient algorithms for semi-parametric estimation of single-index model parameters, for very general link functions.

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- Parameters of many latent variable models (satisfying non-degeneracy conditions) can be efficiently recovered from $O(1)$-order moments.

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- Estimation via **method-of-moments**:
    1. *Estimate* moments → empirical moment tensor $\widehat{\boldsymbol{T}}$.
    2. *Approximately decompose* $\widehat{\boldsymbol{T}}$ → parameter estimate $\hat{\boldsymbol{\theta}}$.

3. Error analysis

Moment estimates

Estimation of $\mathbb{E}[\boldsymbol{X}^{\otimes 3}]$ (say) from iid sample $\{\boldsymbol{x}_i\}_{i=1}^{n}$:

$$\widehat{\mathbb{E}}[\boldsymbol{X}^{\otimes 3}] \;:=\; \frac{1}{n}\sum_{i=1}^{n}\boldsymbol{x}_i^{\otimes 3}\,.$$

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Inevitably expect error of order $n^{-1/2}$ in some norm, e.g.,

$$\|\boldsymbol{T}\| \ := \ \sup_{\|\boldsymbol{x}\|=\|\boldsymbol{y}\|=\|\boldsymbol{z}\|=1} \boldsymbol{T}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{z}) \quad \text{(injective/``spectral'' norm)}\,,$$

$$\|\boldsymbol{T}\|_F \ := \ \left(\sum_{i,j,k} T_{i,j,k}^2\right)^{1/2} \quad \text{(Frobenius norm)}\,.$$

Nearly orthogonally decomposable tensor

(Mu, H., & Goldfarb, 2015)

Let $\varepsilon = \|\boldsymbol{E}\|$ for $\boldsymbol{E} := \widehat{\boldsymbol{T}} - \boldsymbol{T}$.

Claim: Let $\hat{\boldsymbol{v}} := \arg\max_{\|\boldsymbol{x}\|=1} \widehat{\boldsymbol{T}}(\boldsymbol{x}, \boldsymbol{x}, \boldsymbol{x})$ and $\hat{\lambda} := \widehat{\boldsymbol{T}}(\hat{\boldsymbol{v}}, \hat{\boldsymbol{v}}, \hat{\boldsymbol{v}})$.

Then

$$|\hat{\lambda} - \lambda_t| \;\leq\; \varepsilon\,, \qquad \|\hat{\boldsymbol{v}} - \boldsymbol{v}_t\| \;\leq\; O\left(\frac{\varepsilon}{\lambda_t} + \left(\frac{\varepsilon}{\lambda_t}\right)^2\right)$$

for some $t \in [d]$ with $\lambda_t \geq \max_{t'} \lambda_{t'} - 2\varepsilon$.

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for some $t \in [d]$ with $\lambda_t \geq \max_{t'} \lambda_{t'} - 2\varepsilon$.

Many efficient algorithms for solving this approximately, when ε is small enough, like $1/d$ or $1/\sqrt{d}$ (e.g., Anandkumar, Ge, H., Kakade, & Telgarsky, 2014; Ma, Shi, & Steurer, 2016).

Recall: greedy decomposition

(Zhang & Golub, 2001)

Matching moments:

$$\{(\hat{\boldsymbol{v}}_t, \hat{\lambda}_t)\}_{t=1}^{d} \; := \; \operatorname*{arg\,min}_{\{(\boldsymbol{x}_t, \sigma_t)\}_{t=1}^{d}} \left\| \boldsymbol{T} - \sum_{t=1}^{d} \sigma_t \cdot \boldsymbol{x}_t \otimes \boldsymbol{x}_t \otimes \boldsymbol{x}_t \right\|_F^2 .$$

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- Greedy approach:
  - Find best rank-1 approximation:

$$(\hat{\boldsymbol{v}}, \hat{\lambda}) \;:=\; \operatorname*{arg\,min}_{\|\boldsymbol{x}\|=1, \sigma \geq 0} \|\boldsymbol{T} - \sigma \cdot \boldsymbol{x} \otimes \boldsymbol{x} \otimes \boldsymbol{x}\|_F^2 .$$

  - "Deflate" $\boldsymbol{T} := \boldsymbol{T} - \hat{\lambda} \cdot \hat{\boldsymbol{v}} \otimes \hat{\boldsymbol{v}} \otimes \hat{\boldsymbol{v}}$ and repeat.

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Errors from deflation

(For simplicity, assume $\lambda_t = 1$ for all t, so $\boldsymbol{T} = \sum_t \boldsymbol{v}_t^{\otimes 3}$.)

First greedy step:
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Now error seems to have doubled (i.e., of size 2ε) ...

Effect of deflation errors

For any unit vector $\boldsymbol{x}$ orthogonal to $\boldsymbol{v}_1$:

$$\left\| \frac{1}{3} \nabla_{\boldsymbol{x}} \left\{ \left(\boldsymbol{v}_1^{\otimes 3} - \hat{\boldsymbol{v}}_1^{\otimes 3} \right) (\boldsymbol{x}, \boldsymbol{x}, \boldsymbol{x}) \right\} \right\| \quad = \quad \left\| \langle \boldsymbol{v}_1, \boldsymbol{x} \rangle^2 \boldsymbol{v}_1 - \langle \hat{\boldsymbol{v}}_1, \boldsymbol{x} \rangle^2 \hat{\boldsymbol{v}}_1 \right\|$$

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So effect of errors (original and from deflation) $\boldsymbol{E} + \left(\boldsymbol{v}_1^{\otimes 3} - \hat{\boldsymbol{v}}_1^{\otimes 3} \right)$ in directions orthogonal to $\boldsymbol{v}_1$ is $(1 + o(1))\varepsilon$ rather than 2ε.

Effect of deflation errors

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So effect of errors (original and from deflation) $\boldsymbol{E} + \left(\boldsymbol{v}_1^{\otimes 3} - \hat{\boldsymbol{v}}_1^{\otimes 3} \right)$ in directions orthogonal to $\boldsymbol{v}_1$ is $(1 + o(1))\varepsilon$ rather than 2ε.

- Deflation errors have lower-order effect on finding other $\boldsymbol{v}_t$.

  (Analogous statement for deflation with matrices does not hold.)

Summary

- Using method-of-moments with low-order moments, can efficiently estimate parameters for many models.
    - Exploit distributional properties, multi-view structure, and other structure to determine usable moments tensors.
    - Some efficient algorithms for carrying out the tensor decomposition to obtain parameter estimates.

Summary

- Using method-of-moments with low-order moments, can efficiently estimate parameters for many models.
  - Exploit distributional properties, multi-view structure, and other structure to determine usable moments tensors.
  - Some efficient algorithms for carrying out the tensor decomposition to obtain parameter estimates.
- Many issues to resolve!
  - Handle model misspecification, increase robustness.
  - General methodology.
  - Incorporate general prior knowledge and interactive feedback.

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Further reading:

- Anandkumar, Ge, H., Kakade, & Telgarsky.
  Tensor decompositions for learning latent variable models.
  Journal of Machine Learning Research, 15(Aug):2773–2831, 2014.
  `https://goo.gl/F8HudN`

¡Gracias!