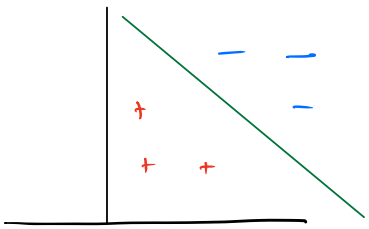
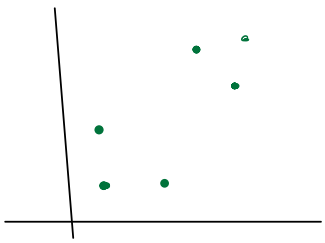
Unsupervised Learning

TODAY: K-means, mixture of Gaussians, EM



Supervised Setting



Unsupervised, no labels!

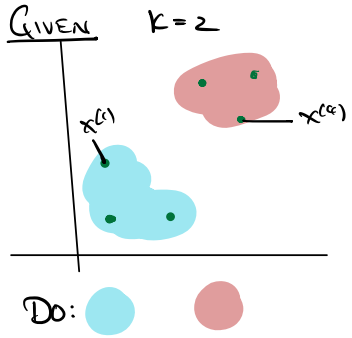
Unsupervised is harder than supervised

allow Stronger assumptions

accept weaker guarantees

Techniques & ideas are valuable

K-MEANS



GIVEN $x^{(1)} \dots x^{(n)} \in \mathbb{R}^d$ & INTEGER K, # of clusters

DO find ASSIGNMENT of $x^{(i)}$ to ONE of K CLUSTERS

$c^{(i)} = j$ Point i IN cluster j

eg. $c^{(3)} = 2$ while $c^{(4)} = 1$

How do we find these clusters? ITERATIVE Approach

1. Randomly init $\mu^{(1)}, \mu^{(2)}$

2. Assign each point to closest cluster $\longleftrightarrow$ $c^{(i)} = \underset{j=1\dots K}{\text{Argmin}} \|\mu^{(j)} - x^{(i)}\|^2$ for each $i = 1 \dots n$

3. Compute New cluster centers for $j = 1 \dots K$

$$\mu^{(j)} = \frac{1}{|\Omega_j|} \sum_{i \in \Omega_j} x^{(i)} \quad \text{s.t. } \Omega_j = \{i : c^{(i)} = j\}$$

Repeat until no points change

Comments

Does k-means terminate? Yes!

$$J(c, \mu) = \sum_{i=1}^{n} \|x^{(i)} - \mu_{c^{(i)}}\|^2$$ decreases monotonically

(see notes)

Does it find a global minimum? not necessarily... NP-hard

Side note: k-means++ from great Stanford students

+ Improved Apx Ratio through Clever Init
+ Default in Sklearn

How do you choose k? No one Right Answer.

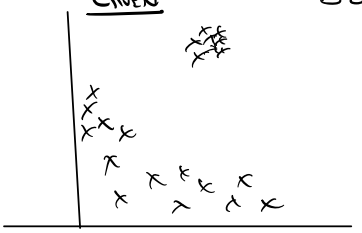
2 clusters 4 clusters

Modeling Question!

Mixture of Gaussians

Toy Astronomy Example (based on a paper from UW)

- Quasars & stars are sources of light
- Both emit light, and we observe photons



Given

Do: Assign each photon to light source $P(z^{(i)} = j)$

"Probability point $z^{(i)}$ belongs to object j"

cf kmeans. this is a **soft** assignment

Challenges + Many sources (say we know K, # of sources)

+ Sources have different intensity & shapes

Assume 1. Sources are well modeled by Gaussian (μ_j, σ_j^2)

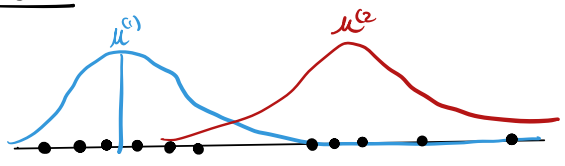
2. We do **not** assume equal # of points per source

→ unknown mixture

NB: Physics folks can check if recovered values make sense.

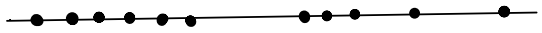
Mixture of Gaussians (model & setup) – 1d for simplicity

Model:



We observe points w/o sources:

$x^{(i)} \in \mathbb{R}$



Observation 1 if we knew "cluster labels" → Solve w/ GDA.

Compute $\mu^{(1)}, \mu^{(2)}$ and be done.

Challenge We don't

GIVEN $x^{(1)}, \dots, x^{(n)} \in \mathbb{R}$ AND POSITIVE INTEGER k

DO find P s.t. for $i = 1 \dots n$ & $j = 1 \dots k$ clusters

$P(z^{(i)} = j)$ SOFT ASSIGNMENT

According to the "GMM MODEL"

$$P(x^{(i)}, z^{(i)}) = P(x^{(i)} \mid z^{(i)}) P(z^{(i)}) \quad \text{Bayes Rule}$$

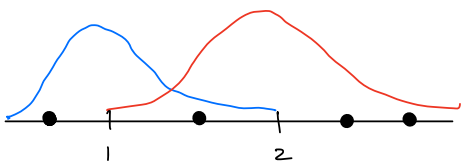
$z^{(i)} \sim \text{Multinomial}(\phi)$ $\phi_j \geq 0$ $\sum_{j=1}^{k} \phi_j = 1$ "which source"

$x^{(i)} \mid z^{(i)} = j \sim N(\mu_j, \sigma_j^2)$ GAUSSIAN IN EACH SOURCE

The PARAMETERS TO BE found ARE highlighted

WE CALL $z^{(i)}$ A hidden or LATENT VARIABLE. $z^{(i)}$ IS NOT DIRECTLY OBSERVED

EXAMPLE "think Sampling"



$\phi_1 = 0.7$ $\phi_2 = 0.3$

$\mu_1 = 1$ $\mu_2 = 2$ $\sigma_1^2 = \sigma_2^2 = \frac{1}{3}$ (roughly)

REPEAT
1. Pick BLUE (w/ Prob 0.7) OR RED (w PROB 0.3)
2. USE APPROPRIATE MEAN μ_1 (RED) or μ_2 (BLUE)

Gmm Algorithm (Famous Algo & Class)

Mirrors K-means

1. (E-STEP) "Guess latent values" of $z^{(i)}$ FOR EACH POINT
2. (M-STEP) UPDATE PARAMETERS

ABSTRACTLY OUR FIRST EXAMPLE of EM-Algorithm (EXPECTATION MAXIMIZATION)

(E-STEP) GIVEN DATA & CURRENT GUESS AT PARAMETERS $(\phi, \mu, \sigma^2 \dots)$

DO PREDICT LATENT VARIABLE $z^{(i)}$ for $i = 1 \dots n$

$$w_j^{(i)} = P(z^{(i)} = j \mid x^{(i)}; \phi, \mu, \sigma) \qquad \text{OUR GOAL}$$

$$= \frac{P(z^{(i)} = j, x^{(i)}; \phi, \mu, \sigma)}{P(x^{(i)}; \phi, \mu, \sigma)} \qquad \text{Bayes Rule}$$

$$= \frac{P(x^{(i)} \mid z^{(i)} = j; \mu, \sigma)\, P(z^{(i)} = j; \phi)}{\sum_{l=1}^{k} P(x^{(i)} \mid z^{(i)} = l; \mu, \sigma)\, P(z^{(i)} = l; \phi)}$$

(2) (2) ϕ_j ϕ_l

- $\propto \exp\left\{-\frac{(x^{(i)} - \mu_j)^2}{\sigma_j^2}\right\}$ "How likely is $x^{(i)}$ according to Gaussian (μ_j, σ_j^2)"
- "How likely point from cluster"

Key Point We can compute all terms! Return $w_j^{(i)}$

M-STEP

GIVEN $w_j^{(i)}$ OUR CURRENT ESTIMATE of $P(z^{(i)} = j)$ for $i = 1 \ldots n$, $j = 1 \ldots k$ clusters

DO ESTIMATE OBSERVED PARAMETERS (USING MLE)

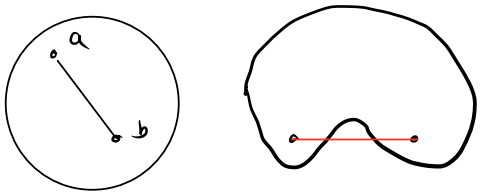
e.g. $\phi_j = \frac{1}{n} \sum_{i=1}^{n} w_j^{(i)} \approx$ fraction of elements in cluster j

$$\mu_j = \frac{\sum w_j^{(i)} x^{(i)}}{\sum w_j^{(i)}} \quad \ldots \text{ etc } \ldots$$

MLE. lets MAKE RIGOROUS!

Detour Convexity & Jensen (This is a key result, we'll go slowly)

A set Ω is convex if for any $a, b \in \Omega$ the line joining a, b is in Ω as well.



Convex

NOT convex!

In symbols,

$\forall \lambda \in [0,1], \quad a, b \in \Omega$

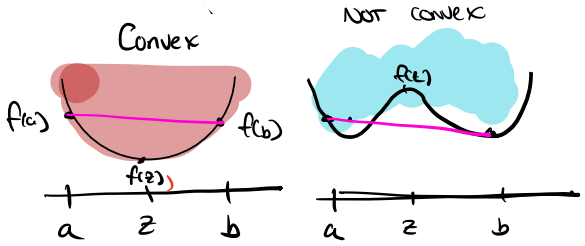
$\lambda a + (1-\lambda) b \in \Omega$

(Need to check $\forall a, b \in \Omega$)

Given a function f, the graph of f G_f is defined as

$$G_f = \{ (x, y) : y \geq f(x) \}$$

A function is convex if its graph is convex (as a set)



"Every chord is above function"

In symbols, $\forall \lambda \in [0,1]$

$\lambda (a, f(a)) + (1-\lambda)(b, f(b)) \in \Omega$

or let $z = \lambda a + (1-\lambda) b$

$\lambda f(a) + (1-\lambda) f(b) \geq f(z)$

If f twice differentiable, $\forall x$ $f''(x) \geq 0 \Rightarrow f$ is convex

Pf $\quad f(a) = f(z) + f'(z)(a-z) + f''(\xi_a)(a-z)^2 \quad \xi_a \in [a, z]$

$f(b) = f(z) + f'(z)(b-z) + f''(\xi_b)(b-z)^2 \quad \xi_b \in [z, b]$

$\lambda f(a) + (1-\lambda) f(b) = f(z) + f'(z)(\lambda a + (1-\lambda) b - z) + C \quad C \geq 0$

$\lambda a + (1-\lambda) b - z = 0$ by def of z.

i.e. $\lambda f(a) + (1-\lambda) f(b) \geq f(z)$ □

We say f is strongly convex if $\forall x \in \text{Dom}(f)$ $f''(x) > 0$.

Ex: $f(x) = x^2 \Rightarrow f'(x) = 2 \Rightarrow$ Strongly convex

$f(x) = x^2(x-1)^2$: graph above (not convex)

Jensen's inequality $\mathbb{E}[f(x)] \geq f(\mathbb{E}[x])$ for convex f.

Ex: x takes value a with prob λ

takes value b with prob $1-\lambda$

$\mathbb{E}[f(x)] = \lambda f(a) + (1-\lambda) f(b)$

$f(\mathbb{E}[x]) = f(z) \qquad z = \lambda a + (1-\lambda) b$

NB: Can prove finitely supported distribution by induction

for convex f, definition implies thm in this case!

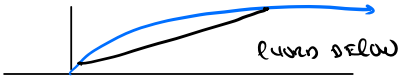
Stronger if f is strongly convex, and $\mathbb{E}[f(x)] = f(\mathbb{E}[x])$

$\Rightarrow$ X is a constant (except: almost surely)

We need concave functions g concave if $-g$ is convex

$$\mathbb{E}[g(x)] \leq g(\mathbb{E}[x])$$

ex: $g(x) = \log(x) \Rightarrow g''(x) = -x^{-2}$ on $(0, \infty)$ negative



What about $h(x) = ax + b$ convex & concave since $h''(x) = 0$.

End detour

EM Algorithm as max likelihood

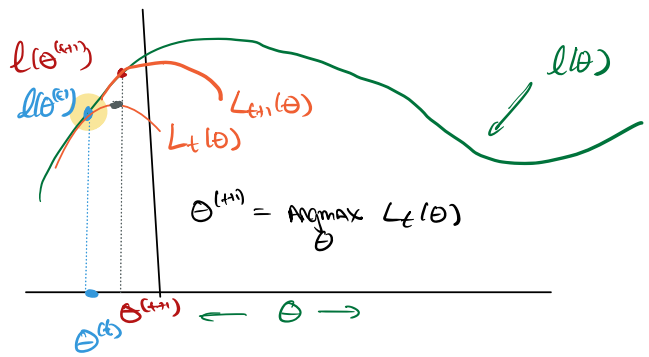
$$\ell(\theta) = \sum_{i=1}^{n} \log P(x^{(i)}; \theta)$$

PARAMETERS

DATA

We assume $P(x;\theta) = \sum_z P(x, z; \theta)$ of GMM latent variable

Picture of Algorithm



$L_t(\theta) \le \ell(\theta)$ (lowerbound)

$L_t(\theta^{(t)}) = \ell(\theta^{(t)})$ (tight)

Hope L_t easier to optimize than $\ell(\theta)$

Rough Algo

(E-step) 1. Given $\theta^{(t)}$ find L_t

(M-step) 2. Given L_t, set $\theta^{(t+1)} = \text{argmax}_\theta L_t(\theta)$

How do we construct L_t?

(Let's look at single point)

$$\log \sum_z P(x, z; \theta) = \log \sum_z \frac{Q(z) P(x, z; \theta)}{Q(z)} \quad \text{for any } Q(z)$$

We Pick $Q(z)$ s.t. $\sum_z Q(z) = 1$ and $Q(z) = 0$ (*)

$$= \log \mathop{E}_z \left[\frac{P(x, z; \theta)}{Q(z)} \right] \quad \text{(Symbol Pushing)}$$

$$\geq \mathop{\mathbb{E}}_{z}\left[\log \frac{P(x,z;\theta)}{Q(z)}\right] \qquad \text{JENSEN'S (log IS CONCAVE)}$$

$$= \sum_{z} Q(z) \log \frac{P(x,z;\theta)}{Q(z)} \qquad \text{(DEF of } \mathbb{E}\text{)}$$

Key step holds for ANY such Q: (*)

This gives a family of lower bounds, one for each choice of Q ($B_t \leq \ell$)

How do we make it tight? Select Q to make inequality tight

What if... $\log \frac{P(x,z;\theta)}{Q(z)} = c$ for some constant, then Jensen's is Equality!

$$P(x,z;\theta) = P(z|x;\theta)P(x;\theta)$$

So, $Q(z) = P(z|x;\theta)$ then

$c = \log P(x;\theta)$ does not depend on z, so constant!

NB: $Q(z|$ does depend on θ & x – we will select a $Q^{(i)}(z)$ for every point independently.

We define Evidenced-based lower bound (ELBO), sum over z

$$\text{ELBO}(x, Q, z) = \sum_{z} Q(z) \log \frac{P(x,z;\theta)}{Q(z)}$$

We've shown $\ell(\theta) \geq \sum_{i=1}^{n} \text{ELBO}(x^{(i)}, Q^{(i)}; \theta)$ for ANY $Q^{(i)}$ satisfying (*)

lower bound

$$\ell(\theta^{(t)}) = \sum_{i=1}^{n} \text{ELBO}(x^{(i)}, Q^{(i)}, \theta^{(t)}) \text{ for choice of } Q^{(i)} \text{ above.}$$

WRAP UP

1. (E-STEP) $Q^{(i)}(z) = P(z^{(i)} | x^{(i)}; \theta)$ for $i = 1 \dots n$
2. (M-STEP) $\theta^{(t+1)} = \underset{\theta}{\text{Argmax}}\ L_t(\theta)$

   in which $L_t(\theta) = \sum_{i=1}^{n} \text{ELBO}(x^{(i)}, Q^{(i)}; \theta)$

WHY DOES THIS TERMINATE? $\ell(\theta^{(t+1)}) \geq \ell(\theta^{(t)})$

IS IT GLOBALLY OPTIMAL? (MAYBE SEE PICTURE)

WE DERIVED HARD & SOFT CLUSTERING METHODS

EM ALGORITHM IN TERMS OF MLE.