IFT 4030/7030, Machine Learning for Signal Processing

Week8: Machine Learning 4, Clustering

Cem Subakan

Admin

- Homework 1 is due soon (tomorrow midnight).
  - Homework 1 est du très bientot.
- I will release Homework 2 soon.
  - On va publier le homework 2 bientot!
- I hope you have started working on your projects!.
  - J'espère que vous avez déjà commencé vos projets.
- Today: Clustering
  - Aujourd'hui: Clustering

Clustering

- Let's kick things off with clustering. / On va commencer avec clustering.
- We were doing supervised learning for the past two classes. Now we will change.
  - On faisait de l'apprentissage supervisé pour les deux derniers classes.

Clustering

- Let's kick things off with clustering. / On va commencer avec clustering.
- We were doing supervised learning for the past two classes. Now we will change.
  - On faisait de l'apprentissage supervisé pour les deux derniers classes.
- What if we do not have the labels?
  - Et si on n'avait pas d'étiquettes?

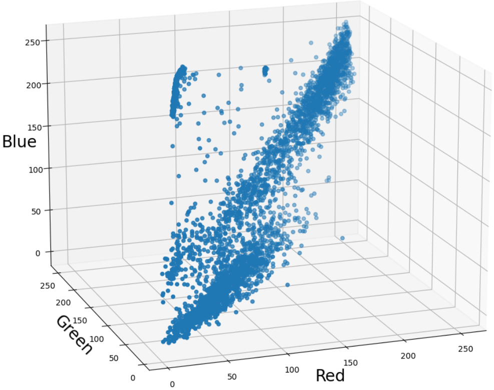
Clustering

- Let's kick things off with clustering. / On va commencer avec clustering.
- We were doing supervised learning for the past two classes. Now we will change.
    - On faisait de l'apprentissage supervisé pour les deux derniers classes.
- What if we do not have the labels?
    - Et si on n'avait pas d'étiquettes?
- Today's lecture's goal / Le but d'aujourd'hui.
    - I will try to acclimate you with clustering./Je vais essayer de vous introduire des concepts de base de clustering.
    - But in a sneaky way I will introduce powerful tools from probabilistic machine learning. / Je vais vous bombarder silenciusement avec des outils des l'apprentissage automatique probabilistique.

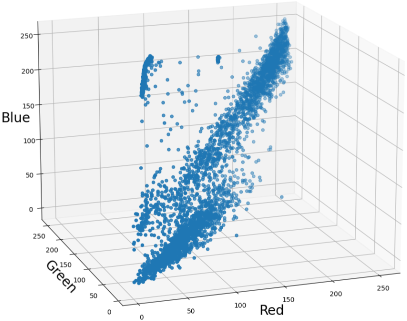
Some motivation

El Capitan, Yosemite National Park, California

How many clusters?

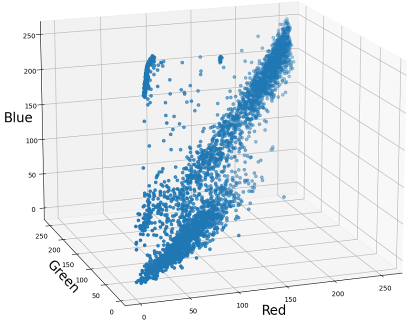


Clustering



- We see clusters, but how do we find them?
  - On voit des groupes, mais comment on les trouve?
- Can I find an algorithm for this? / Peut-on trouver un algorithme pour cela?

Clustering



- We see clusters, but how do we find them?
  - On voit des groupes, mais comment on les trouve?
- Can I find an algorithm for this? / Peut-on trouver un algorithme pour cela?
- Clustering!

Clustering

- **Clustering:** We discover clusters/groups in the data.
  - **Clustering:** On découvre des groupes dans les données.
- Fundamentally **ill defined** problem. There is often no correct solution.
  - Clustering n'est pas un problème bien défini.
- Relies on user choices.
  - Ça dépend sur les choix de l'utilisateur.

Clustering process

- **Features**

  Describe your data using features. / Quels features utilise-t-on pour répresenter les données?

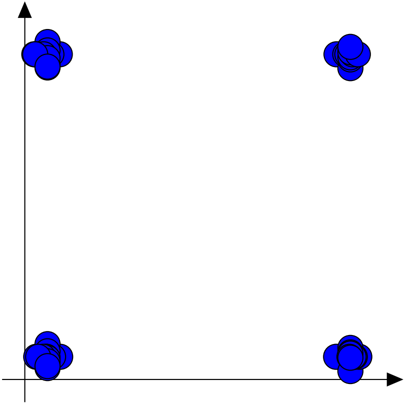
- **Cluster Shapes**

  Decide what your clusters should look like / Il faut décider comment on veut que les clusters se forment.

Clustering process

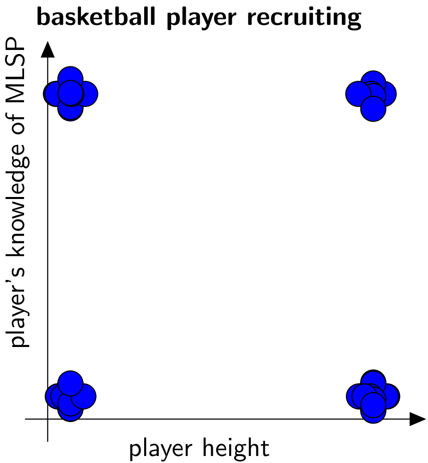
- **Features**
  Describe your data using features. / Quels features utilise-t-on pour répresenter les données?
- **Cluster Shapes**
  Decide what your clusters should look like / Il faut décider comment on veut que les clusters se forment.
- **Distance**
  Define a distance function / promixity measure.
  - Définissons une notion de distance / proximité.

Features



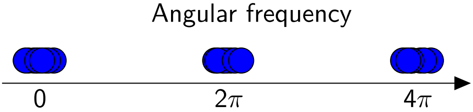
- How many clusters? / Combien de groupes?

Features

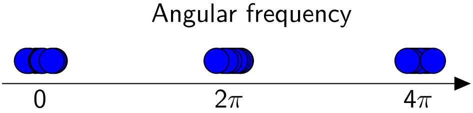


- How many clusters? / Combien de groupes?
- How many clusters? / Combien de groupes?

Use a sensible distance function

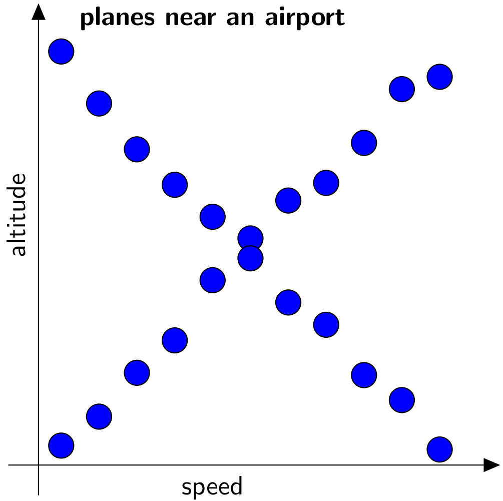


Use a sensible distance function

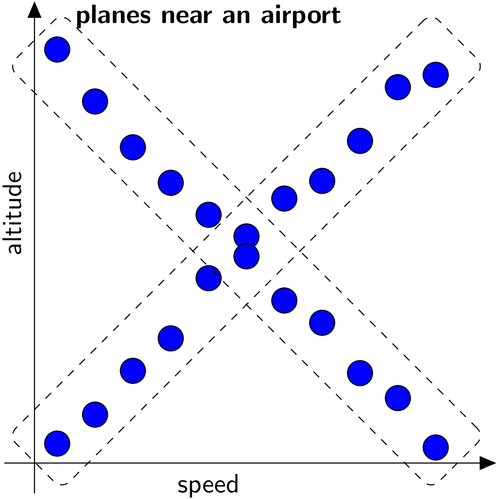


- Probably using euclidean distance is not a good idea here!
    - Très probable qu’il faut pas utiliser la distance euclidienne içi!!

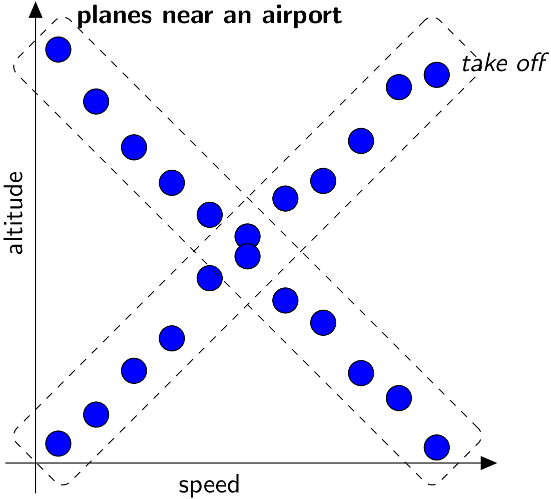
What forms clusters in your space?



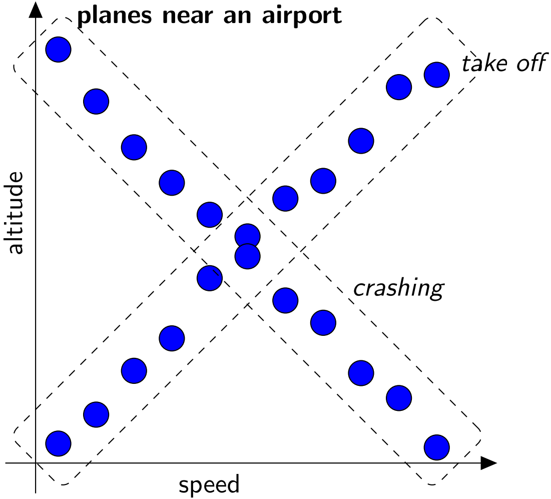
What forms clusters in your space?



What forms clusters in your space?

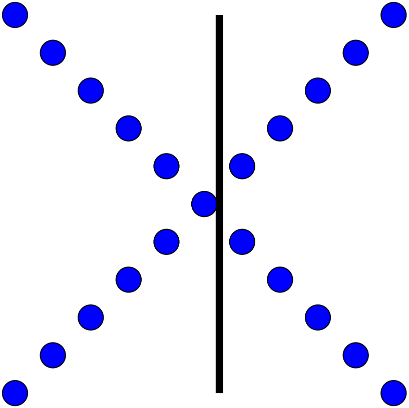


What forms clusters in your space?



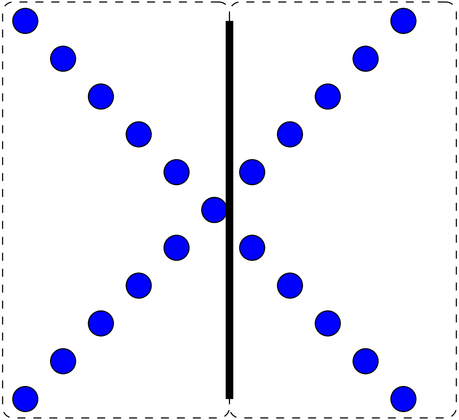
What forms clusters in your space?

ball trajectories bouncing off a wall

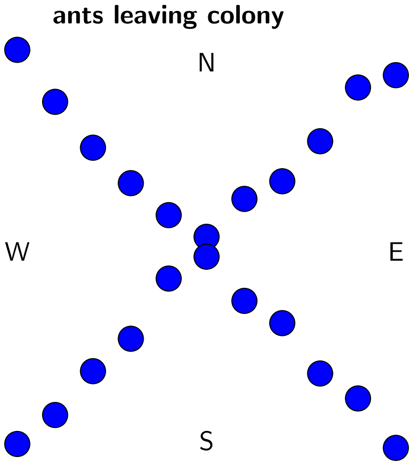


What forms clusters in your space?

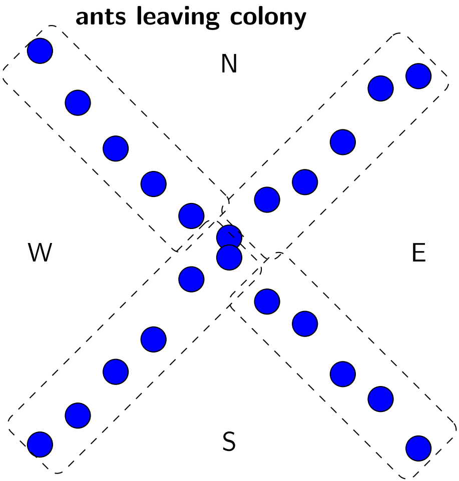
ball trajectories bouncing off a wall



What forms clusters in your space?



What forms clusters in your space?



There usually are not %100 correct answers

- Clustering is partly an art
  - Clustering de partie est un art
- You need to experiment with different things to get there
  - On a besoin d'experimenter afin d'y arriver

How to cluster

- Many approaches. Today we'll talk about
  - Centroid based approaches
    - K-means
    - Mixture Models
  - Hierarchical clustering
  - Spectral clustering

Table of Contents

Centroid based approaches

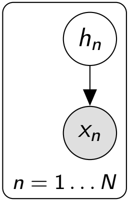
- K-means clustering
- Gaussian Mixture Model
- More Advanced GMM Learning Methods

Spectral Clustering

Hierarchical Clustering

Gaussian Mixture Model

- Model:



$$\begin{aligned} h_n &\sim \text{Discrete}(\pi) \\ x_n | h_n &\sim \mathcal{N}(x; \mu_{h_n}, \sigma^2 I), \text{ for } n \in \{1, \dots N\} \end{aligned}$$

- $h_n \in \{1, \dots, K\}$, cluster indicators / indicateur de groupes.
- $x_n \in \mathbb{R}^L$, observed data items / des données observées.
- $\theta = \{\mu_1, \mu_2, \dots, \mu_K\}$ parameters/cluster centers (or centroids) (les paramètres, centres de groupes).

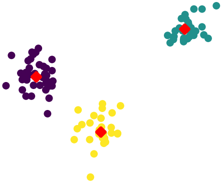


Table of Contents

Centroid based approaches

K-means clustering

Gaussian Mixture Model

More Advanced GMM Learning Methods

Spectral Clustering

Hierarchical Clustering

Learning Variant 1 for GMM

- Find cluster indicators $\widehat{h}_{1:N}$ and parameters $\widehat{\theta}$ such that: / On trouve des indicateurs de clusters et des centroids telle que:

$$\widehat{h}_{1:N}, \widehat{\theta} = \arg\max_{h_{1:N}, \theta} p(x_{1:N} | h_{1:N}, \theta)$$

Learning Variant 1 for GMM

- Find cluster indicators $\widehat{h}_{1:N}$ and parameters $\widehat{\theta}$ such that: / On trouve des indicateurs de clusters et des centroids telle que:

$$\widehat{h}_{1:N}, \widehat{\theta} = \arg\max_{h_{1:N}, \theta} p(x_{1:N} | h_{1:N}, \theta)$$

- Write down log-likelihood: / On écrit le log-likelihood:

$$\begin{aligned}
\log p(x_{1:N}, h_{1:N} | \theta) &= \log \prod_{n=1}^{N} p(x_n | h_n, \theta) p(h_n | \theta) \\
&= \log \prod_{n=1}^{N} \left(\prod_{k=1}^{K} \mathcal{N}(x_n; \mu_k, \sigma^2 I)^{[h_n = k]} \times \prod_{k=1}^{K} \pi_k^{[h_n = k]} \right) \\
&=^{+} \sum_{n=1}^{N} \left(\sum_{k=1}^{K} [h_n = k] \left(\frac{-\|x_n - \mu_k\|_2^2}{2\sigma^2} + \log \pi_k \right) \right)
\end{aligned}$$

How to learn with this objective function?

$$\mathcal{L}(\mu_{1:K}, \pi_{1:K}, h_{1:N}) = \sum_{n=1}^{N} \left(\sum_{k=1}^{K} [h_n = k] \left(\frac{\|x_n - \mu_k\|_2^2}{2\sigma^2} + \log \pi_k \right) \right)$$

- Notice that $h_{1:N}$ are discrete variables. / Notez que $h_{1:N}$ sont discrets.
- We can not directly take the gradient and optimize. / On ne peut pas juste calculer le gradient et l'optimiser.

How to learn with this objective function?

$$\mathcal{L}(\mu_{1:K}, \pi_{1:K}, h_{1:N}) = \sum_{n=1}^{N} \left(\sum_{k=1}^{K} [h_n = k] \left(\frac{\|x_n - \mu_k\|_2^2}{2\sigma^2} + \log \pi_k \right) \right)$$

- Notice that $h_{1:N}$ are discrete variables. / Notez que $h_{1:N}$ sont discrets.
- We can not directly take the gradient and optimize. / On ne peut pas juste calculer le gradient et l'optimiser.
- Any ideas? / Idées?

Learning Variant 1 for GMM

- Algorithm: Fix θ, update *h*. Fix *h*, update θ, repeat until convergence (and fix $\pi_k = 1/K$). / On alterne entre l'optimization des parametres θ et les indicateurs *h*.

Learning Variant 1 for GMM

- Algorithm: Fix θ, update h. Fix h, update θ, repeat until convergence (and fix $\pi_k = 1/K$). / On alterne entre l'optimization des parametres θ et les indicateurs h.
- Update $\mu_{k'}$: compute the gradient while $h_{1:N}$ is fixed: / calcule le gradient par rapport à $\mu_{k'}$ quand $h_{1:N}$ est fixé.

$$\frac{\partial \log p(x_{1:N}, h_{1:N}|\theta)}{\partial \mu_k} = \frac{\partial \sum_{n=1}^{N} \left(\sum_{k=1}^{K} [h_n = k] \left(\frac{-\|x_n - \mu_k\|_2^2}{2\sigma^2} + \log \pi_k \right) \right)}{\partial \mu_{k'}}$$

$$= \sum_{n=1}^{N} [h_n = k'] \frac{(x_n - \mu_{k'})}{\sigma^2} = \sum_{n=1}^{N} [h_n = k'] \frac{x_n}{\sigma^2} - [h_n = k'] \frac{\mu_{k'}}{\sigma^2}$$

set the gradient equal to 0 / mettez le gradient à 0, solve for / résoudre pour

$\mu_{k'} \to \widehat{\mu}_{k'} = \frac{\sum_{n=1}^{N} [h_n = k'] x_n}{\sum_{n=1}^{N} [h_n = k']}$.

Learning Variant 1 for GMM

- Algorithm: Fix θ, update h. Fix h, update θ, repeat until convergence (and fix $\pi_k = 1/K$). / On alterne entre l'optimization des parametres θ et les indicateurs h.
- Update $\mu_{k'}$: compute the gradient while $h_{1:N}$ is fixed: / calcule le gradient par rapport à $\mu_{k'}$ quand $h_{1:N}$ est fixé.

$$\frac{\partial \log p(x_{1:N}, h_{1:N}|\theta)}{\partial \mu_k} = \frac{\partial \sum_{n=1}^{N} \left(\sum_{k=1}^{K} [h_n = k] \left(\frac{-\|x_n - \mu_k\|_2^2}{2\sigma^2} + \log \pi_k \right) \right)}{\partial \mu_{k'}}$$

$$= \sum_{n=1}^{N} [h_n = k'] \frac{(x_n - \mu_{k'})}{\sigma^2} = \sum_{n=1}^{N} [h_n = k'] \frac{x_n}{\sigma^2} - [h_n = k'] \frac{\mu_{k'}}{\sigma^2}$$

set the gradient equal to 0 / mettez le gradient à 0, solve for / résoudre pour

$\mu_{k'} \to \widehat{\mu}_{k'} = \frac{\sum_{n=1}^{N} [h_n = k'] x_n}{\sum_{n=1}^{N} [h_n = k']}$.

- Update $h_{1:N}$ while $\mu_{k'}$ is fixed: / Mettez $h_{1:N}$ à jour quand $\mu_{k'}$ est fixé:

$$\widehat{h}_n = \arg\max_{h_n} \log p(x_n, h_n|\theta) = \arg\min_{k} \|x_n - \mu_k\|_2^2,$$

we therefore assign h_n as the index of the mean closest to x_n. / On assigne h_n au centroid plus proche.

Learning Variant 1 for GMM

- Algorithm: Fix θ, update h. Fix h, update θ, repeat until convergence (and fix $\pi_k = 1/K$). / On alterne entre l'optimization des parametres θ et les indicateurs h.
- Update $\mu_{k'}$: compute the gradient while $h_{1:N}$ is fixed: / calcule le gradient par rapport à $\mu_{k'}$ quand $h_{1:N}$ est fixé.

$$\frac{\partial \log p(x_{1:N}, h_{1:N}|\theta)}{\partial \mu_k} = \frac{\partial \sum_{n=1}^{N} \left(\sum_{k=1}^{K} [h_n = k] \left(\frac{-\|x_n - \mu_k\|_2^2}{2\sigma^2} + \log \pi_k \right) \right)}{\partial \mu_{k'}}$$

$$= \sum_{n=1}^{N} [h_n = k'] \frac{(x_n - \mu_{k'})}{\sigma^2} = \sum_{n=1}^{N} [h_n = k'] \frac{x_n}{\sigma^2} - [h_n = k'] \frac{\mu_{k'}}{\sigma^2}$$

set the gradient equal to 0 / mettez le gradient à 0, solve for / résoudre pour

$\mu_{k'} \to \widehat{\mu}_{k'} = \frac{\sum_{n=1}^{N} [h_n = k'] x_n}{\sum_{n=1}^{N} [h_n = k']}$.

- Update $h_{1:N}$ while $\mu_{k'}$ is fixed: / Mettez $h_{1:N}$ à jour quand $\mu_{k'}$ est fixé:

$$\widehat{h}_n = \arg\max_{h_n} \log p(x_n, h_n|\theta) = \arg\min_{k} \|x_n - \mu_k\|_2^2,$$

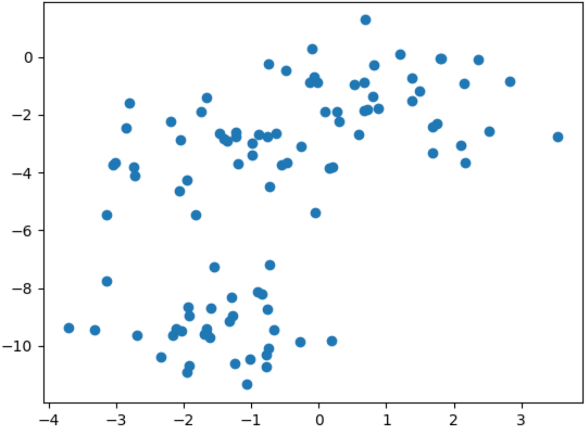
we therefore assign h_n as the index of the mean closest to x_n. / On assigne h_n au centroid plus proche.

- Looks like a familiar algorithm? / Vous connaissez ça?

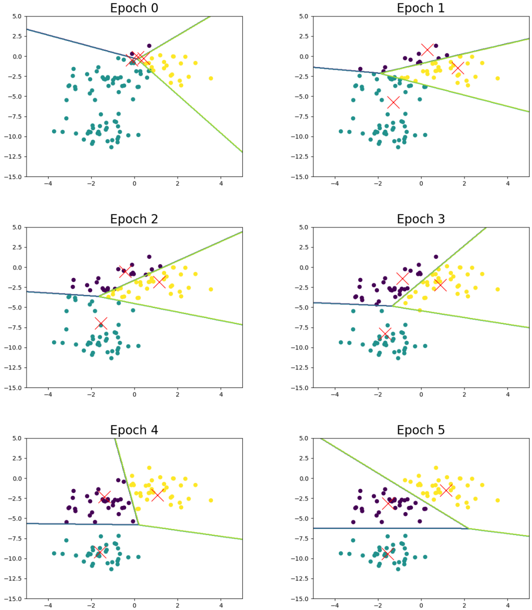
Kmeans Clustering

```
Randomly initialize $\mu_{1:K}$.
while Not converged do
    E-step:
        $\widehat{h}_n = \arg\max_{h_n} \log p(x_n, h_n|\theta) = \arg\min_k \|x_n - \mu_k\|_2^2$
    M-step:
        $\widehat{\mu}_{k'} = \frac{\sum_{n=1}^N [h_n = k'] x_n}{\sum_{n=1}^N [h_n = k']}$
end while
```

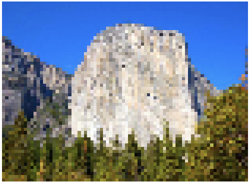
Kmeans Example

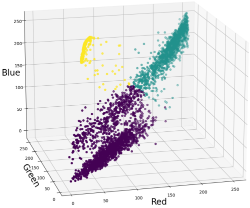


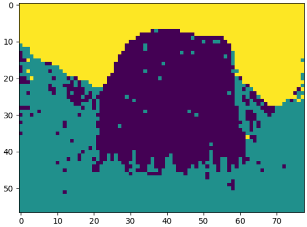
Kmeans Updates



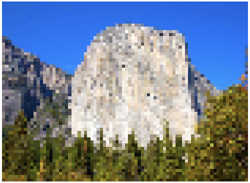
Applying K-means on El-Capitan ($K = 3$)

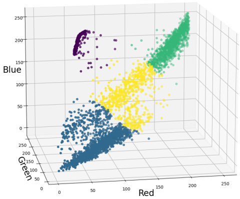


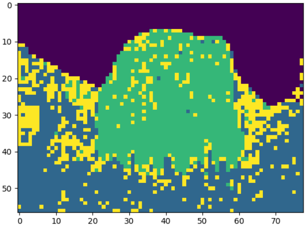




Applying K-means on El-Capitan ($K = 4$)

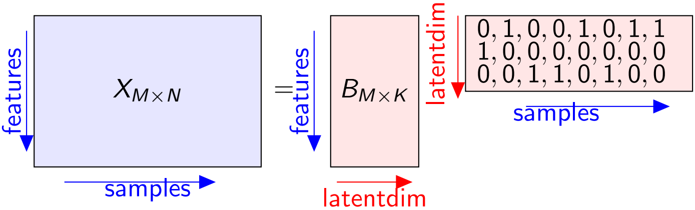






A sidenote

- K-means is a matrix-factorization algorithm

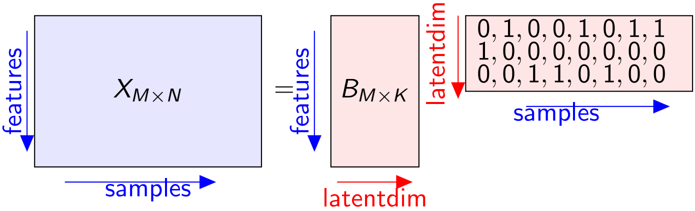


0, 1, 0, 0, 1, 0, 1, 1
1, 0, 0, 0, 0, 0, 0, 0
0, 0, 1, 1, 0, 1, 0, 0

- B in this case has the cluster means in columns / B dans ce cas-ci a les cluster means dans ses colonnes.

A sidenote

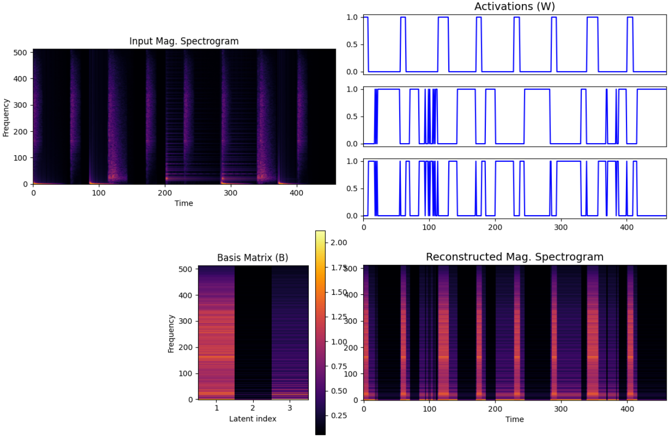
- K-means is a matrix-factorization algorithm



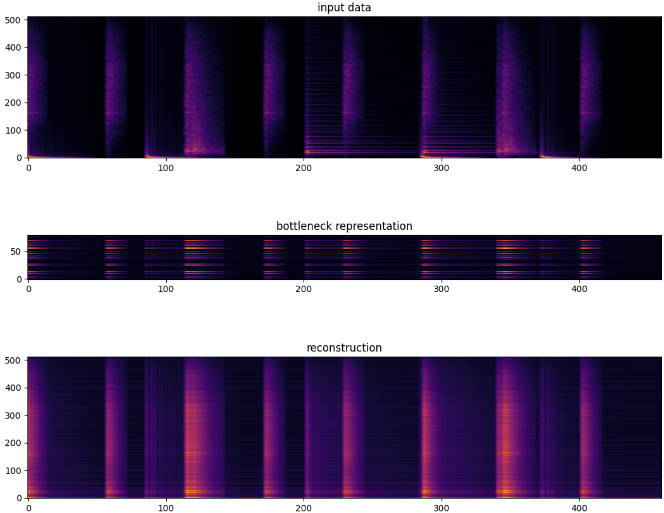
$$\begin{matrix}0,1,0,0,1,0,1,1\\1,0,0,0,0,0,0,0\\0,0,1,1,0,1,0,0\end{matrix}$$

- B in this case has the cluster means in columns / B dans ce cas-ci a les cluster means dans ses colonnes.
- Kmeans is a tokenizer! (It's a buzzword these days)

Kmeans on a familiar picture



Kmeans in the latent space



Cluster the latents!

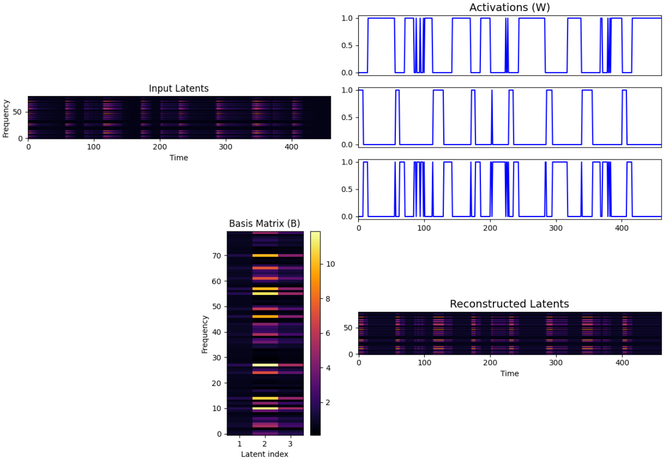


Table of Contents

Centroid based approaches

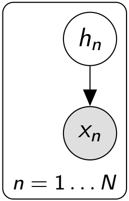
- K-means clustering
- Gaussian Mixture Model
- More Advanced GMM Learning Methods

Spectral Clustering

Hierarchical Clustering

Extending K-means

- Kmeans is good and all, but only learns Isotropic Gaussians. / Kmeans ne peut apprendre que des Gaussiennes Isotropiques.

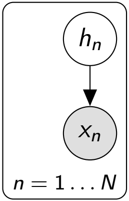


$$\begin{aligned} h_n &\sim \text{Discrete}(\pi) \\ x_n | h_n &\sim \mathcal{N}(x; \mu_{h_n}, \Sigma_{h_n}), \text{ for } n \in \{1, \dots N\} \end{aligned}$$

- $h_n \in \{1, \dots, K\}$, cluster indicators / indicateur de groupes.
- $x_n \in \mathbb{R}^L$, observed data items / des données observées.
- $\theta = \{\mu_1, \mu_2, \dots, \mu_K, \Sigma_1, \Sigma_2, \dots, \Sigma_K, \pi_1, \pi_2, \dots, \pi_K\}$ parameters (les paramètres).

Extending K-means

- Kmeans is good and all, but only learns Isotropic Gaussians. / Kmeans ne peut apprendre que des Gaussiennes Isotropiques.



$$\begin{aligned} h_n &\sim \text{Discrete}(\pi) \\ x_n | h_n &\sim \mathcal{N}(x; \mu_{h_n}, \Sigma_{h_n}), \text{ for } n \in \{1, \dots N\} \end{aligned}$$

- $h_n \in \{1, \dots, K\}$, cluster indicators / indicateur de groupes.
- $x_n \in \mathbb{R}^L$, observed data items / des données observées.
- $\theta = \{\mu_1, \mu_2, \dots, \mu_K, \Sigma_1, \Sigma_2, \dots, \Sigma_K, \pi_1, \pi_2, \dots, \pi_K\}$ parameters (les paramètres).
- Full Covariance matrix for each cluster, and cluster prior probabilities are estimated also.
  - Une matrice de covariance est appris pour chaque cluster, puis les probabilités a prioris de chaque cluster.

Learning Variant 2 for GMM

- In addition, we want to estimate probabilities for $h_{1:N}$. / On estimer des probabilités pour des indicateurs des clusters.
- Find cluster indicator parameters $\widehat{\theta}$ while integrating out hidden variables, such that: / On marginalise sur $h_{1:N}$

$$\begin{aligned}\widehat{\theta} &= \arg\max_{\theta} p(x_{1:N}|\theta) \\ &= \arg\max_{\theta} \sum_{h_{1:N}} p(x_{1:N}, h_{1:N}|\theta)\end{aligned}$$

Learning Variant 2 for GMM

- In addition, we want to estimate probabilities for $h_{1:N}$. / On estimer des probabilités pour des indicateurs des clusters.
- Find cluster indicator parameters $\widehat{\theta}$ while integrating out hidden variables, such that: / On marginalise sur $h_{1:N}$

$$\begin{aligned}\widehat{\theta} &= \arg\max_{\theta} p(x_{1:N}|\theta)\\ &= \arg\max_{\theta} \sum_{h_{1:N}} p(x_{1:N}, h_{1:N}|\theta)\end{aligned}$$

- Write down/Écrit log-likelihood:

$$\log p(x_{1:N}|\theta) = \log \sum_{h_{1:N}} \frac{p(x_{1:N}, h_{1:N}|\theta)}{q(h_{1:N})} q(h_{1:N}) = \log \mathbb{E}_q \left[\frac{p(x_{1:N}, h_{1:N}|\theta)}{q(h_{1:N})} \right]$$

Learning Variant 2 for GMM

- In addition, we want to estimate probabilities for $h_{1:N}$. / On estimer des probabilités pour des indicateurs des clusters.
- Find cluster indicator parameters $\widehat{\theta}$ while integrating out hidden variables, such that: / On marginalise sur $h_{1:N}$

$$\begin{aligned}\widehat{\theta} &= \arg\max_{\theta} p(x_{1:N}|\theta) \\ &= \arg\max_{\theta} \sum_{h_{1:N}} p(x_{1:N}, h_{1:N}|\theta)\end{aligned}$$

- Write down/Écrit log-likelihood:

$$\begin{aligned}\log p(x_{1:N}|\theta) &= \log \sum_{h_{1:N}} \frac{p(x_{1:N}, h_{1:N}|\theta)}{q(h_{1:N})} q(h_{1:N}) = \log \mathbb{E}_q \left[\frac{p(x_{1:N}, h_{1:N}|\theta)}{q(h_{1:N})} \right] \\ &\geq VLB := \mathbb{E}_q \left[\log \frac{p(x_{1:N}, h_{1:N}|\theta)}{q(h_{1:N})} \right] =^{+} \mathbb{E}_q \left[\log p(x_{1:N}, h_{1:N}|\theta) \right] \\ &=^{+} \sum_{n=1}^{N} \left(\sum_{k=1}^{K} \mathbb{E}_q[h_n = k] \left(\frac{-\|x_n - \mu_k\|_2^2}{2\sigma^2} + \log \pi_k \right) \right)\end{aligned}$$

Learning Variant 2 for GMM

- Algorithm: Fix θ, update q. Fix q, update θ, repeat until convergence. / On alterne entre l'optimization de q et θ.

Learning Variant 2 for GMM

- Algorithm: Fix θ, update q. Fix q, update θ, repeat until convergence. / On alterne entre l'optimization de q et θ.
- Update $\mu_{k'}$: compute the gradient while $q(h_{1:N})$ is fixed:

$$\frac{\partial VLB}{\partial \mu_{k'}} = \frac{\partial \sum_{n=1}^{N} \left(\sum_{k=1}^{K} \mathbb{E}[h_n = k] \left(\frac{-\|x_n - \mu_k\|_2^2}{2\sigma^2} + \log \pi_k \right) \right)}{\partial \mu_{k'}}$$

$$= \sum_{n=1}^{N} [h_n = k'] \frac{(x_n - \mu_{k'})}{\sigma^2} = \sum_{n=1}^{N} \mathbb{E}[h_n = k'] \frac{x_n}{\sigma^2} - \mathbb{E}[h_n = k'] \frac{\mu_{k'}}{\sigma^2}$$

set the gradient equal to 0, solve for $\mu_{k'} \to \widehat{\mu}_{k'} = \frac{\sum_{n=1}^{N} \mathbb{E}[h_n = k'] x_n}{\sum_{n=1}^{N} \mathbb{E}[h_n = k']}$.

Learning Variant 2 for GMM

- Algorithm: Fix θ, update q. Fix q, update θ, repeat until convergence. / On alterne entre l'optimization de q et θ.
- Update $\mu_{k'}$: compute the gradient while $q(h_{1:N})$ is fixed:

$$\frac{\partial VLB}{\partial \mu_{k'}} = \frac{\partial \sum_{n=1}^{N} \left(\sum_{k=1}^{K} \mathbb{E}[h_n = k] \left(\frac{-\|x_n - \mu_k\|_2^2}{2\sigma^2} + \log \pi_k \right) \right)}{\partial \mu_{k'}}$$

$$= \sum_{n=1}^{N} [h_n = k'] \frac{(x_n - \mu_{k'})}{\sigma^2} = \sum_{n=1}^{N} \mathbb{E}[h_n = k'] \frac{x_n}{\sigma^2} - \mathbb{E}[h_n = k'] \frac{\mu_{k'}}{\sigma^2}$$

  set the gradient equal to 0, solve for $\mu_{k'} \rightarrow \widehat{\mu}_{k'} = \frac{\sum_{n=1}^{N} \mathbb{E}[h_n = k'] x_n}{\sum_{n=1}^{N} \mathbb{E}[h_n = k']}$.
- Update $\widehat{\sigma}_{k'} = \frac{\sum_{n=1}^{N} \mathbb{E}[h_n = k'](x_n - \mu_k)^2}{\sum_{n=1}^{N} \mathbb{E}[h_n = k']}$.
- Update $\widehat{\pi}_{k'} = \frac{1}{N} \sum_{n=1}^{N} \mathbb{E}[h_n = k']$.

Learning Variant 2 for GMM - optimal $q(h)$

- Update $q(h_{1:N})$ while θ is fixed. Notice that:

$$VLB = \mathbb{E}_q\left[\log \frac{p(x_{1:N}, h_{1:N}|\theta)}{q(h_{1:N})}\right] = KL(q(h)\|p(x, h|\theta)).$$

What is the variational distribution that would minimize this divergence?

Learning Variant 2 for GMM - optimal $q(h)$

- Update $q(h_{1:N})$ while θ is fixed. Notice that:

$$VLB = \mathbb{E}_q \left[\log \frac{p(x_{1:N}, h_{1:N}|\theta)}{q(h_{1:N})} \right] = KL(q(h) \| p(x, h|\theta)).$$

  What is the variational distribution that would minimize this divergence?

- The derivation.

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial q} =& \frac{\partial}{\partial q} \left(\int q(h) \log p(x, h|\theta) dh - \int q(h) \log q(h) dh + \lambda \left(\int q(h) dh - 1 \right) \right) \\
&= \log p(x, h) - \log q(h) - 1 + \lambda = 0 \\
&\rightarrow q(h) = \frac{p(x, h|\theta)}{\exp(1 - \lambda)} \\
&\rightarrow \exp(1 - \lambda) = p(x|\theta) \\
&\rightarrow q(h) = \frac{p(x, h|\theta)}{p(x|\theta)} = p(h|x, \theta)
\end{aligned}$$

Learning Variant 2 for GMM - optimal $q(h)$

- Update $q(h_{1:N})$ while θ is fixed. Notice that:

$$VLB = \mathbb{E}_q\left[\log \frac{p(x_{1:N}, h_{1:N}|\theta)}{q(h_{1:N})}\right] = KL(q(h)\|p(x, h|\theta)).$$

  What is the variational distribution that would minimize this divergence?

- The derivation.

$$\begin{aligned}
\frac{\partial \mathcal{L}}{\partial q} =& \frac{\partial}{\partial q}\left(\int q(h)\log p(x, h|\theta)dh - \int q(h)\log q(h)dh + \lambda\left(\int q(h)dh - 1\right)\right)\\
&= \log p(x, h) - \log q(h) - 1 + \lambda = 0\\
&\rightarrow q(h) = \frac{p(x, h|\theta)}{\exp(1-\lambda)}\\
&\rightarrow \exp(1-\lambda) = p(x|\theta)\\
&\rightarrow q(h) = \frac{p(x, h|\theta)}{p(x|\theta)} = p(h|x, \theta)
\end{aligned}$$

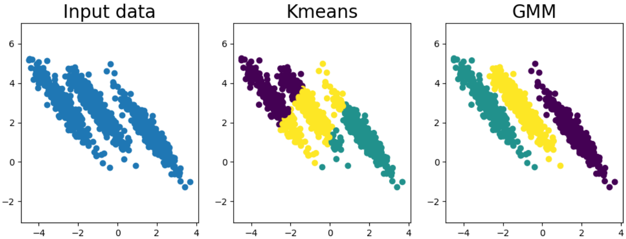
- Note that in our case $q(h) = q(h_{1:N}) = \prod_n q(h_n)$, where

$$q(h_n = k) = \frac{p(x_n, h_n = k|\theta)}{p(x_n|\theta)} = \frac{\pi_k \mathcal{N}(x_n; \mu_k, \sigma^2 I)}{\sum_{k'} \pi_{k'} \mathcal{N}(x_n; \mu_{k'}, \sigma^2 I)}$$

Learning Variant 2 for GMM - Summary for ICM and EM

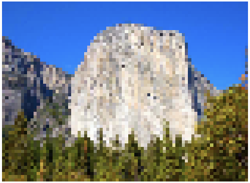
```
Randomly initialize $\mu_{1:K}$.
while Not converged do
  E-step:
    if ICM then
      $\widehat{h}_n = \arg\max_{h_n} \log p(x_n, h_n|\theta) = \arg\min_k \|x_n - \mu_k\|_2^2$
    else if EM then
      $q(h_n = k) = \frac{\pi_k \mathcal{N}(x_n; \mu_k, \sigma^2 I)}{\sum_{k'} \pi_{k'} \mathcal{N}(x_n; \mu_{k'}, \sigma^2 I)}$
    end if
  M-step:
    if ICM then
      $\widehat{\mu}_{k'} = \frac{\sum_{n=1}^{N} [h_n = k'] x_n}{\sum_{n=1}^{N} [h_n = k']}$
    else if EM then
      $\widehat{\mu}_{k'} = \frac{\sum_{n=1}^{N} \mathbb{E}_q [h_n = k'] x_n}{\sum_{n=1}^{N} \mathbb{E}_q [h_n = k']}$
    end if
end while
```

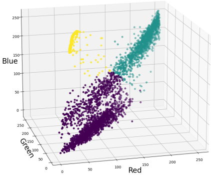
Kmeans vs GMM

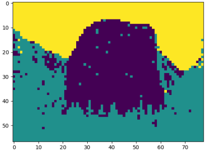


GMM on El Capitan

With Kmeans

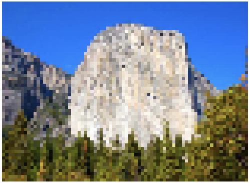


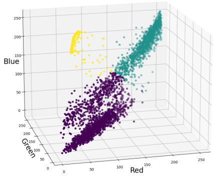


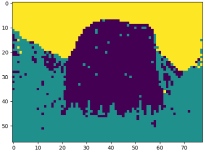


GMM on El Capitan

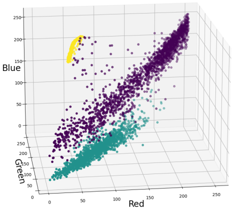
With Kmeans







With GMM



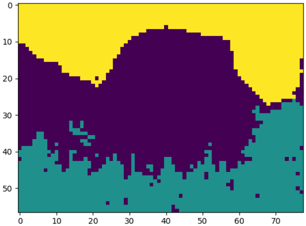


Table of Contents

Centroid based approaches

K-means clustering

Gaussian Mixture Model

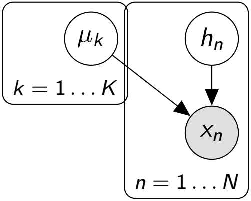
More Advanced GMM Learning Methods

Spectral Clustering

Hierarchical Clustering

Learning Variant 3 for GMM - Going Full Bayesian

- Model:



$$\begin{aligned} \mu_k &\sim \mathcal{N}(\mu_k; 0, \sigma_0^2 I), \text{ for } k \in \{1, \ldots, K\} \\ h_n &\sim \text{Categorical}(\pi) \\ x_n | h_n &\sim \mathcal{N}(x; \mu_h, \sigma^2 I), \text{ for } n \in \{1, \ldots, N\} \end{aligned}$$

- $h_n \in \{1, \ldots, K\}$, cluster indicators / indicateur des clusters.
- $x_n \in \mathbb{R}^L$, observed data items / données observées.
- $\theta = \{\mu_1, \mu_2, \ldots, \mu_K\}$ parameters/cluster centers. But we are not treating these guys as parameters anymore. / On ne traite plus ça comme des parametres mais des distributions.

Inference for Variant 3 GMM

- Approximate the posterior distribution $p(h, \theta|x)$, with a variational distribution $\widehat{q}$ such that, / On va approximer la posterior telle que,

$$\widehat{q}(h, \theta) = \arg\min_q KL(q(h, \theta) \| p(x, h, \theta))$$

- We will use the mean field approximation. English: $q(h, \theta) = q_h(h) q_\theta(\theta)$.

Inference for Variant 3 GMM

- Approximate the posterior distribution $p(h, \theta|x)$, with a variational distribution $\widehat{q}$ such that, / On va approximer la posterior telle que,

$$\widehat{q}(h, \theta) = \arg\min_{q} KL(q(h, \theta) \| p(x, h, \theta))$$

- We will use the mean field approximation. English: $q(h, \theta) = q_h(h) q_\theta(\theta)$.
- Algorithm: Fix q_h, update q_θ. We can show that: (via same process as the EM case)

$$\widehat{q}_\theta(\theta) = \arg\min_{q_\theta} KL(q_h(h) q_\theta(\theta) \| p(x, h, \theta)) = \frac{1}{Z} \exp\left(\mathbb{E}_{q_h}[\log p(x, h, \theta)]\right)$$

where Z is the normalization constant (constant de normalization). Similarly,

Inference for Variant 3 GMM

- Approximate the posterior distribution $p(h, \theta|x)$, with a variational distribution $\widehat{q}$ such that, / On va approximer la posterior telle que,

$$\widehat{q}(h, \theta) = \arg\min_{q} KL(q(h, \theta) \| p(x, h, \theta))$$

- We will use the mean field approximation. English: $q(h, \theta) = q_h(h) q_\theta(\theta)$.
- Algorithm: Fix q_h, update q_θ. We can show that: (via same process as the EM case)

$$\widehat{q}_\theta(\theta) = \arg\min_{q_\theta} KL(q_h(h) q_\theta(\theta) \| p(x, h, \theta)) = \frac{1}{Z} \exp\left(\mathbb{E}_{q_h}[\log p(x, h, \theta)]\right)$$

  where Z is the normalization constant (constant de normalization). Similarly,

- Fix q_θ, update q_h:

$$\widehat{q}_h(h) = \arg\min_{q_h} KL(q_h(h) q_\theta(\theta) \| p(x, h, \theta)) = \frac{1}{Z} \exp\left(\mathbb{E}_{q_\theta}[\log p(x, h, \theta)]\right)$$

Inference for Variant 3 GMM - Specifics:

$$
\begin{aligned}
\log \widehat{q}_\theta(\mu_k) &=^{+} \mathbb{E}_{q_h}[\log p(x, h, \mu_k)] \\
&=^{+} \sum_{n=1}^{N} \mathbb{E}[h_n = k] \frac{-(x_n^\top x_n - 2x_n^\top \mu_k + \mu_k^\top \mu_k)}{2\sigma^2} - \frac{\mu_k^\top \mu_k}{2\sigma_0^2} \\
&=^{+} \frac{\sum_{n=1}^{N} \mathbb{E}[h_n = k] 2x_n^\top \mu_k - (\sum_{n=1}^{N} \mathbb{E}[h_n = k] + \sigma^2)\mu_k^\top \mu_k)}{2\sigma^2\sigma_0^2} \\
&=^{+} \log \mathcal{N}\left(\mu_k; \frac{\sum_n \mathbb{E}[h_n = k] x_n}{\sum_n \mathbb{E}[h_n = k] + \sigma^2}, \frac{\sigma^2\sigma_0^2}{\sum_n \mathbb{E}[h_n = k] + \sigma^2}\right)
\end{aligned}
$$

Inference for Variant 3 GMM - Specifics:

$$
\begin{aligned}
\log \widehat{q}_\theta(\mu_k) &=^+ \mathbb{E}_{q_h}[\log p(x, h, \mu_k)] \\
&=^+ \sum_{n=1}^{N} \mathbb{E}[h_n = k] \frac{-(x_n^\top x_n - 2x_n^\top \mu_k + \mu_k^\top \mu_k)}{2\sigma^2} - \frac{\mu_k^\top \mu_k}{2\sigma_0^2} \\
&=^+ \frac{\sum_{n=1}^{N} \mathbb{E}[h_n = k] 2x_n^\top \mu_k - (\sum_{n=1}^{N} \mathbb{E}[h_n = k] + \sigma^2)\mu_k^\top \mu_k)}{2\sigma^2 \sigma_0^2} \\
&=^+ \log \mathcal{N}\left(\mu_k; \frac{\sum_n \mathbb{E}[h_n = k] x_n}{\sum_n \mathbb{E}[h_n = k] + \sigma^2}, \frac{\sigma^2 \sigma_0^2}{\sum_n \mathbb{E}[h_n = k] + \sigma^2}\right)
\end{aligned}
$$

Inference for Variant 3 GMM - Specifics:

$$\log \widehat{q}_h(h_n = k) = \left(\frac{\mathbb{E}[-\|x_n - \mu_k\|_2^2]}{2\sigma^2} + \log \pi_k \right)$$

$$\rightarrow \widehat{q}_h(h_n = k) = \frac{\exp\left(\frac{\mathbb{E}[-\|x_n - \mu_k\|_2^2]}{2\sigma^2} + \log \pi_k \right)}{\sum_k \exp\left(\frac{\mathbb{E}[-\|x_n - \mu_k\|_2^2]}{2\sigma^2} + \log \pi_k \right)}$$

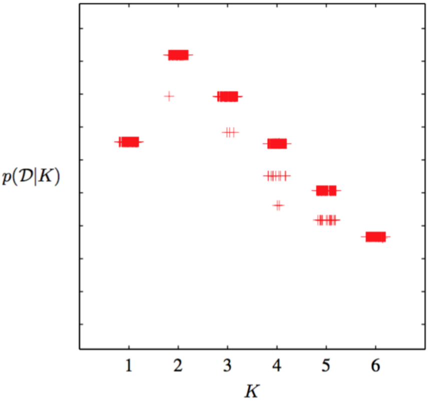
Inference for Variant 3 GMM - Why:

- Variational lower bound:

$$\int p(x,h,\theta)dhd\theta \geq \mathbb{E}_{q(h)q(\theta)}[\log p(x,h,\theta)] - \mathbb{E}_{q(h)q(\theta)}[\log q(h) + \log q(\theta)]$$

- You can use VLB to determine K: (plot taken from Bishop, 2006)

Plot of the variational lower bound $\mathcal{L}$ versus the number K of components in the Gaussian mixture model, for the Old Faithful data, showing a distinct peak at $K = 2$ components. For each value of K, the model is trained from 100 different random starts, and the results shown as '+' symbols plotted with small random horizontal perturbations so that they can be distinguished. Note that some solutions find suboptimal local maxima, but that this happens infrequently.



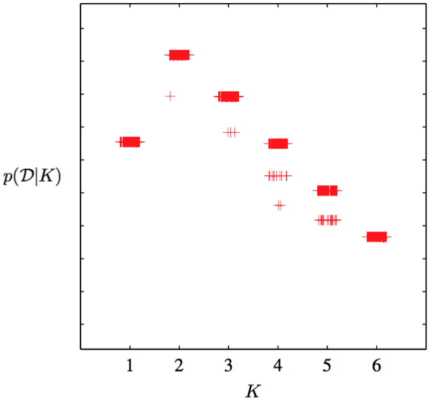
Inference for Variant 3 GMM - Why:

- Variational lower bound:

$$\int p(x,h,\theta)dhd\theta \geq \mathbb{E}_{q(h)q(\theta)}[\log p(x,h,\theta)] - \mathbb{E}_{q(h)q(\theta)}[\log q(h) + \log q(\theta)]$$

- You can use VLB to determine K: (plot taken from Bishop, 2006)

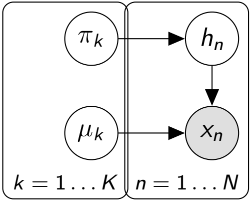
Plot of the variational lower bound $\mathcal{L}$ versus the number K of components in the Gaussian mixture model, for the Old Faithful data, showing a distinct peak at $K = 2$ components. For each value of K, the model is trained from 100 different random starts, and the results shown as '+' symbols plotted with small random horizontal perturbations so that they can be distinguished. Note that some solutions find suboptimal local maxima, but that this happens infrequently.



- But admittedly the algebra gets tiring./C'est évident que les

Variant 4 for GMM - Going Ultra Bayesian

- Model:



$$\begin{aligned} \pi &\sim \text{Dirichlet}(1/K, \dots, 1/K) \\ \mu_k &\sim \mathcal{N}(\mu_k; 0, \sigma_0^2 I), \text{ for } k \in \{1, \dots, K\} \\ h_n &\sim \text{Categorical}(\pi) \\ x_n | h_n &\sim \mathcal{N}(x; \mu_h, \sigma^2 I), \text{ for } n \in \{1, \dots, N\} \end{aligned}$$

- $h_n \in \{1, \dots, K\}$, cluster indicators / indicateurs de clusters.
- $x_n \in \mathbb{R}^L$, observed data items / données.
- $\theta = \{\mu_1, \mu_2, \dots, \mu_K\} \cup \{\pi\}$

Variant 4 for GMM - Infinite Mixture Model

- Integrate out the parameters, sample from the full conditionals / On va éliminer les parameters, et échantilloner en utilisant les full conditionals:

$$
\begin{aligned}
p(h_n = k | h_{-n}, x_{1:N}) \; & \propto \; \int p(x_{1:N}, h_{1:N}, \pi, \mu_{1:K}) d\mu_{1:K} d\pi \\
& \propto \frac{\alpha/K + N_k^{-n}}{\alpha + N - 1} p(x_n | \{x_m : m \neq n, h_m = k\})
\end{aligned}
$$

- And, sample from these full conditionals!

Variant 4 for GMM - Infinite Mixture Model

- Integrate out the parameters, sample from the full conditionals / On va éliminer les parameters, et échantilloner en utilisant les full conditionals:

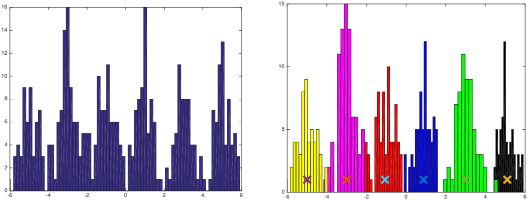
$$
\begin{aligned}
p(h_n = k | h_{-n}, x_{1:N}) \; &\propto \int p(x_{1:N}, h_{1:N}, \pi, \mu_{1:K}) d\mu_{1:K} d\pi \\
&\propto \frac{\alpha/K + N_k^{-n}}{\alpha + N - 1} p(x_n | \{x_m : m \neq n, h_m = k\})
\end{aligned}
$$

- Take K to infinity:

$$
\begin{aligned}
p(h_n = k, k \text{ occupied} | h_{-n}, x_{1:N}) &\propto \frac{N_k^{-n}}{\alpha + N - 1} p(x_n | \{x_m : m \neq n, h_m = k\}) \\
p(h_n = k, k \text{ empty} | h_{-n}, x_{1:N}) &\propto \frac{\alpha}{\alpha + N - 1} p(x_n)
\end{aligned}
$$

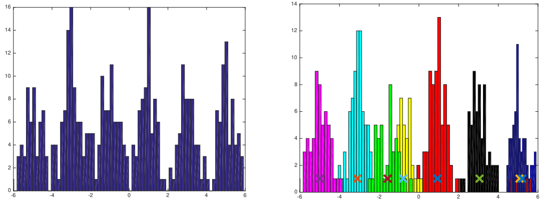
- And, sample from these full conditionals!

Collapsed Gibbs sampling in Infinite GMM



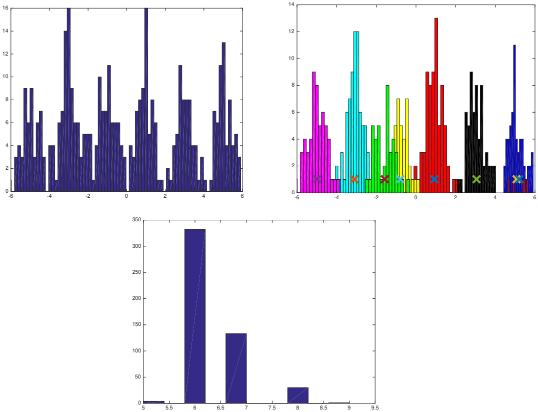
Top left: Histogram of observed data (données observés), Top right: Samples from full conditional of $h_{1:N}$, Bottom: Histogram of K (nombre de clusters)

Collapsed Gibbs sampling in Infinite GMM



Top left: Histogram of observed data (données observés), Top right: Samples from full conditional of $h_{1:N}$, Bottom: Histogram of K (nombre de clusters)

Collapsed Gibbs sampling in Infinite GMM



Top left: Histogram of observed data (données observés), Top right: Samples from full conditional of $h_{1:N}$, Bottom: Histogram of K (nombre de clusters)

What's the point of going all Bayesian then

- (Automatic) Model Selection for Unsupervised Learning / Sélection automatique du complexité du modèle

What's the point of going all Bayesian then

- (Automatic) Model Selection for Unsupervised Learning / Sélection automatique du complexité du modèle
- Model Averaging (Model plays all its cards) / On calcule un moyenne sur les modèles

What's the point of going all Bayesian then

- (Automatic) Model Selection for Unsupervised Learning / Sélection automatique du complexité du modèle
- Model Averaging (Model plays all its cards) / On calcule un moyenne sur les modèles
- Principled way of regularization / Un moyenne de regularization

What's the point of going all Bayesian then

- (Automatic) Model Selection for Unsupervised Learning / Sélection automatique du complexité du modèle
- Model Averaging (Model plays all its cards) / On calcule un moyenne sur les modèles
- Principled way of regularization / Un moyenne de regularization
- All of these 4 variants are extendable for other models. We can play with: / Ces 4 idées sont extremement puissants, on peut capturer pleins de modèles.
  - Distribution of h.
  - Impose structure on h. / Imposition d'une structure sur h (semaine prochaine)
  - We can change the conditional distribution $p(x|h, \theta)$. (Application decides) / Dépend sur l'output.
  - We can play with how we do inference and learning. / On peut changer comment on fait apprentissage.

Table of Contents

Centroid based approaches

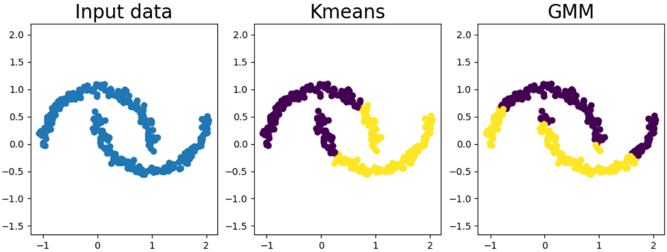
- K-means clustering
- Gaussian Mixture Model
- More Advanced GMM Learning Methods

Spectral Clustering

Hierarchical Clustering

Failure case for Centroid Based Methods

- What if we have something like this? / Et si on avait qqch comme ċa?



- Any ideas / Idées?

Remember KPCA?

- Do you remember KPCA? / Vous souvenez-vous de KPCA?
- Let's calculate a pairwise distance matrix

Spectral Clustering

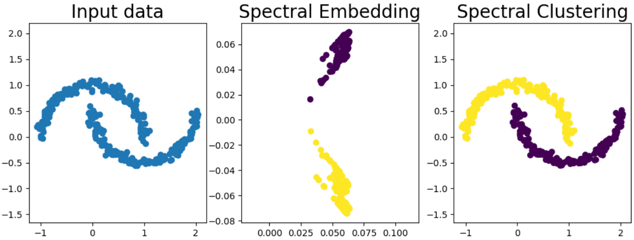
- $A_{ij} = \exp\left(-\gamma \|x_i - x_j\|_2^2\right),\ i \neq j.\ A_{ij} = 0\ i = j.$
- Compute Graph Laplacian

$$L := D^{-1/2} A D^{-1/2},\ D_{ii} = \sum_j A_{ij}$$

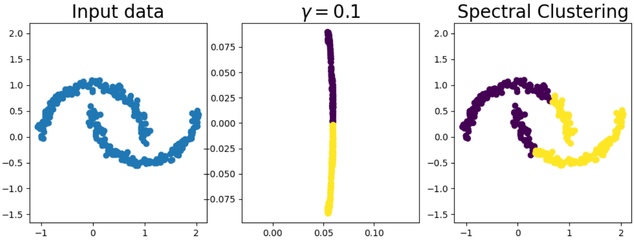
.

- K-means cluster the first k-eigenvectors of L.

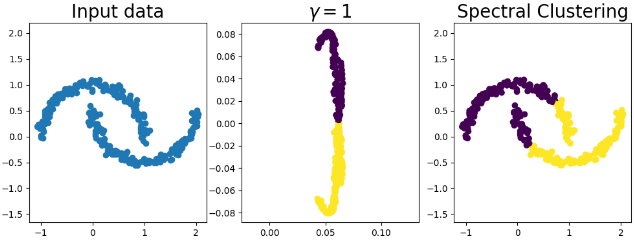
Spectral Clustering in Action



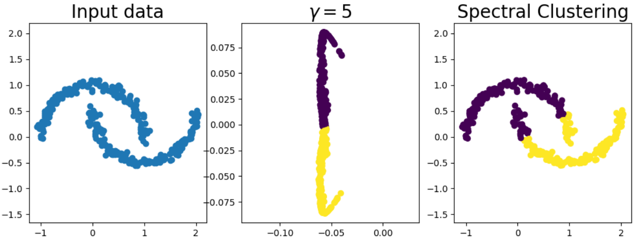
Spectral Clustering, effect of Gamma



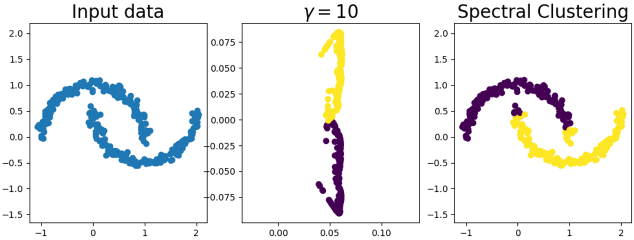
Spectral Clustering, effect of Gamma



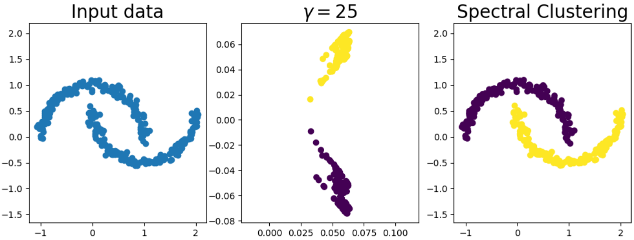
Spectral Clustering, effect of Gamma



Spectral Clustering, effect of Gamma



Spectral Clustering, effect of Gamma



Spectral Clustering, effect of Gamma

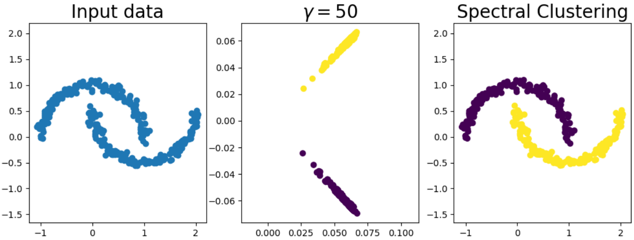


Table of Contents

Centroid based approaches

- K-means clustering
- Gaussian Mixture Model
- More Advanced GMM Learning Methods

Spectral Clustering

Hierarchical Clustering

Agglomerative Clustering

- Choose $R_0 = \{C_i = \{x_i\}, i = 1, \dots N\}$. We start from each data item being a cluster. / On commence avec chaque data étant un cluster.

Agglomerative Clustering

- Choose $R_0 = \{C_i = \{x_i\}, i = 1, \dots N\}$. We start from each data item being a cluster. / On commence avec chaque data étant un cluster.
- For $t = 1, \dots$

Agglomerative Clustering

- Choose $R_0 = \{C_i = \{x_i\}, i = 1, \dots N\}$. We start from each data item being a cluster. / On commence avec chaque data étant un cluster.
- For $t = 1, \dots$
  - Among all clusters in / Parmi tous les clusters dans R_{t-1}, find cluster pair / on trouve un paire $\{C_i, C_j\}$ such that / telle que,

$$i, j = \arg\min_{i', j'} d(C_{i'}, C_{j'})$$

.

Agglomerative Clustering

- Choose $R_0 = \{C_i = \{x_i\}, i = 1, \dots N\}$. We start from each data item being a cluster. / On commence avec chaque data étant un cluster.
- For $t = 1, \dots$
  - Among all clusters in / Parmi tous les clusters dans R_{t-1}, find cluster pair / on trouve un paire $\{C_i, C_j\}$ such that / telle que,

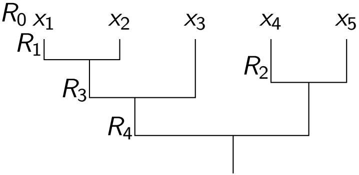
$$i, j = \arg\min_{i', j'} d(C_{i'}, C_{j'})$$

.

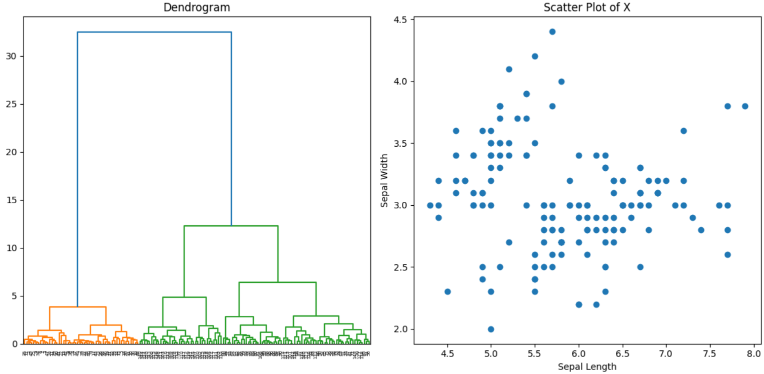
  - Form new cluster pair, remove the pair / Forme un nouvelle paire de clusters, enlève l'ancien,

$$C_q = C_i \cup C_j,\ R_t = (R_{t-1} - C_i \cup C_j) \cup C_q$$

Dendrogram



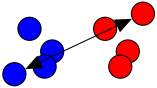
Example Dendrogram on IRIS



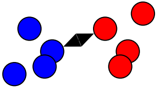
With Ward Linkage

How do we measure distances between clusters

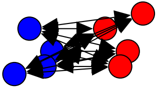
- Linkage functions
  - Complete linkage



  - Single linkage

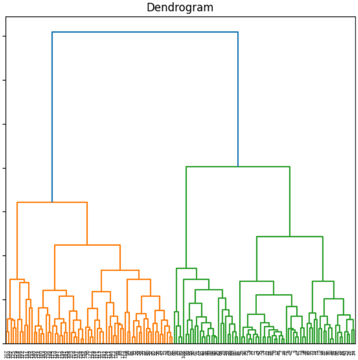


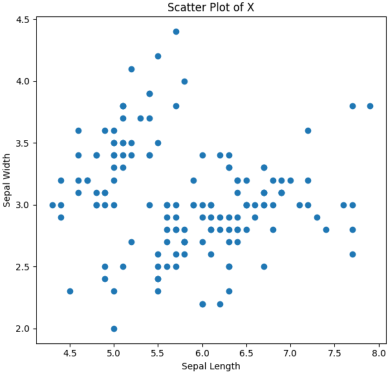
  - Average linkage



- There's more / Il y en a d'autres.

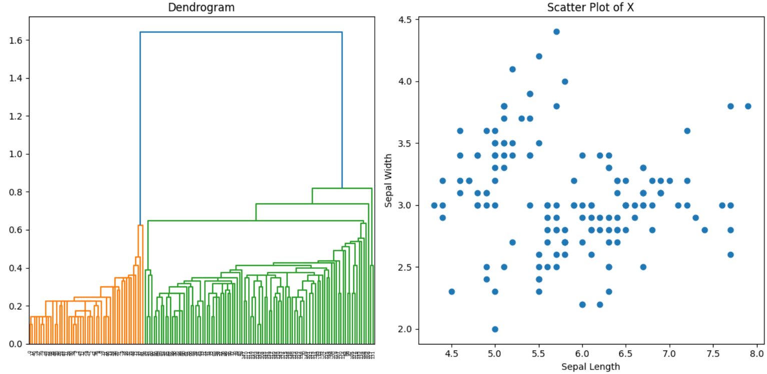
Example Dendrogram on IRIS





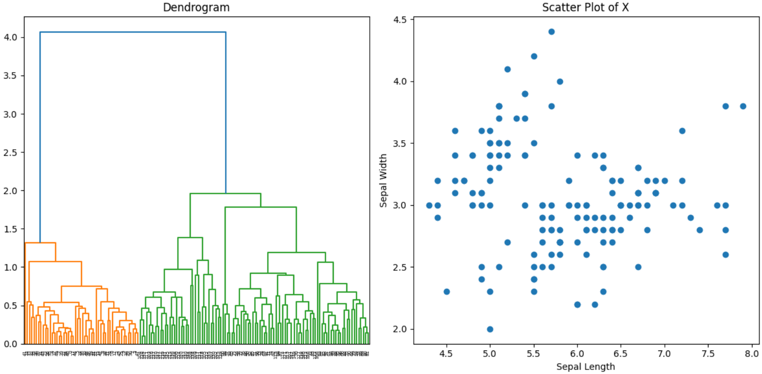
Complete Linkage

Example Dendrogram on IRIS



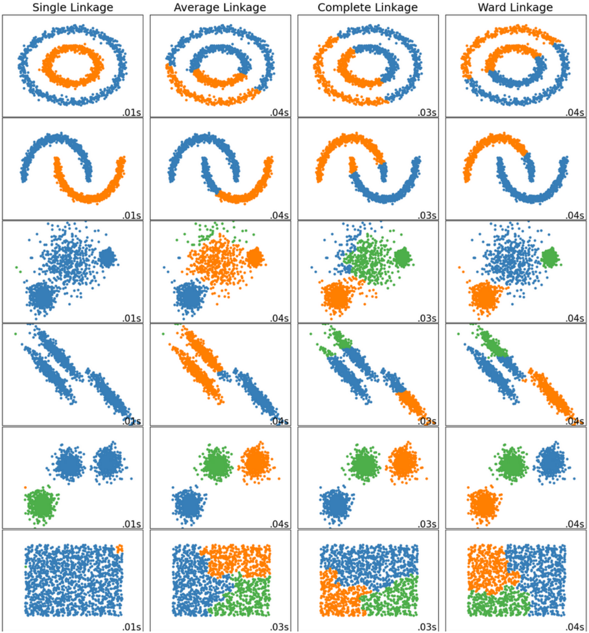
Single Linkage

Example Dendrogram on IRIS



Average Linkage

How does linkage change things



Computational Complexity

- At level t we have $N - t$ clusters / Au niveau t, on a $N - t$ clusters.
- How many pairs of clusters do we need to deal with? Combien de pairs?

Computational Complexity

- At level t we have $N-t$ clusters / Au niveau t, on a $N-t$ clusters.
- How many pairs of clusters do we need to deal with? Combien de pairs?
  - $\binom{N-t}{2} = \frac{(N-t)(N-t-1)}{2}$.
- In total / Au totale:
  - $\sum_{t=0}^{N-1} \binom{N-t}{2} = \frac{(N-1)N(N+1)}{6}$

Computational Complexity

- At level t we have $N - t$ clusters / Au niveau t, on a $N - t$ clusters.
- How many pairs of clusters do we need to deal with? Combien de pairs?
  - $\binom{N-t}{2} = \frac{(N-t)(N-t-1)}{2}$.
- In total / Au totale:
  - $\sum_{t=0}^{N-1} \binom{N-t}{2} = \frac{(N-1)N(N+1)}{6}$
- So N^3. In the original El-Capitan Image we had $N \approx 500000$. That would give something like 2.083×10^{16}. / Dans l'image originale El-Capitan on avait $N \approx 500000$. Donc.. merci mais non merci..

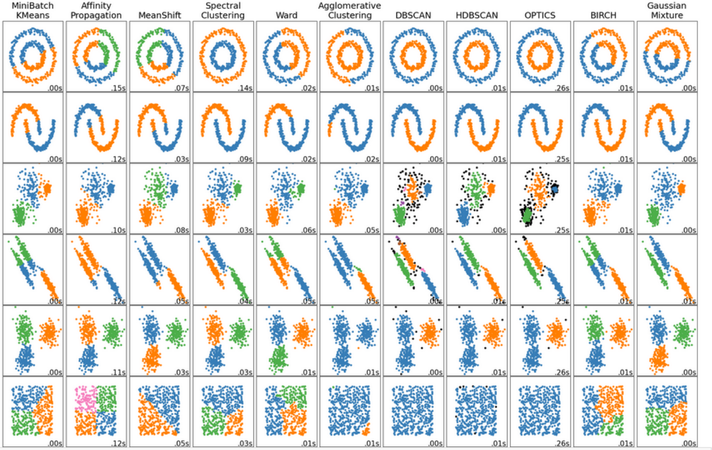
Divisive Clustering

- We start with the whole dataset forming a giant cluster. / On commence avec une seule cluster.
- Then we divide by picking out the least similar clusters / Puis on divise en choissisant les cluster les moins similaires.
- They say that divisive usually works better than agglomerative since it sees the global picture better.
  - C'est accepté que la divisive travaille mieux car il voit le paysage globale mieux.
- Agglomerative is typically faster / Agglomerative est typiquement plus rapide.

Clustering recap

- Kmeans
  - Reliable (Fiable), quick and dirty
- GMMs
  - More powerful than Kmeans but still a centroid method in heart / Plus puissant que Kmeans mais une méthode de centroids si on y pense.
- Spectral Clustering
  - The non-linear get around to find manifold-like clusters / Une cheminement alternative pour trouver des clusters qui sont comme des manifolds. Not suitable for large datasets / N'est pas approprié pour des grands datasets.
- Hiearchical Clustering
  - Gives a dendrogram, but expensive! Donne un dendrogram, est un bon utile, mais cher!

There’s more!

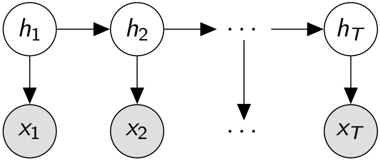

MiniBatch KMeans
Affinity Propagation
MeanShift
Spectral Clustering
Ward
Agglomerative Clustering
DBSCAN
HDBSCAN
OPTICS
BIRCH
Gaussian Mixture
.00s
.15s
.07s
.14s
.02s
.01s
.00s
.01s
.26s
.01s
.00s
.00s
.12s
.03s
.09s
.02s
.02s
.00s
.01s
.25s
.01s
.00s
.00s
.10s
.08s
.03s
.06s
.05s
.00s
.00s
.25s
.01s
.00s
.00s
.12s
.05s
.04s
.05s
.05s
.00s
.01s
.25s
.01s
.01s
.00s
.11s
.03s
.03s
.01s
.01s
.00s
.01s
.26s
.01s
.00s
.00s
.12s
.05s
.03s
.01s
.01s
.00s
.01s
.26s
.01s
.00s

Suggested reading

- Spectral clustering: `http://ai.stanford.edu/~ang/papers/nips01-spectral.pdf`
- Bishop chapter 9.

Next week/class

- Well, next week we are off as it is the reading week.
- But after that, in the next class we will add connections between h_n's!


h_1
h_2
$\cdots$
h_T
x_1
x_2
$\cdots$
x_T