# Polynomial Methods in Learning and Statistics

## Ankur Moitra, MIT

July 11, 2013

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### Outline

- Mixtures of Gaussians
  - Highlights: method of moments and the heat equation
  - based on [Kalai, Moitra, Valiant] (see also [Belkin and Sinha])
- Topic Models
  - Highlights: tensor methods and Chang's Lemma
  - based on [Anandkumar, Foster, Hsu, Kakade and Liu]
- Nonnegative Matrix Factorization
  - Highlights: separability and more general topic models

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• based on [Arora, Ge, Kannan, Moitra]

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## Pearson (1894) and the Naples Crabs

(figure due to Peter Macdonald)



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$$F(x) = w_1 F_1(x) + (1 - w_1) F_2(x)$$
, where  $F_i(x) = \mathcal{N}(\mu_i, \sigma_i^2, x)$ 

In particular, with probability  $w_1$  output a sample from  $F_1$ , otherwise output a sample from  $F_2$ 

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*Can we learn these parameters approximately, given enough random samples from F*?

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Pearson invented the method of moments, to attack this problem...

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Claim

 $E_{x \leftarrow F(x)}[x^r]$  is a polynomial in  $\theta = (w_1, \mu_1, \sigma_1, \mu_2, \sigma_2)$ 

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- Dasgupta (1999) and many others: Clustering assumes almost **non-overlapping** components

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#### Question

To learn the parameters to within an additive  $\epsilon$ , is there an algorithm whose sample complexity and running time are bounded by  $(1/\epsilon)^C$ ?

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### (Kalai, Moitra, Valiant):

Given an *n*-dimensional mixture of two Gaussians, our algorithm requires poly(n, <sup>1</sup>/<sub>ε</sub>) samples and running time to output a mixture that is ε-close to the true parameters

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- Given an *n*-dimensional mixture of two Gaussians, our algorithm requires poly(n, <sup>1</sup>/<sub>ε</sub>) samples and running time to output a mixture that is ε-close to the true parameters
- Reduce to the one-dimensional case
- Analyze Pearson's sixth moment test (with noisy moments)

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Does this uniquely determine the parameters of the mixture? (up to a relabeling of the components)

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#### Question

Do any two different mixtures F and  $\hat{F}$  differ on at least one of the first six moments?

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### Method of Moments



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**Proof:** 

$$0 < \left| \int_{x} p(x)f(x)dx \right| = \left| \int_{x} \sum_{r=1}^{6} p_{r}x^{r}f(x)dx \right|$$

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So  $\exists_{r\in\{1,2,...,6\}}$  such that  $|M_r(F) - M_r(\hat{F})| > 0$ 

If  $f(x) = \sum_{i=1}^{k} \alpha_i \mathcal{N}(\mu_i, \sigma_i^2, x)$  is not identically zero, f(x) has at most 2k - 2 zero crossings ( $\alpha_i$  can be negative).

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#### Theorem (Hummel, Gidas)

Suppose  $f(x) : \mathbb{R} \to \mathbb{R}$  is analytic and has n zeros. Then  $f(x) \circ \mathcal{N}(0, \sigma^2, x)$  has at most n zeros (for any  $\sigma^2 > 0$ ).

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#### Fact

$$\mathcal{N}(\mathbf{0}, \sigma_1^2, \mathbf{x}) \circ \mathcal{N}(\mathbf{0}, \sigma_2^2, \mathbf{x}) = \mathcal{N}(\mathbf{0}, \sigma_1^2 + \sigma_2^2, \mathbf{x})$$



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### An algebraic restatement:

Let  $\Gamma = \{$ **valid** parameters $\}$  (in particular  $w_i \in [0, 1], \sigma_i \geq 0$ )

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### Claim

Let  $\theta$  be the true parameters; then the variety

$$\{ heta'\in \Gamma|M_r( heta')=M_r( heta) ext{ for } r=1,2,...6\}$$

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contains only  $(w_1, \mu_1, \sigma_1, \mu_2, \sigma_2)$  and  $(1 - w_1, \mu_2, \sigma_2, \mu_1, \sigma_1)$ 

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Are these equations stable, when we are given noisy estimates?

Using deconvolution to isolate components, we show:

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There are constants c, C such that if  $\epsilon < c$ , the means and variances are bounded by  $\frac{1}{\epsilon}$ , the mixing weights are in  $[\epsilon, 1 - \epsilon]$  and

$$|M_r(\theta) - M_r(\theta')| \le \epsilon^C$$

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for r = 1, 2, ...6 then there is a permutation  $\pi$  such that

$$\sum_{i=1}^{2} |w_{i} - w_{\pi(i)}'| + |\mu_{i} - \mu_{\pi(i)}'| + |\sigma_{i}^{2} - \sigma_{\pi(i)}'^{2}| \le \epsilon$$

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Hence, close enough estimates for the first six moments guarantee that the parameters are close too!

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And  $\theta'$  must be close to  $\theta$ , because solutions to this system of polynomial equations are **stable** 

(Belkin, Sinha)



(Belkin, Sinha): Consider a family of distributions  $F(\theta)$ 

#### Fact

If the moment generating function converges in a neighborhood around zero, then  $M_r(\theta) = M_r(\theta')$  for all r implies  $F(\theta) = F(\theta')$ .

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### e.g. a mixture of Gaussians

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Hence for some N,  $I_N = I_{N+1} = ...$ ; i.e.

$$Q_{N+j}(\theta, \theta') = \sum_{r=1}^{N} \alpha(\theta, \theta') Q_r(\theta, \theta')$$

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## Definition $Q_r(\theta, \theta') = M_r(\theta) - M_r(\theta')$

Consider the ideals  $I_1 = \langle Q_1 \rangle \subseteq I_2 = \langle Q_1, Q_2 \rangle ... \subseteq \mathbb{R}[\theta, \theta']$ 

#### Fact

 $\mathbb{R}[\theta, \theta']$  is a Noetherian Ring (Hilbert's Basis Theorem)

Hence for some N,  $I_N = I_{N+1} = ...$ ; i.e.

$$Q_{N+j}(\theta, \theta') = \sum_{r=1}^{N} \alpha(\theta, \theta') Q_r(\theta, \theta')$$

 $\sum_{i=1}^{N} |M_i(\theta) - M_i(\theta')| = 0 \Rightarrow$ all moments are equal  $\Rightarrow F(\theta) = F(\theta')$ 

# If $\sum_{r=1}^{N} |M_r(\theta) - M_r(\theta')| < \delta$ , for what $\epsilon(\delta)$ is $|\theta - \theta'| < \epsilon$ ?

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**Caveat:** This uses Hilbert's Basis Theorem, hence no **effective** bound for number of moments (or *C*)

# Outline

- Mixtures of Gaussians
  - Highlights: method of moments and the heat equation
  - based on [Kalai, Moitra, Valiant] (see also [Belkin and Sinha])
- Topic Models
  - Highlights: tensor methods and Chang's Lemma
  - based on [Anandkumar, Foster, Hsu, Kakade and Liu]
- Nonnegative Matrix Factorization
  - Highlights: separability and more general topic models

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• based on [Arora, Ge, Kannan, Moitra]

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# **Topic Models**

Large collection of articles, say from the New York Times:



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### Question

How can we automatically organize them by topic? (unsupervised learning)

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### Question

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**Challenge:** Develop tools for automatic comprehension of data - e.g. newspaper articles, webpages, images, genetic sequences, user ratings...

# Parceling Out a Nest Egg, Without Emptying It

What clients often forget are fixed costs — homes, cars, insurance — that must come down but take time to reduce, she said. Beyond that is her clients' skittish approach to risk; putting all of their money in cash may make them feel safe, she said, but it probably will not support the lifestyle they want for decades.

A generational disconnect is at work here: most people plan to retire at 65, the retirement age established for <u>Social Security</u> in 1935, when the average <u>life expectancy</u> was 61. Today the average is over 80 for men and women with a college degree.

So the \$5.12 million gift exemption — created in a compromise between President Obama and Congress in 2010 — presents the well-off with a decision laden with short- and long-term consequences. How much should they give heirs now — and thus avoid giving the government in <u>estate taxes</u> later — while maintaining their lifestyle over a probably longer but still unpredictable remaining life span?

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Politics: (President Obama, 0.10), (congress, 0.08), (government, 0.07), ...

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- Each document is a distribution on topics
- Each topic is a distribution on words



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document #1: (1.0, personal finance)



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## Latent Dirichlet Allocation (Blei, Ng, Jordan)



document #2: (0.5, baseball); (0.5, movie review)

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### Correlated Topic Model (Blei, Lafferty)



document #2: (0.5, baseball); (0.5, movie review)

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## Pachinko Allocation Model (Li, McCallum)



document #2: (0.5, baseball); (0.5, movie review)

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document #2: (0.5, baseball); (0.5, movie review)

These models differ only in how W is generated

• **Maximum Likelihood:** Find the parameters that maximize the likelihood of generating the observed data.

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- **Spectral:** Compute the singular value decomposition of  $\widehat{M}$ . [Papadimitriou et al], [Azar et al], ...

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# Algorithms

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- **Tensors:** Use powerful tensor decompositions to recover *A*, when the topic model can be "diagonalized". [Anandkumar et al]
- **Nonnegative Matrix Factorization:** When *A* is separable, works for any topic model [Arora et al]

Given 
$$T = \sum_i u_i \otimes v_i \otimes w_i$$

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Given  $T = \sum_{i} u_i \otimes v_i \otimes w_i$ 

• Suppose that  $\{u_i\}, \{v_i\}$  and  $\{w_i\}$  are linearly independent

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• Choose random unit vectors *a*, *b* 

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• Set 
$$T(\cdot, \cdot, a) = \sum_i (w_i^T a) u_i v_i^T = U D_a V^T$$
, similarly for  $T(\cdot, \cdot, b)$ 

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• Then  $T(\cdot, \cdot, a)(T(\cdot, \cdot, b))^{-1} = UD_a D_b^{-1} U^{-1}$ , similarly for V

Hence we compute find U and V through eigen-decomposition (can also recover W) if diagonals of  $D_a D_b^{-1}$  are distinct

(Mossel, Roch): Applications to phylogenetic reconstruction and HMMs, when transition matrices are full-rank

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Let  $T = Pr[word_1 = \alpha, word_2 = \beta, word_3 = \gamma]$  in a random document of length  $\geq 3$ .

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Hence we can recover A if it is full rank and each document is about only one topic

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The challenge is T has a more complicated form: (D is not necessarily diagonal)

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### Definition

A Tucker decomposition of T is a set of  $n \times r$  matrices U, V, W and an  $r \times r$  matrix D, such that

$$T = \sum_{i,j,k \in [r]} D_{i,j,k} U_i \otimes V_j \otimes W_k$$

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In our setting, U = V = W = A, but *D* corresponds to **moments** of the Dirichlet distribution

Let 
$$\mu = \Pr[word_1 = \alpha]$$
 and  $M = \Pr[word_1 = \alpha, word_2 = \beta]$ 

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We can form new tensors, e.g.  $\mu \otimes \mu \otimes \mu$  or  $M \otimes \mu$ 

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#### Claim

Given Tucker decompositions T and T' with same U, V, W

$$T - T' = \sum_{i,j,k \in [r]} (D_{i,j,k} - D'_{i,j,k}) U_i \otimes V_j \otimes W_k$$

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(Anandkumar, Foster, Hsu, Kakade, Liu): The formula

$$T+2\mu\otimes\mu\otimes\mu-M\otimes\mu$$
 (all three ways)

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**diagonalizes** the decomposition, and hence we can recover *A* if it is full rank for LDA topic models!

### Outline

- Mixtures of Gaussians
  - Highlights: method of moments and the heat equation
  - based on [Kalai, Moitra, Valiant] (see also [Belkin and Sinha])
- Topic Models
  - Highlights: tensor methods and Chang's Lemma
  - based on [Anandkumar, Foster, Hsu, Kakade and Liu]
- Nonnegative Matrix Factorization
  - Highlights: separability and more general topic models

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• based on [Arora, Ge, Kannan, Moitra]

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# rank



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• Known to fail on worst-case inputs (stuck in local minima)

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### Question (theoretical)

Is there an algorithm that (provably) works on all inputs?

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[Arora, Ge, Kannan, Moitra]: There is an  $(nm)^{O(r^2)}$  time algorithm but improving this to  $(nm)^{o(r)}$  would imply a subexponential time algorithm for 3-SAT

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Question

Can we do better for natural instances?

### topics (r)


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If an **anchor word** occurs then the document is at least partially about the topic

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### topics (r) personal finance



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### topics (r) baseball



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#### oscar-winning



If an anchor word occurs then the document is at least partially about the topic

A is **p-separable** if each topic has an anchor word that occurs with probability ≥ p

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Question How do anchor words help?







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#### Observation

If A is separable, then rows of W appear as (scaled) rows of M, we just need to find the anchor words!

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How do anchor words help?

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If A is separable, then rows of W appear as (scaled) rows of M, we just need to find the anchor words!

#### Question

How can we find the anchor words?

Anchor words are extreme points; can be found by linear programming (or a combinatorial distance-based algorithm)

(Arora, Ge, Kannan, Moitra):

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(Arora, Ge, Kannan, Moitra):

• Find the anchor words (linear programming):

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• Find the anchor words (linear programming):

If a word cannot be written as a convex combination of the other words, it is an anchor word

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- Find the nonnegative A so that  $AW \approx M$  (convex programming)

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- Paste these vectors in as rows of W
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#### Claim

The following greedy algorithm works too: repeatedly find the word furthest from the span of the ones we have found so far!

### Back to Topic Models

Question What if documents are **short**; can we still find A?

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### Back to Topic Models

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Crucial observation: We can work with the Gram matrix (define next) to find the anchor words

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Anchor words are extreme rows of the Gram matrix!

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How can we use the anchor words to find the rest of A?

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The posterior distribution Pr[topic|word] is supported on just one topic, for an anchor word

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We will find *Pr*[*topic*|*word*] for all the other words...

# points are now (normalized) rows of $\widehat{M} \widehat{M}^{T}$







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## word #3: (0.5, anchor #2); (0.5, anchor #3)

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what we have:

Pr[topic|word]

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(Arora, Ge, Halpern, Mimno, Moitra, Sontag, Wu, Zhu):

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- Write each word as a convex combination of the anchor words to find *Pr*[*topic*|*word*]

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 $Pr[word|topic] = \frac{Pr[topic|word]Pr[word]}{\sum_{word'} Pr[topic|word']Pr[word']}$ 

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$$Pr[word|topic] = rac{Pr[topic|word]Pr[word]}{\sum_{word'} Pr[topic|word']Pr[word']}$$

This algorithm provably works for **any** topic model (LDA, CTM, PAM, ...) provided A is separable and R is non-singular!

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(Hsu, Kakade): Improved algorithm for spherical GMMs



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**Open Question** 

Are there better algorithm for general GMMs?



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Are there better algorithm for general GMMs?

There are powerful uniqueness theorems for tensors (beyond Chang's Lemma):

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Is there an algorithmic proof of Kruskal's Theorem?

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Other uses of the polynomial method?

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**Open Question** 

Is there an algorithmic proof of Kruskal's Theorem?

Other uses of the polynomial method? (Moitra, Saks): Applications to inverse problems, population recovery

# Thanks!

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