Learning mixtures of Gaussians

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McGill University
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III. *Contributions to the Mathematical Theory of Evolution.*

By KARL PEARSON, *University College, London.*

Communicated by Professor HENRICI, *F.R.*

Received October 18,—Read November 16, 1893.

[PLATES 1—5.]

CONTENTS.

(9.) The whole method may be illustrated by the following numerical example :—

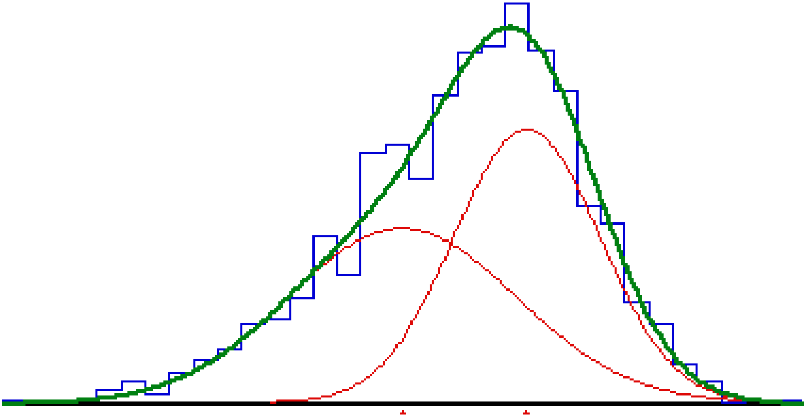
Breadth of "Forehead" of Crabs.—Professor W. F. R. WELDON has very kindly given me the following statistics from among his measurements on crabs. They are for 1000 individuals from Naples. The abscissæ of the curve are the ratio of "forehead" to body-length, and one unit of abscissa = ·004 of body-length. No. 1 of the abscissæ corresponds to ·580 — ·583 of body-length. The ordinates represent the number of individual crabs corresponding to each set of ratios of forehead to body-length. Thus there was one crab fell into the range ·580 — ·583, three fell into the range ·584 — ·587, five into the range ·588 — ·591, and so on. The average length of animals measured 35 millims., and measurements were recorded to ·1 millim.

Abscissæ.	Ordinates.	Abscissæ.	Ordinates.
1	1	16	74
2	3	17	84
3	5	18	86
4	2	19	96
5	7	20	85
6	10	21	75
7	13	22	47
8	19	23	43
9	20	24	24
10	25	25	19
11	40	26	9
12	31	27	5
13	60	28	0
14	62	29	1
15	54		

Observation: data is asymmetric.

Hypothesis: may be a mixture of two Gaussians.

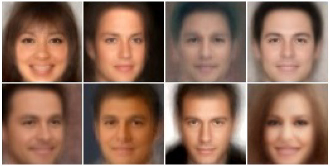
Method: numerically matching the moments.



Learning mixtures of Gaussians in modern times

These days trying to fit data with mixtures of Gaussians is popular in data science.

Modern applications: high-dimensional data



[Richardson and Weiss, Neurips 2018]

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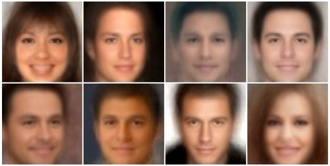

[Richardson and Weiss, Neurips 2018]

Why mixtures of Gaussians?

- ✓ fit some natural data well
- ✓ universal approximators
- ✓ clustering

High-dimensional Gaussians

Multivariate normal distribution:

$$\mathcal{N}_{\mu,\Sigma}(x) = \frac{\exp\left(-\frac{1}{2}(x-\mu)^{\mathsf{T}}\Sigma^{-1}(x-\mu)\right)}{(2\pi)^{d/2}\sqrt{\det(\Sigma)}} \qquad \text{for } x \in \mathbb{R}^d$$

$$X \sim \mathcal{N}_{\mu,\Sigma}\colon\ \mathbb{E}[X] = \mu \in \mathbb{R}^d, \mathbb{E}\left[(X-\mu)(X-\mu)^{\mathsf{T}}\right] = \Sigma \in \mathbb{R}^{d\times d}$$

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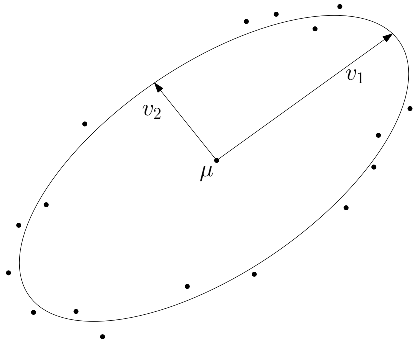

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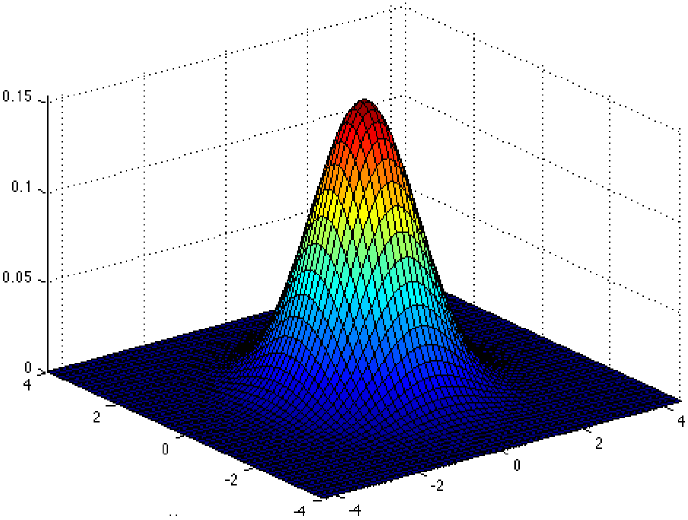
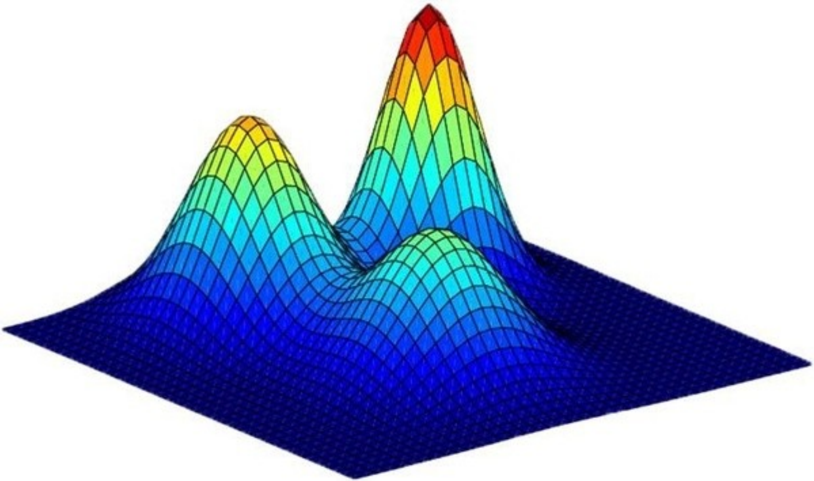
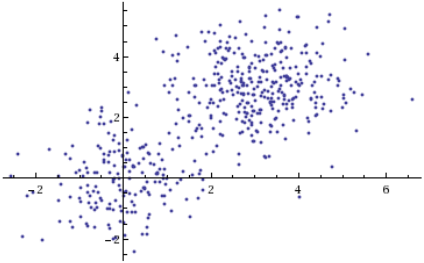
Mixture of k Gaussians in $\mathbb{R}^d$: $\sum_{i=1}^{k} w_i \mathcal{N}_{\mu_i,\Sigma_i}$

mixture weights satisfy $w_i \geq 0$, $\sum w_i = 1$

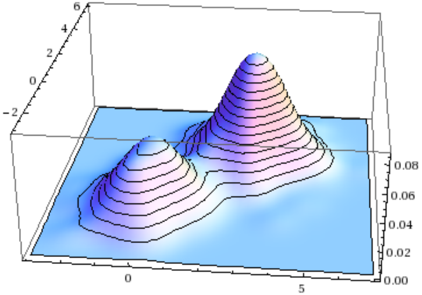
Parameters of the model: $(w_i, \mu_i, \Sigma_i)_{i=1}^{k}$: $\Theta(kd^2)$ parameters


0.15
0.1
0.05
0
4
2
0
-2
-4
-4
-2
0
2
4





-2
2
4
6
4
2
-2



6
4
2
0
-2
0.08
0.06
0.04
0.02
0.00
0
5

What does it mean to learn/estimate a mixture of Gaussians given data?

First answer: maximum likelihood estimation

Given samples $x_1, \ldots, x_n$, find parameters that maximize the likelihood:

$$\prod_{i=1}^{n} \left(\sum_{j=1}^{k} w_j \mathcal{N}_{\mu_j, \Sigma_j}(x_i) \right)$$

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- ✓ Non-convex optimization problem, NP-hard
- ✓ Widely used in practice: expectation-maximization (EM) an iterative algorithm
- ✓ Convergence not well understood, very sensitive to initialization

Second answer: parameter estimation

Given samples from some unknown mixture of Gaussians $\sum_{i=1}^{k} w_i \mathcal{N}(\mu_i, \Sigma_i)$, find each of the parameters within ε.

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Given samples from some unknown mixture of Gaussians $\sum_{i=1}^{k} w_i \mathcal{N}(\mu_i, \Sigma_i)$, find each of the parameters within ε.

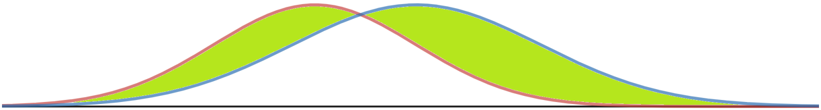
- ✓ Active area of research in theoretical computer science [Dasgupta 1999]
- ✓ Computational complexity: polynomial in d and $1/\varepsilon$ [Kalai, Moitra, Valiant 2010] [Belkin, Sinha 2010]
- ✓ Any algorithm has sample complexity exponential in k [Moitra, Valiant 2010]

Third answer: density estimation

Given samples from an unknown mixture of Gaussians f, output a density $\widehat{f}$ that is close to f with high probability, 99%.

Close in L^1 distance:

$$\left\| f - \widehat{f} \right\|_1 = \int_{\mathbb{R}^d} \left| f(x) - \widehat{f}(x) \right| \mathrm{d}x = 2 \sup_{A \subseteq \mathbb{R}^d} \left| \int_A f - \int_A \widehat{f} \right|$$



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Bounds for parameter estimation do not translate to bounds for density estimation: zero-mean 2-dimensional Gaussians with

$$\Sigma_1=\begin{pmatrix}1 & -0.99\\ -0.99 & 1\end{pmatrix}\text{ and }\Sigma_2=\begin{pmatrix}1 & -1\\ -1 & 1\end{pmatrix}$$

Close parameters, large L^1 distance.

Density estimation

Given samples from an unknown density f from some known family C of densities, output a density $\widehat{f}$ that is close to f.

REMARKS ON SOME NONPARAMETRIC ESTIMATES OF A DENSITY FUNCTION[1]

By Murray Rosenblatt[2]

University of Chicago

1956

On the Learnability of Discrete Distributions

(EXTENDED ABSTRACT)

1994

Michael Kearns
AT&T Bell Laboratories

Yishay Mansour
Tel-Aviv University

Dana Ron
Hebrew University

Ronitt Rubinfeld
Cornell University

Robert E. Schapire
AT&T Bell Laboratories

Linda Sellie
University of Chicago

Precise question we study today

Question

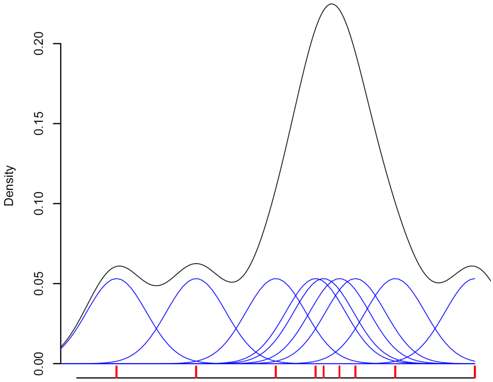
Let f be an unknown mixture of k Gaussians in $\mathbb{R}^d$. How many i.i.d. samples from f is needed to produce, with high probability, a density $\widehat{f}$ satisfying $\|f - \widehat{f}\|_1 \leq \varepsilon$?

Remarks:

1. Algorithm knows k
2. Focus is on sample complexity
3. Equivalent formulation: given n samples from $f \in \mathcal{C}$, how small can you make $\mathbb{E}\left[\|f - \widehat{f}\|_1\right]$? Minimax risk
4. Unbounded for $L^{p>1}$ or KL

Popular method in practice for density estimation

Kernel density estimation



Unfortunately, sample complexity is exponential in d.

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$k = 1$: sample complexity $\le O(d^2/\varepsilon^2)$
compute empirical mean and covariance, and use Gaussian concentration

$d = 1$: sample complexity $\le O(k/\varepsilon^2)$
approximate by piecewise polynomials
[Chan, Diakonikolas, Servedio, Sun 2014]

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Question: sample complexity $\leq$ number of parameters divided by ε^2?
Indeed we will show
sample complexity $\leq kd^2/\varepsilon^2 \times \log^2(d)\log(k) = \widetilde{O}(kd^2/\varepsilon^2)$

Known results - 1

Definition

Given an i.i.d. sample from an unknown density $f \in \mathcal{C}$, output $\widehat{f}$ satisfying $\|f - \widehat{f}\|_1 \leq \varepsilon$ with high probability.

$m_{\mathcal{C}}(\varepsilon)$ = the smallest number of required samples.

k-mix$(\mathcal{C})$ = class of distributions formed by taking k-mixtures of elements of $\mathcal{C}$

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Theorem (Ashtiani, Ben-david, M2017)

For any class $\mathcal{C}$, sample complexity for learning $k\text{-}mix(\mathcal{C}) \leq O(m_{\mathcal{C}}(\varepsilon) \times k \log k / \varepsilon^2)$

Corollary

Sample complexity for learning mixtures of Gaussians $\leq O((d^2/\varepsilon^2) \times k \log k/\varepsilon^2) = O(kd^2 \log(k)/\varepsilon^4)$

Known results - 2

$$Y(\mathcal{C}) = \left\{ \{x \in \mathbb{R}^d : f_1(x) > f_2(x)\} : f_1, f_2 \in \mathcal{C} \right\}$$

1. $m_{\mathcal{C}}(\varepsilon) \leq O(\text{VC-dim}(Y(\mathcal{C}))/\varepsilon^2)$ [Devroye and Lugosi 2001]

Known results - 2

$$Y(\mathcal{C}) = \left\{ \{x \in \mathbb{R}^d : f_1(x) > f_2(x)\} : f_1, f_2 \in \mathcal{C} \right\}$$

1. $m_{\mathcal{C}}(\varepsilon) \leq O(\text{VC-dim}(Y(\mathcal{C}))/\varepsilon^2)$ [Devroye and Lugosi 2001]
2. When $\mathcal{C}$ = mixtures of Gaussians, VC-dim$(Y(\mathcal{C})) \leq O(k^4 d^4)$ [Khovanskii 1991], [Karpinski and Macintyre 1997], [Anthony and Bartlett 1999]
3. Gives an upper bound of $O(k^4 d^4/\varepsilon^2)$ for the sample complexity of mixtures of Gaussians.

We will improve this to kd^2/ε^2.

Lower bounds

Lower bounds?

Best known lower bound was $\Omega(kd/\varepsilon^2)$.
[Suresh, Orlitsky, Acharya, and Jafarpour 2014]

Theorem (Ashtiani, Ben-David, Harvey, Liaw, M, Plan'18)

Any algorithm that learns mixtures of Gaussians has sample complexity $\Omega(kd^2/\varepsilon^2)$.

Suffices to show lower bound of $\Omega(d^2/\varepsilon^2)$ for a single Gaussian.

Lower bound proof

Suffices to show lower bound of $\Omega(d^2/\varepsilon^2)$ for a single Gaussian.

General idea: find lots of distributions that are hard to distinguish but far in L^1 distance.
[LeCam 1973], [Hasminskii 1976], [Assoud 1983]

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[LeCam 1973], [Hasminskii 1976], [Assoud 1983]

Hasminskii+Fano's inequality: find $2^{\Omega(d^2)}$ Gaussians with pairwise KL-divergence $\leq \varepsilon^2$ and pairwise L^1 distance $> \varepsilon$.

$$\mathrm{KL}(f_1 \parallel f_2) := \int f_1(x) \log \frac{f_1(x)}{f_2(x)} \mathrm{d}x \qquad [\mathit{Kullback} - \mathit{Leibler}]$$

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Need to build $2^{\Omega(d^2)}$ Gaussians with pairwise KL-divergence $\leq \varepsilon^2$ and pairwise L^1 distance $> \varepsilon$.

We will use zero-mean Gaussians, so just need to specify the covariance matrices.

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First construction [Ashtiani, Ben-David, Harvey, Liaw, M, Plan'18]. Repeat 2^{d^2} times: start with an identity covariance matrix, then choose a random subspace of dimension $d/9$ and slightly increase the eigenvalues corresponding to this eigenspace: $\Sigma = I + \frac{\varepsilon}{\sqrt{d}} UU^\intercal$, with $U \in \mathbb{R}^{d \times d/9}$ orthonormal. Then prove that with large probability, any two of these have L^1 distance $> \varepsilon$.

Lower bound proof

Need to build $2^{\Omega(d^2)}$ Gaussians with pairwise KL-divergence $\leq \varepsilon^2$ and pairwise L^1 distance $> \varepsilon$.

We will use zero-mean Gaussians, so just need to specify the covariance matrices.

Second construction (combinatorial) [Devroye,M,Reddad 2018]. For $d = 3$, consider the following inverse covariance matrices:

$$\begin{pmatrix} 0 & -\delta & -\delta \\ -\delta & 0 & -\delta \\ -\delta & -\delta & 0 \end{pmatrix}, \begin{pmatrix} 0 & \delta & \delta \\ \delta & 0 & -\delta \\ \delta & -\delta & 0 \end{pmatrix}, \begin{pmatrix} 0 & \delta & -\delta \\ \delta & 0 & \delta \\ -\delta & \delta & 0 \end{pmatrix}, \begin{pmatrix} 0 & -\delta & \delta \\ -\delta & 0 & \delta \\ \delta & \delta & 0 \end{pmatrix}$$

For general d, build $2^{d^2/10}$ inverse covariance matrices so that any two of them are different in at least $d^2/3$ coordinates (Gilbert-Varshamov bound in coding theory).

Theorem (Ashtiani, Ben-David, Harvey, Liaw, M, Plan'18)

Any algorithm that learns mixtures of Gaussians has sample complexity $\Omega(kd^2/\varepsilon^2)$*.*

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Any algorithm that learns mixtures of Gaussians has sample complexity $\Omega(kd^2/\varepsilon^2)$.

Next: upper bound

Our upper bound

$m_{\mathcal{C}}(\varepsilon)$ = sample complexity for learning a density from class $\mathcal{C}$.

Theorem (Ashtiani, Ben-David, Harvey, Liaw, M, Plan'18)

If $\mathcal{C}$ = mixtures of k Gaussians in $\mathbb{R}^d$, then
$m_{\mathcal{C}}(\varepsilon) = \widetilde{O}(kd^2/\varepsilon^2)$.

Covering number argument

Lemma (Yatracos 1985)

Suppose there exist $f_1, \ldots, f_M \in C$ such that for any $f \in C$, there exists some i with $\|f - f_i\|_1 \leq \varepsilon$. Then $m_C(\varepsilon) = O(\log(M)/\varepsilon^2)$.

Proved by a clever combination of Hoeffding's inequality and the union bound.

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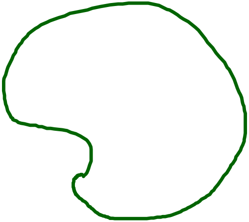

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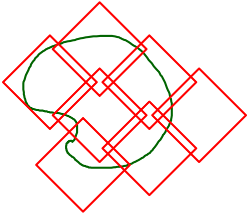
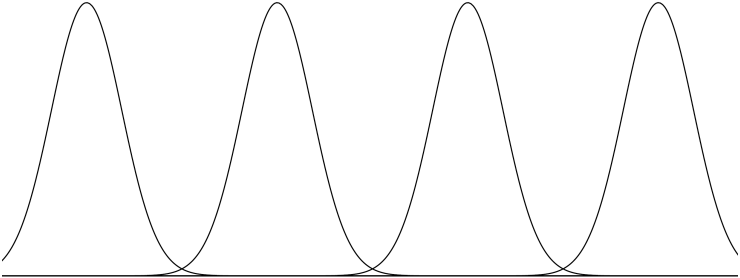


A bound on the covering number of a distribution class bounds its sample complexity.

covering number= ε-net number= packing number= ε-Kolmogorov entropy= metric entropy

Gaussians are not bounded

Unfortunately, Gaussian distributions have infinite covering number, even if the mean is bounded.



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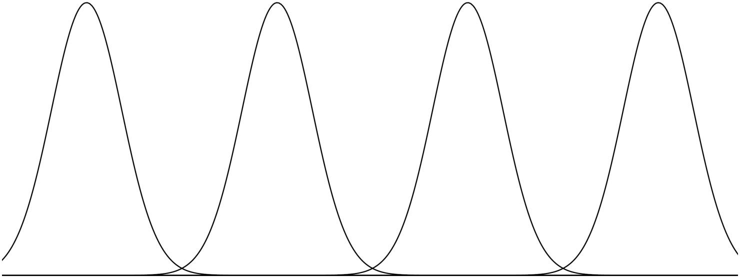

Our novel idea to solve this: Use some of the data to reduce the search space significantly. To formalize this idea, we introduce the notion of compression.

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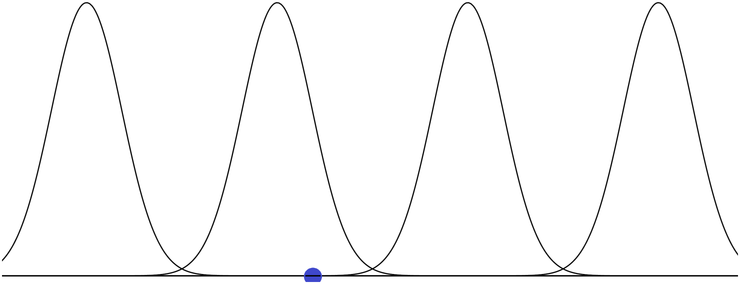

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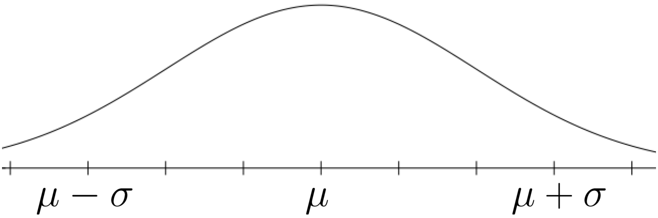
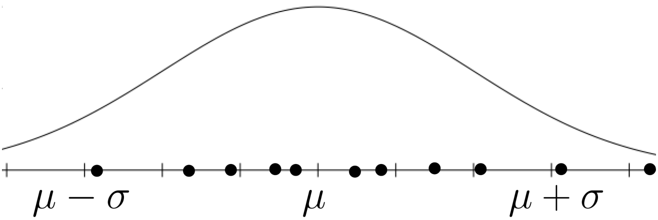
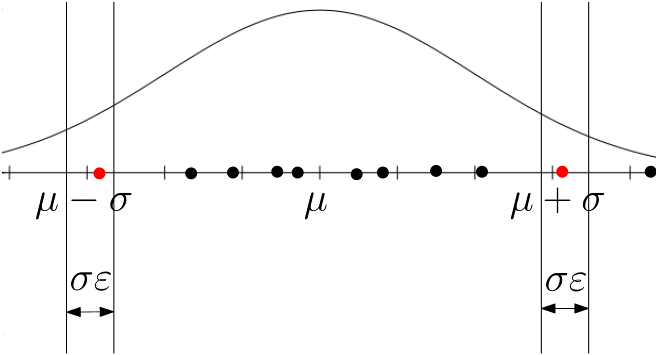

$\mu - \sigma$
μ
$\mu + \sigma$


$\mu - \sigma$
μ
$\mu + \sigma$



$\mu - \sigma$
μ
$\mu + \sigma$
$\sigma\varepsilon$
$\sigma\varepsilon$

$$\widehat{\mu} = \frac{x_1 + x_2}{2}$$

$$\widehat{\sigma} = \frac{|x_1 - x_2|}{2}$$

$$\left\| N(\widehat{\mu}, \widehat{\sigma}) - N(\mu, \sigma) \right\|_1 \leq \varepsilon$$

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One-dimensional Gaussians admit $(100/\varepsilon, 2)$-compression.

Compression implies learnability

Definition (compression)

Class $\mathcal{C}$ admits $(n(\varepsilon), \tau(\varepsilon))$-compression if, for any $f \in \mathcal{C}$, after $n(\varepsilon)$ i.i.d. samples from f are generated, with high probability there exist $\tau(\varepsilon)$ of the samples from which $\widehat{f}$ can be constructed satisfying $\|f - \widehat{f}\|_1 \leq \varepsilon$.

Lemma (compression implies learnability)

If $\mathcal{C}$ admits (n, τ)-compression, $m_{\mathcal{C}}(\varepsilon) = O\left(n + \frac{\tau \log n}{\varepsilon^2}\right)$.

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Algorithm: Exhaustive search + Yatracos' algorithm

Running time: n^τ

Proof of upper bound: compression

1. Compressing d-dimensional Gaussians

d-dimensional Gaussians admit $\widetilde{O}(d, d^2)$-compression.

2. Compressing mixtures

If $\mathcal{C}$ admits (n, τ)-compression, then k-mix$(\mathcal{C})$ admits $\widetilde{O}(kn, k\tau)$-compression.

3. Compression implies learnability

If $\mathcal{C}$ admits (n, τ)-compression, $m_{\mathcal{C}}(\varepsilon) = \widetilde{O}(n + \tau/\varepsilon^2)$.

Theorem (Ashtiani, Ben-David, Harvey, Liaw, M, Plan'18)

If $\mathcal{C}$ is mixtures of k Gaussians in $\mathbb{R}^d$ then $m_{\mathcal{C}}(\varepsilon) = \widetilde{O}(kd^2/\varepsilon^2)$.

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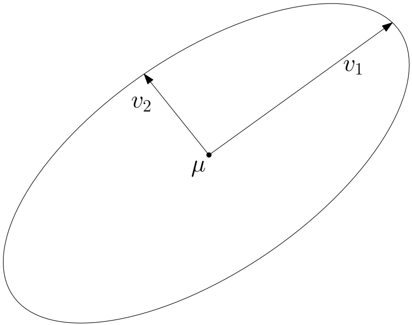
$$\mathcal{N}(\mu, \Sigma) = \mathcal{N}(\mu, v_1 v_1^\mathsf{T} + v_2 v_2^\mathsf{T}).$$



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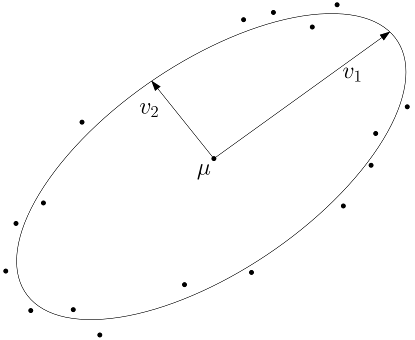

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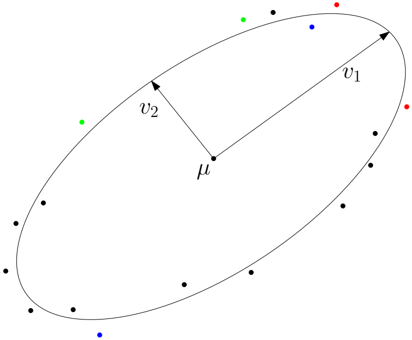
$\mathcal{N}(\mu, \Sigma) = \mathcal{N}(\mu, v_1 v_1^{\mathsf{T}} + v_2 v_2^{\mathsf{T}})$.



Proof of upper bound: compression

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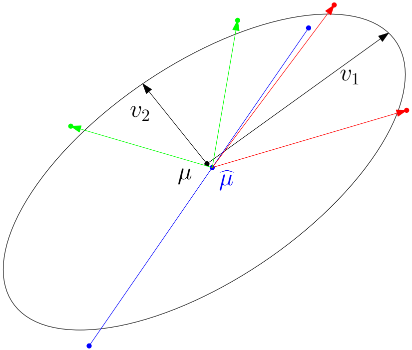

Proof of upper bound: compression

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d-dimensional Gaussians admit $\widetilde{O}(d, d^2)$-compression.

In general, use $d \log^2(d/\varepsilon)$ data points to encode the mean, and $d \log^2(d/\varepsilon)$ data points for each eigenvector.

Lemma (Litvak, Pajor, Rudelson, Tomczak-Jaegermann 2005)

If we take $O(d \log d)$ samples from $\mathcal{N}(0, I_d)$, their convex hull with high probability contains $\frac{1}{20} B_2^d$

Main result

Theorem (Ashtiani, Ben-David, Harvey, Liaw, M, Plan, NeurIPS 2018)

Given $\widetilde{O}(kd^2/\varepsilon^2)$ samples from an unknown mixture of k Gaussians in d dimensions, we can output a density that is ε-close in L^1 to the underlying density with high probability. Moreover, any algorithm achieving this task requires at least $\Omega(kd^2/\varepsilon^2)$ many samples.

improve previous upper bounds of $\widetilde{O}(kd^2/\varepsilon^4)$ and $O(k^4d^4/\varepsilon^2)$, and the lower bound of $\Omega(kd/\varepsilon^2)$.

Upper bound. a novel technique for distribution learning based on compressions, high-dimensional geometry + Yatracos' algorithm.

Lower bound. a packing argument, Fano's inequality.

Open questions

Open questions

1. Polynomial time algorithm?
2. What if k is not known?
3. Sample complexity for general classes?

Thanks to my co-authors

Hassan Ashtiani
(McMaster)

Shai Ben-David
(Waterloo)

Nick Harvey
(UBC)

Chris Liaw
(UBC)

Yaniv Plan
(UBC)

Research direction 1

What is the sample complexity for learning a class C?

- ✓ Relate this to some notion of dimension of the class?
- ✓ Apply the compression idea to other classes?

- ✓ Probabilistic graphical models, e.g. the Ising model [Devroye, M, Reddad'18]
- ✓ Distributions generated by neural networks

Picture taken from the work of Karras, Aila, Laine, and Lehtinen 2017

Research direction 2: computational complexity

Which classes are learnable in polynomial time?

Polynomial time algorithm for mixtures of Gaussians?

Exists for mixtures of spherical Gaussians.
[Suresh, Orlitsky, Acharya, and Jafarpour 2014]

Research direction 2: computational complexity

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Research direction 3: robustness

Design learners that are robust against noisy data.

Our algorithm works in agnostic learning.

What if a small fraction of the data is corrupted in an adversarial way?

Research direction 4: online learning

What if data is not revealed at once, but is received in an online manner? Can we compete against a batch algorithm that sees all the data at once?

Research direction 5: model selection

Can we learn the class C itself from data?

What if the number of Gaussian components, k, is not known?

Popular method in practice for density estimation

Kernel density estimation–continued

Table 4.2 *Sample size required (accurate to about 3 significant figures) to ensure that the relative mean square error at zero is less than* 0.1, *when estimating a standard multivariate normal density using a normal kernel and the window width that minimizes the mean square error at zero*

Dimensionality	*Required sample size*
1	4
2	19
3	67
4	223
5	768
6	2 790
7	10 700
8	43 700
9	187 000
10	842 000

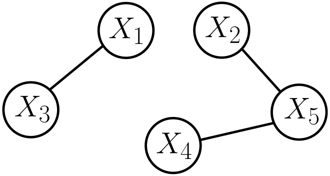
Silverman 1998, Density estimation for Statistics and Data Analysis

VC-dimension

For a family $\mathcal{Y}$ of subsets of X, the VC-dimension of $\mathcal{Y}$ is the size of the largest set $A \subseteq X$, such that for any $B \subseteq A$ there exists some $Y \in \mathcal{Y}$ with $Y \cap A = B$.

Interesting classes - 1

Probabilistic graphical models



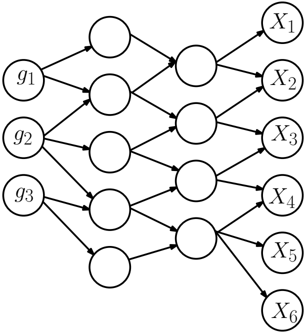
Example (The Ising model). Each $X_i \in \{-1, +1\}$ and

$$\mathbb{P}\left[X_1 = x_1, \ldots, X_d = x_d\right] \propto \exp\left(\sum_{ij \in E(G)} w_{i,j} x_i x_j\right)$$

Theorem (Devroye, M, Reddad'18)

Let $\mathcal{I}_G$ = Ising models on G. Then, $m_{\mathcal{I}_G}(\varepsilon) = \Theta(|E(G)|/\varepsilon^2)$.

Interesting classes - 2



[Karras, Aila, Laine, and Lehtinen 2017]

Proof of mixture lemma

Compressing mixtures

If $\mathcal{C}$ admits (n, τ)-compression, then k-mix$(\mathcal{C})$ admits $(nk\log(k), k\tau + k\log k)$-compression.

Let $\mathbf{P} = \frac{1}{3}P_1 + \frac{1}{3}P_2 + \frac{1}{3}P_3$, where each P_i is 2-compressible.

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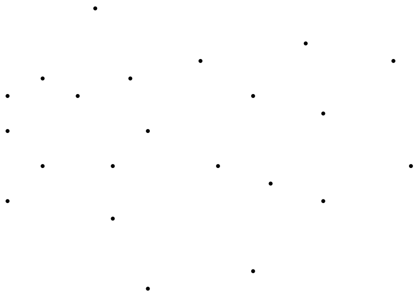

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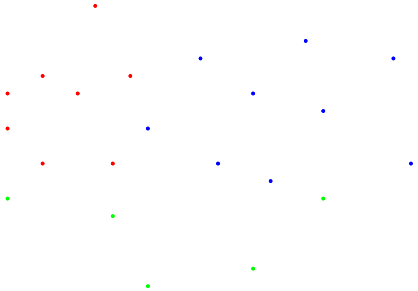

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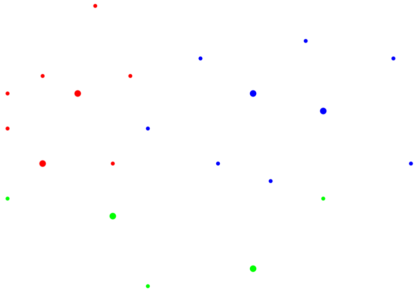

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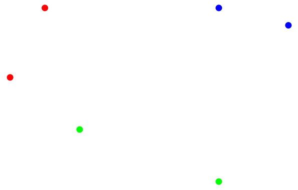

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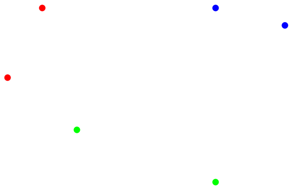

Let $\widehat{\mathbf{P}} = \frac{1}{3}\widehat{P_1} + \frac{1}{3}\widehat{P_2} + \frac{1}{3}\widehat{P_3}$

Lemma (Yatracos 1985)

Suppose there exist $f_1, \ldots, f_M \in \mathcal{C}$ *such that for any* $f \in \mathcal{C}$*, there exists some* i *with* $\|f - f_i\|_1 \leq \varepsilon/5$*. Then* $m_{\mathcal{C}}(\varepsilon) = O(\log(M)/\varepsilon^2)$*.*

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Let $Y := \left\{ \{x : f_i(x) > f_j(x)\} \text{ for } i, j = 1, \ldots, m \right\}$ and let S be an i.i.d. sample of size $50 \log(M)/\varepsilon^2$ from f. For density f, let $f(A) := \int_A f$. $|S \cap A| \sim \text{binomial}(|S|, f(A))$. By Hoeffding [1963] and a union bound over $A \in Y$,

$$\text{err}(f) := \sup_{A \in Y} \left| f(A) - \frac{|S \cap A|}{|S|} \right| \leq \varepsilon/5$$

with probability $1 - 2M^2 \exp(-|S|\varepsilon^2/25) \geq 99\%$.
Thus there exists some i with $\text{err}(f_i) \leq 2\varepsilon/5$.
So $\min_j \text{err}(f_j) \leq 2\varepsilon/5$, and it can be shown that the argmin here is within L1 distance ε of f.

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Output

$$\min_{j=1,\dots,M} \sup_{A \in Y} \left| f_j(A) - \frac{|S \cap A|}{|S|} \right|$$

An application of density estimation

detecting breast cancer

- ✓ Training data consists of normal (non-cancerous) X-ray images.
- ✓ A probability density function $f : \mathbb{R}^d \to \mathbb{R}$ is learned from the data.
- ✓ When a new input x is presented, a high value for $f(x)$ indicates a normal image, while a low value indicates a novel input, which might be characteristic of an abnormality.

[Tarassenko, Hayton, Cerneaz, Brady 1995: Novelty detection for the identification of masses in mammograms]

An example of density estimation

Generating random faces for computer games

- ✓ Training data consists of actual faces.
- ✓ A probability density function $f : \mathbb{R}^d \to \mathbb{R}$ is learned from the data.
- ✓ New random faces are generated using the learned distribution.

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A popular approach: generative adversarial networks (GANs), based on deep neural networks.

Density estimation in action

Top: generated images using generative adversarial networks

Bottom: a small part of the training data

Picture from Karras, Aila, Laine, and Lehtinen (NVIDIA and Aalto University), October 2017