Disentangling Gaussians

Ankur Moitra, MIT

November 6th, 2014 — Dean's Breakfast

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The Gaussian Distribution

The Gaussian distribution is defined as ($\mu = \text{mean}, \sigma^2 = \text{variance}$):

$$\mathcal{N}(\mu, \sigma^2, x) = rac{1}{\sqrt{2\pi\sigma^2}}e^{-rac{(x-\mu)^2}{2\sigma^2}}$$

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Central Limit Theorem: The sum of independent random variables $X_1, X_2, ..., X_s$ converges in distribution to a Gaussian:

$$\frac{1}{\sqrt{s}}\sum_{i=1}^{s}X_{i}\rightarrow_{d}\mathcal{N}(\mu,\sigma^{2})$$

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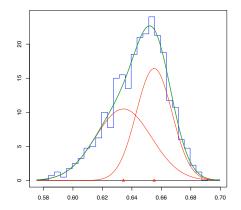
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This distribution is ubiquitous — e.g. used to model height, velocities in an ideal gas, annual rainfall, ...

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

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$$E_{x \leftarrow F(x)}[x^r]$$
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 for $r = 1, 2, ..., 6$

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• Compute simultaneous roots of $\{M_r(\theta) = \widetilde{M}_r\}_{r=1,2,\dots,5}$, select root θ that is closest in sixth moment

Provable Guarantees?

In <u>Contributions to the Mathematical Theory of Evolution</u> (attributed to George Darwin):

"Given the probable error of every ordinate of a frequency curve, what are the probable errors of the elements of the two normal curves into which it may be dissected?"

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• Are these polynomial equations robust to errors?

A View from Theoretical Computer Science

Suppose our goal is to **provably** learn the parameters of each component within an additive ϵ :

Goal

Output a mixture $\widehat{F} = \widehat{w}_1 \widehat{F}_1 + \widehat{w}_2 \widehat{F}_2$ so that there is a permutation $\pi : \{1, 2\} \rightarrow \{1, 2\}$ and for $i = \{1, 2\}$

$$|w_i - \widehat{w}_{\pi(i)}|, |\mu_i - \widehat{\mu}_{\pi(i)}|, |\sigma_i^2 - \widehat{\sigma}_{\pi(i)}^2| \le \epsilon$$

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 $|w_i - \widehat{w}_{\pi(i)}|, |\mu_i - \widehat{\mu}_{\pi(i)}|, |\sigma_i^2 - \widehat{\sigma}_{\pi(i)}^2| < \epsilon$

Is there an algorithm that takes $\mathsf{poly}(1/\epsilon)$ samples and runs in time $\mathsf{poly}(1/\epsilon)$?

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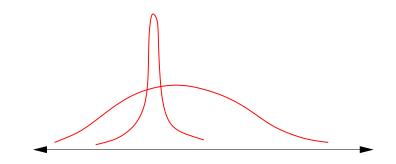
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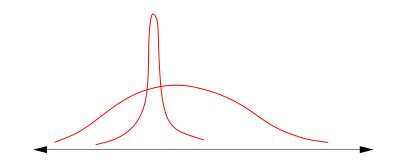
Identifiability through the Tails



Approach: Find the parameters of the component with largest variance (it dominates the behavior of F(x) at infinity)

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Identifiability through the Tails



Approach: Find the parameters of the component with largest variance (it dominates the behavior of F(x) at infinity); subtract it off and continue

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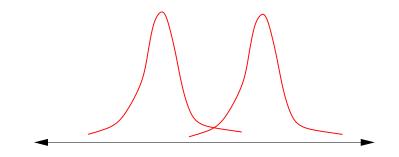
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Clustering Well-separated Mixtures

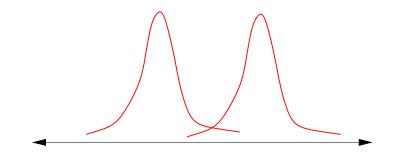


Approach: Cluster samples based on which component generated them

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Clustering Well-separated Mixtures



Approach: Cluster samples based on which component generated them; output the empirical mean and variance of each cluster

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A Conceptual History

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- Dempster, Laird, Rubin (1977): Expectation-Maximization (EM) gets stuck in local maxima
- Dasgupta (1999) and many others: Clustering assumes almost **non-overlapping** components

In summary, these approaches are heuristic, computationally intractable or make a separation assumption about the mixture

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[Kalai, Moitra, Valiant] (studies *n*-dimensional version too):

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• Reduce to the one-dimensional case

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[Kalai, Moitra, Valiant] (studies *n*-dimensional version too):

- Reduce to the one-dimensional case
- Analyze Pearson's sixth moment test (with noisy estimates)

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Suppose $w_1 \in [\epsilon^{10}, 1 - \epsilon^{10}]$ and $\int |F_1(x) - F_2(x)| dx \ge \epsilon^{10}$

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Theorem (Kalai, Moitra, Valiant)

There is an algorithm that (with probability at least $1 - \delta$) learns the parameters of F within an additive ϵ , and the running time and number of samples needed are $poly(\frac{1}{\epsilon}, \log \frac{1}{\delta})$.

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See also [Moitra, Valiant] and [Belkin, Sinha] for mixtures of k Gaussians

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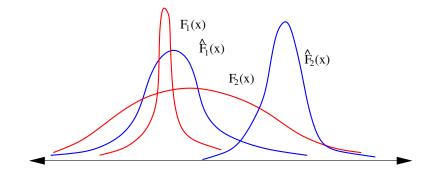
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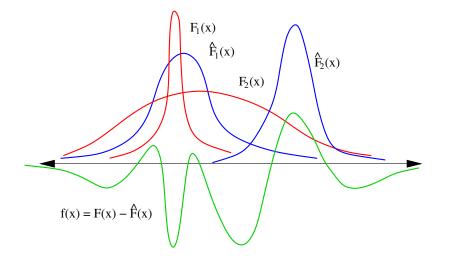
Do any two different mixtures F and \hat{F} differ on at least one of the first six moments?

Method of Moments



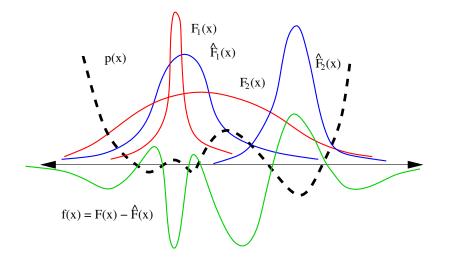
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So $\exists_{r \in \{1,2,...,6\}}$ such that $|M_r(F) - M_r(\widehat{F})| > 0$

Our goal is to prove the following:

Proposition

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 (α_i 's can be negative).

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We will do it through properties of the heat equation

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The Heat Equation

Question

If the initial heat distribution on a one-dimensional infinite rod (κ) is f(x) = f(x, 0) what is the heat distribution f(x, t) at time t?

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There is a probabilistic interpretation ($\sigma^2 = 2\kappa t$):

$$f(x,t) = \mathbb{E}_{z \leftarrow \mathcal{N}(0,\sigma^2)}[f(x+z,0)]$$

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Alternatively, this is called a **convolution**:

$$f(x,t) = \int_{z=-\infty}^{\infty} f(x+z)\mathcal{N}(0,\sigma^2,z)dz = f(x)*\mathcal{N}(0,\sigma^2)$$

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The Key Facts

Theorem (Hummel, Gidas)

Suppose $f(x) : \mathbb{R} \to \mathbb{R}$ is analytic and has N zeros. Then

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Fact

$$\mathcal{N}(\mu_1, \sigma_1^2, x) * \mathcal{N}(\mu_2, \sigma_2^2, x) = \mathcal{N}(\mu_1 + \mu_2, \sigma_1^2 + \sigma_2^2, x)$$

Recall, our goal is to prove the following:

Proposition

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 (α_i 's can be negative).

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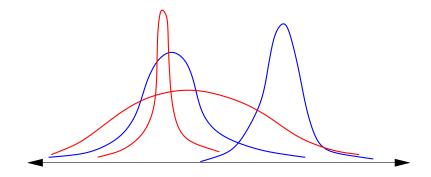
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Start with k = 3 (at most 4 zero crossings), Let's prove it for k = 4 (at most 6 zero crossings)

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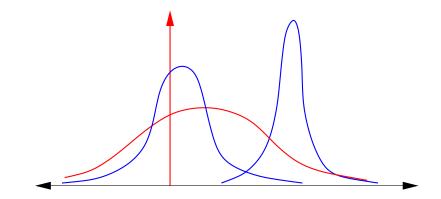
Bounding the Number of Zero Crossings



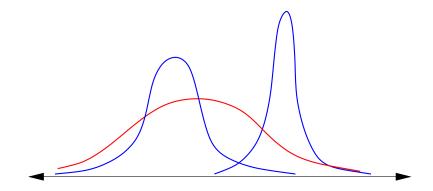
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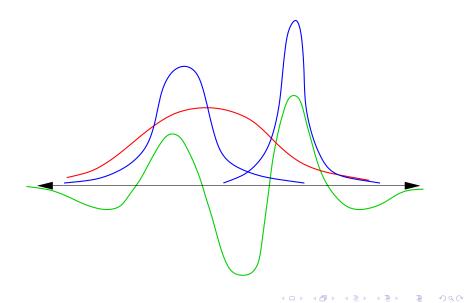
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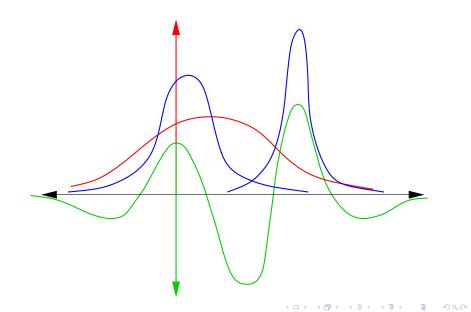


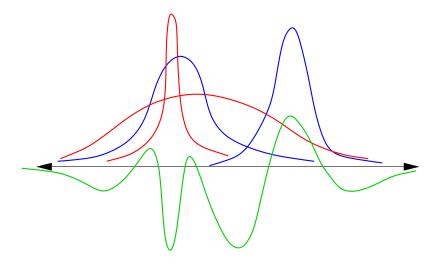
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Let $\Theta = \{$ **valid** parameters $\}$ (in particular $w_i \in [0, 1], \sigma_i \geq 0$)

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Claim

Let θ be the true parameters; then the only solutions to

$$\left\{ \widehat{ heta} \in \Theta | M_r(\widehat{ heta}) = M_r(heta) ext{ for } r = 1, 2, ...6
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are $(w_1, \mu_1, \sigma_1, \mu_2, \sigma_2)$ and the relabeling $(1 - w_1, \mu_2, \sigma_2, \mu_1, \sigma_1)$

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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

$$|M_r(\theta) - M_r(\widehat{\theta})| \le \epsilon^{C}$$

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for r = 1, 2, ...6 then there is a permutation π such that

$$\sum_{i=1}^{2} |w_{i} - \widehat{w}_{\pi(i)}| + |\mu_{i} - \widehat{\mu}_{\pi(i)}| + |\sigma_{i}^{2} - \widehat{\sigma}_{\pi(i)}^{2}| \le \epsilon$$

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

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Our algorithm:

Our algorithm:

• Take enough samples S so that $\widetilde{M}_r = \frac{1}{|S|} \sum_{i \in S} x_i^r$ is w.h.p. close to $M_r(\theta)$ for r = 1, 2...6

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Take enough samples S so that M
r = 1/|S| Σ{i∈S} x_i^r is w.h.p. close to M_r(θ) for r = 1, 2...6 (within an additive ε^C/2)

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• Compute $\widehat{\theta}$ such that $M_r(\widehat{\theta})$ is close to \widetilde{M}_r for r = 1, 2...6

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Take enough samples S so that M̃_r = 1/|S| ∑_{i∈S} x_i^r is w.h.p. close to M_r(θ) for r = 1, 2...6 (within an additive ^{ε^C}/₂)

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Take enough samples S so that M̃_r = 1/|S| ∑_{i∈S} x_i^r is w.h.p. close to M_r(θ) for r = 1, 2...6 (within an additive ε^C/2)
Compute θ̂ such that M_r(θ̂) is close to M̃_r for r = 1, 2...6

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And $\hat{\theta}$ must be close to θ , because solutions to this system of polynomial equations are **stable**

• Here we gave the first efficient algorithms for learning mixtures of Gaussians with provably minimal assumptions

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Key words: method of moments, polynomials, heat equation

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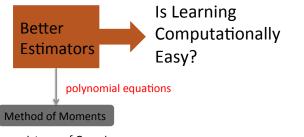
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• Can we design new algorithms for some of the fundamental problems in these fields?

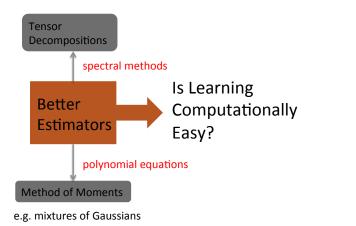
Is Learning Computationally Easy?

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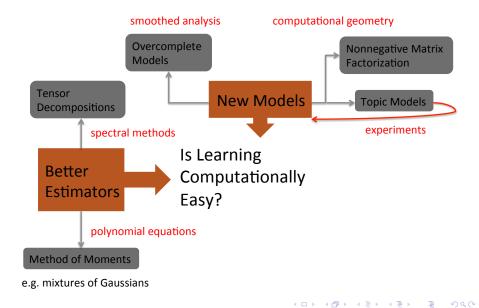


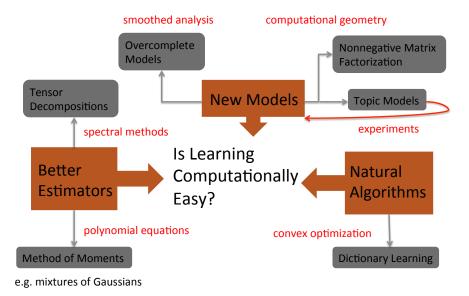
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e.g. mixtures of Gaussians



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Thanks!

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