

IFT 4030/7030,
Machine Learning for Signal Processing
Week9: Machine Learning 4
Clustering

Cem Subakan



UNIVERSITÉ
Laval



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

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- What if we do not have the labels?
 - ▶ Et si on n'avait pas d'étiquettes?

Clustering

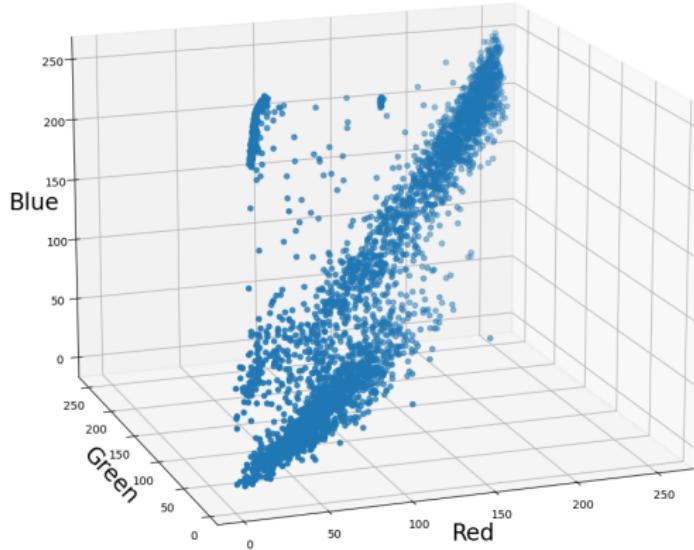
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- What if we do not have the labels?
 - ▶ Et si on n'avait pas d'étiquettes?
- Today's lecture's goal / Le but d'aujourd'hui.
 - ▶ I will try to acclimate you with clustering./Je vais essayer de vous introduire des concepts de base de clustering.
 - ▶ But in a sneaky way I will introduce powerful tools from probabilistic machine learning. / Je vais vous bombarder silencieusement avec des outils de l'apprentissage automatique probabilistique.

Some motivation

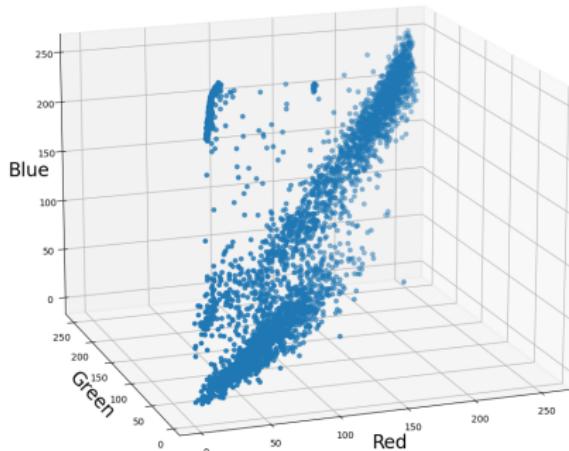


El Capitan, Yosemite National Park, California

How many clusters?

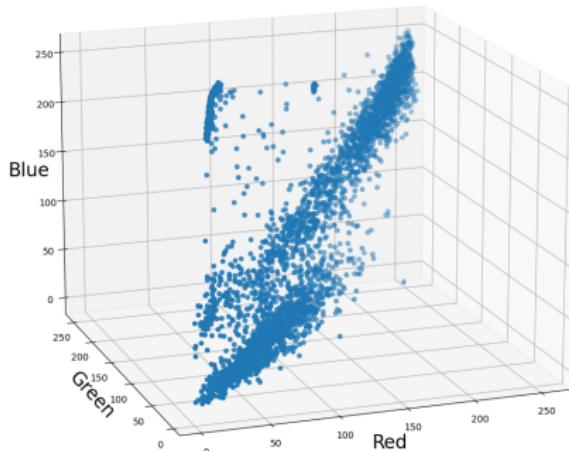


Clustering



- 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 représenter les données?

■ Cluster Shapes

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

Clustering process

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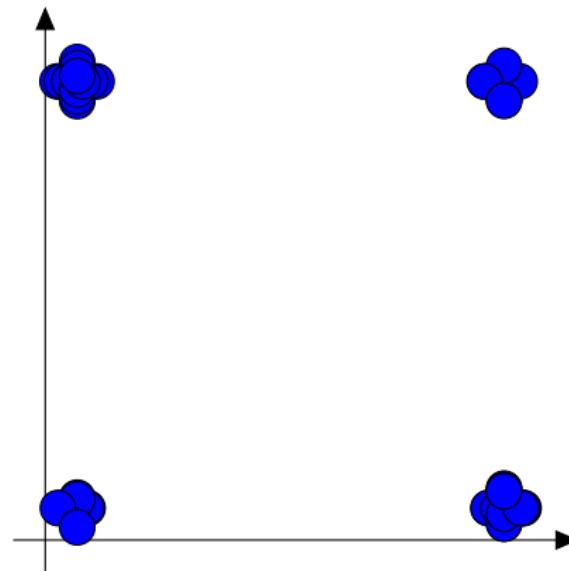
Decide what your clusters should look like / Il faut décider comment on veut que les clusters se forment.

■ Distance

Define a distance function / proximity measure.

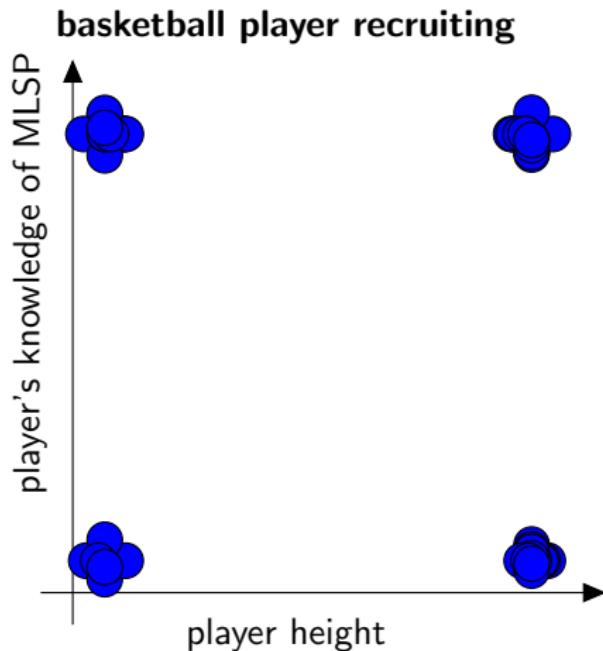
- ▶ Définissons une notion de distance / proximité.

Features



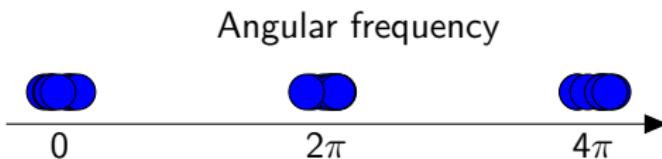
- How many clusters? / Combien de groupes?

Features

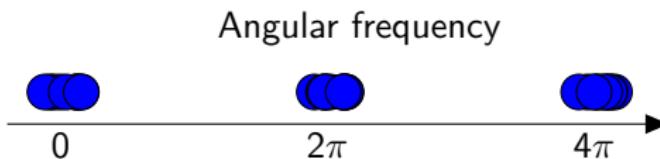


- How many clusters? / Combien de groupes?
- How many clusters? / Combien de groupes?

Use a sensible distance function

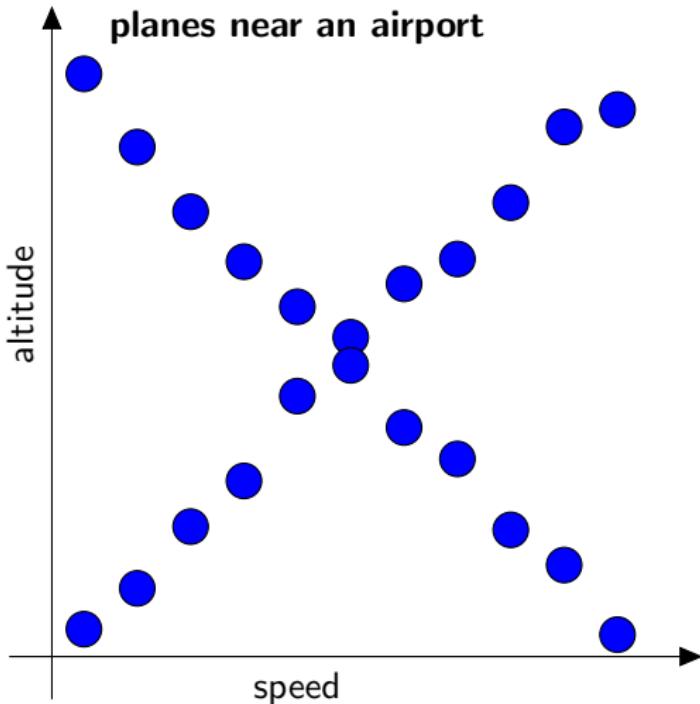


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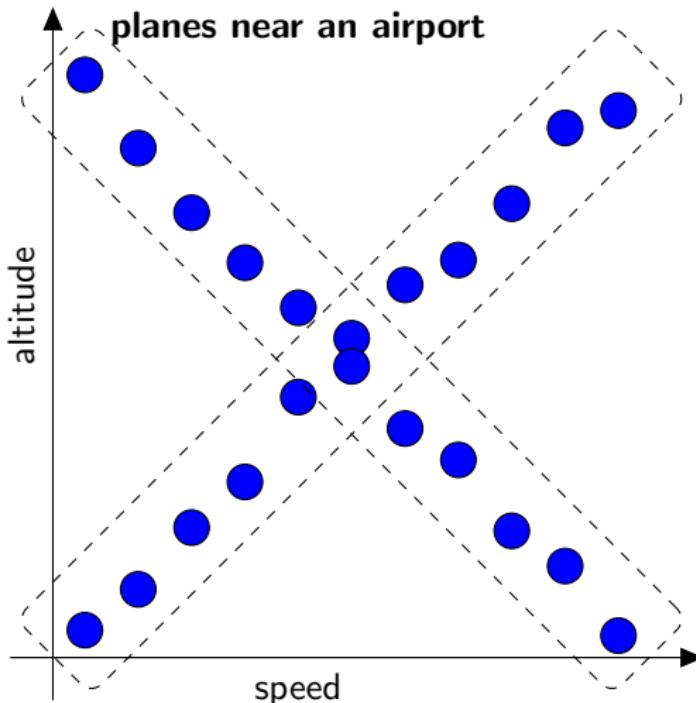


- Probably using euclidean distance is not a good idea here!
 - ▶ Très probable qu'il faut pas utiliser la distance euclidienne ici!!

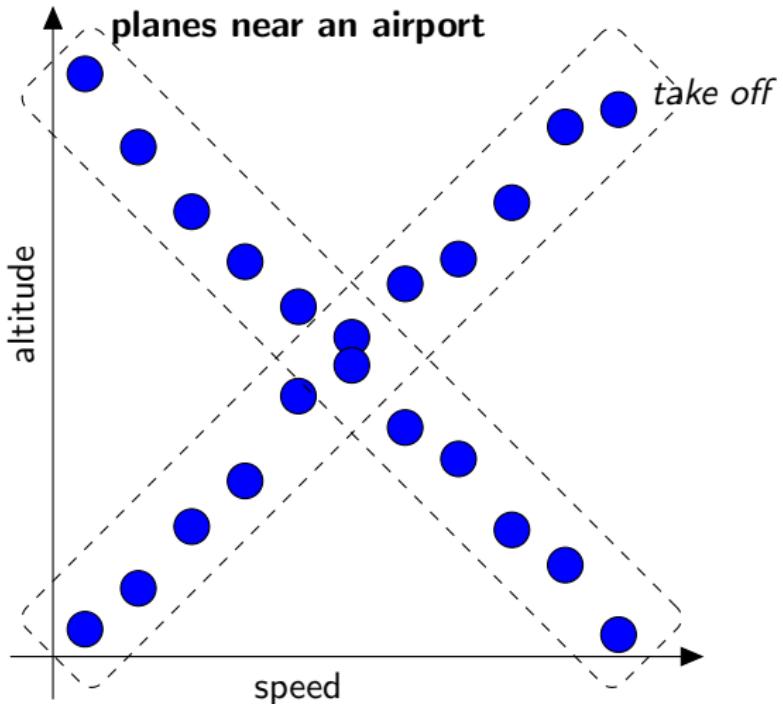
What forms clusters in your space?



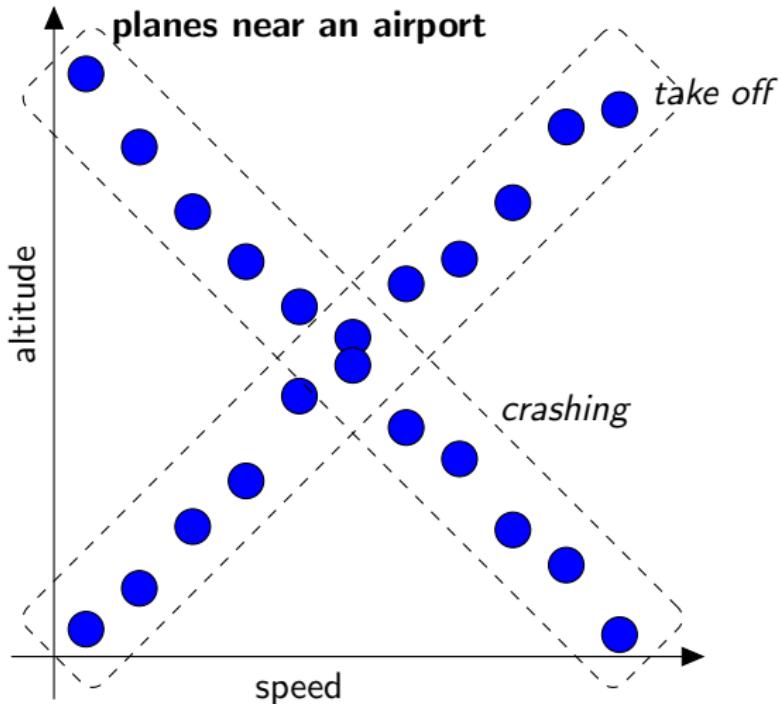
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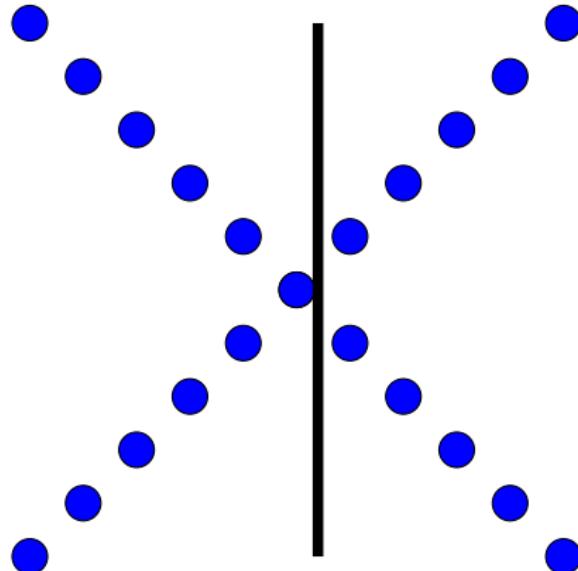


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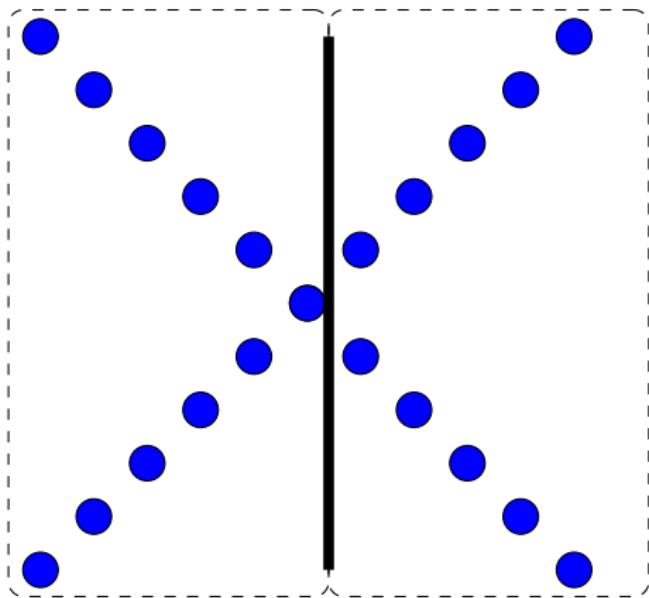
What forms clusters in your space?

ball trajectories bouncing off a wall

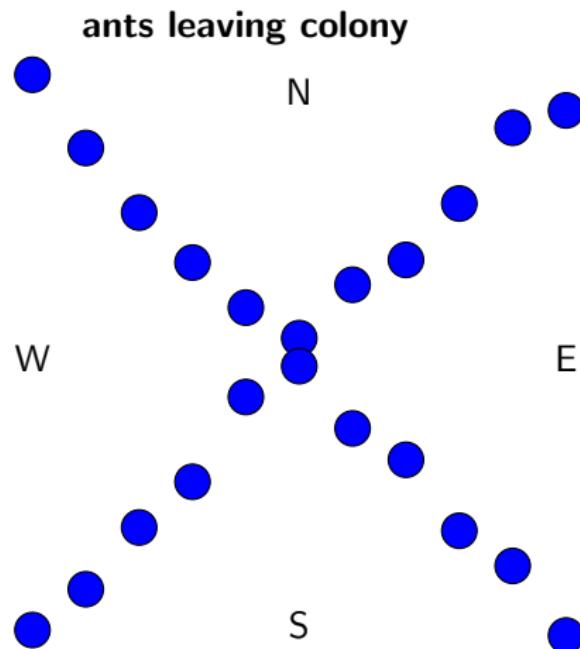


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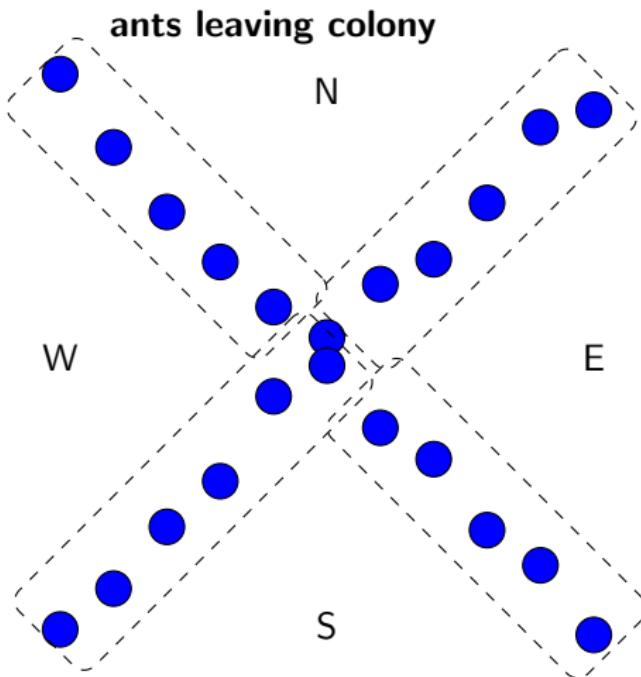
ball trajectories bouncing off a wall



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'expérimenter 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

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Centroid based approaches

K-means clustering

Gaussian Mixture Model

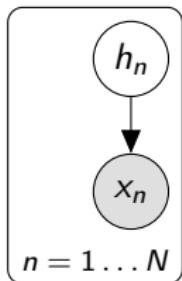
More Advanced GMM Learning Methods

Spectral Clustering

Hierarchical Clustering

Gaussian Mixture Model

■ Model:



$$h_n \sim \text{Discrete}(\pi)$$

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

- $h_n \in \{1, \dots, K\}$, 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).

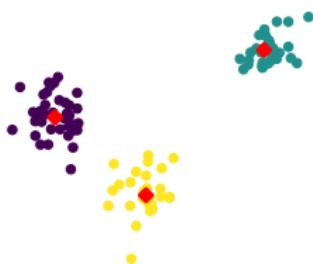


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Learning Variant 1 for GMM

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

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

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- 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.

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- 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 paramètres θ et les indicateurs h .

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- 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.

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

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

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

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

Kmeans Clustering

Randomly initialize $\mu_{1:K}$.

while Not converged **do**

E-step:

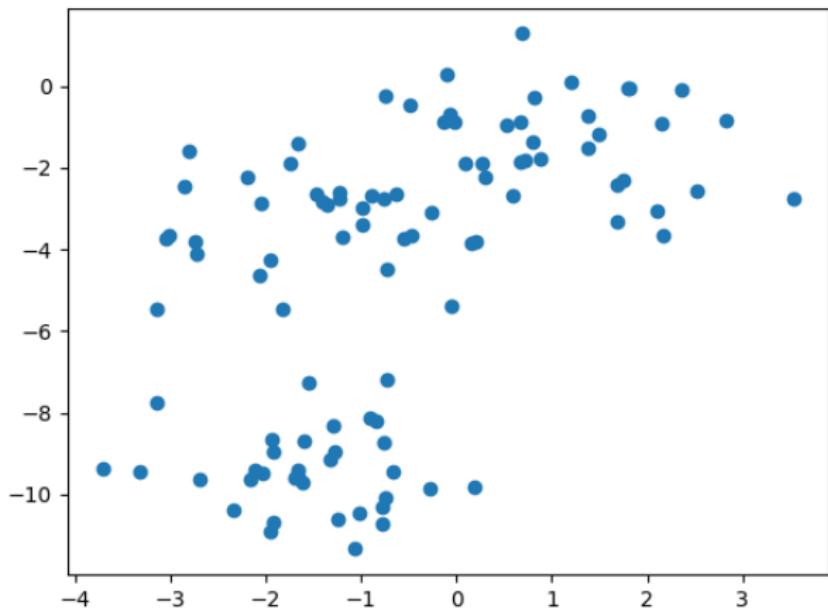
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M-step:

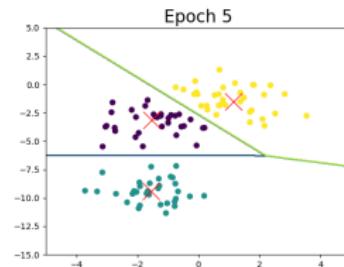
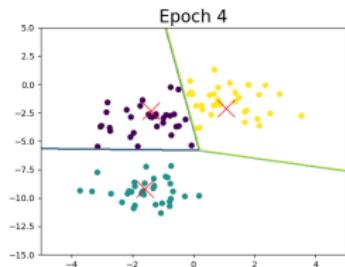
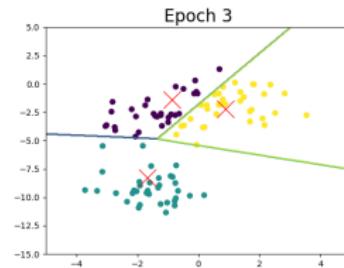
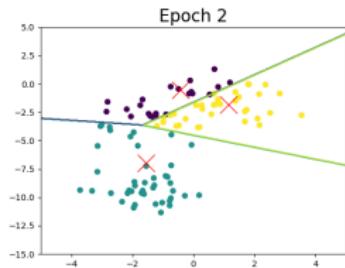
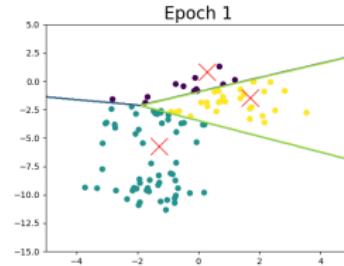
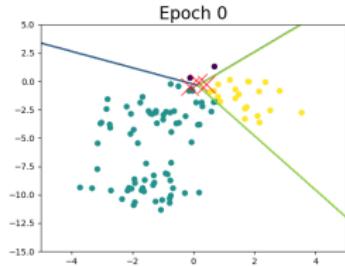
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end while

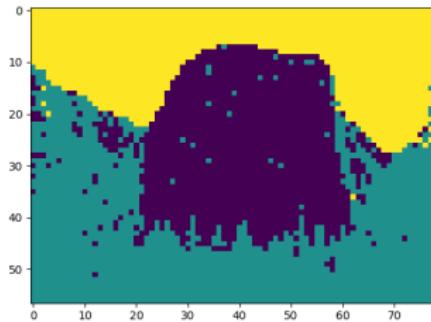
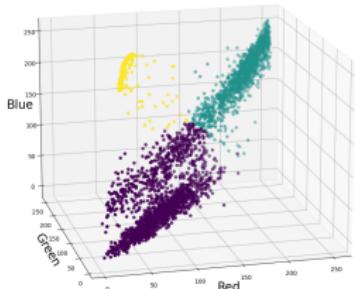
Kmeans Example



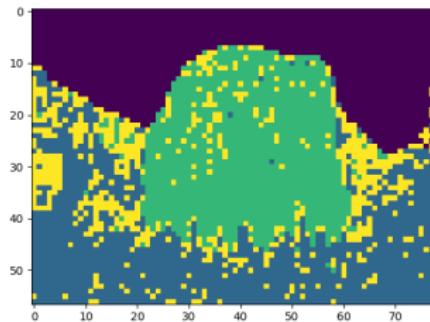
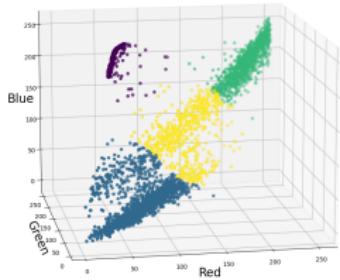
Kmeans Updates



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

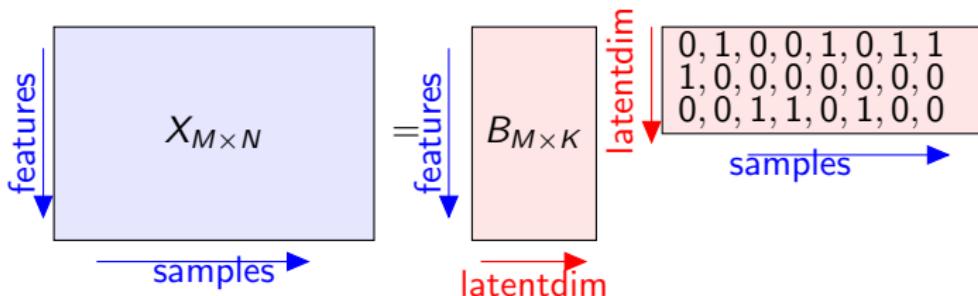


Applying K-means on El-Capitan ($K = 4$)



A sidenote

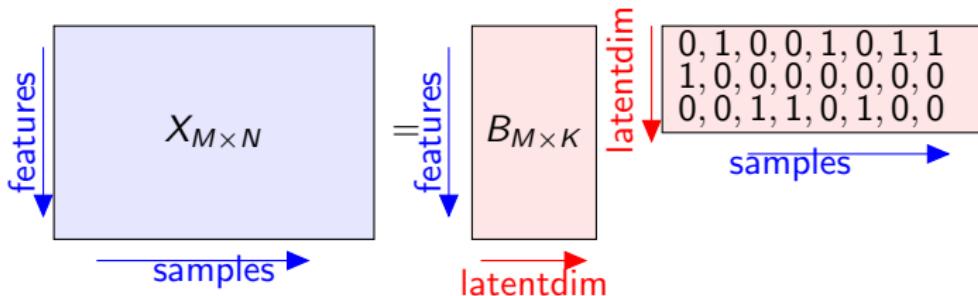
- K-means is a matrix-factorization algorithm



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

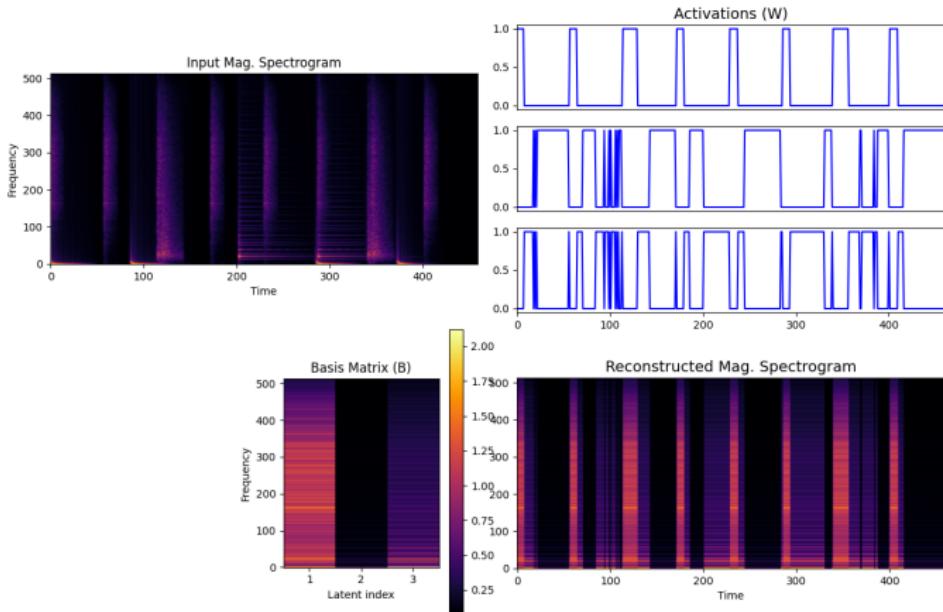
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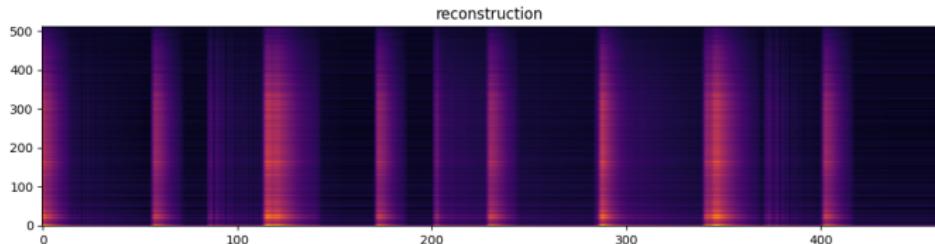
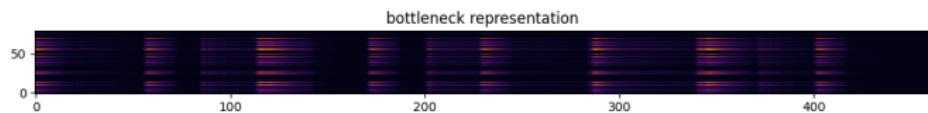
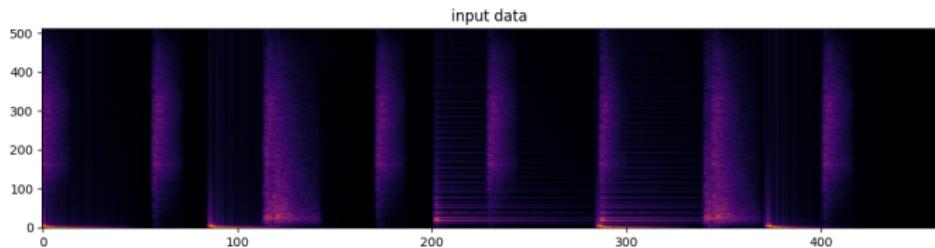


- B in this case has the cluster means in columns / B dans ce cas-ci a les cluster means dans ses colonnes.
- Kmeans is a tokenizer! (It's a buzzword these days)

Kmeans on a familiar picture



Kmeans in the latent space



Cluster the latents!

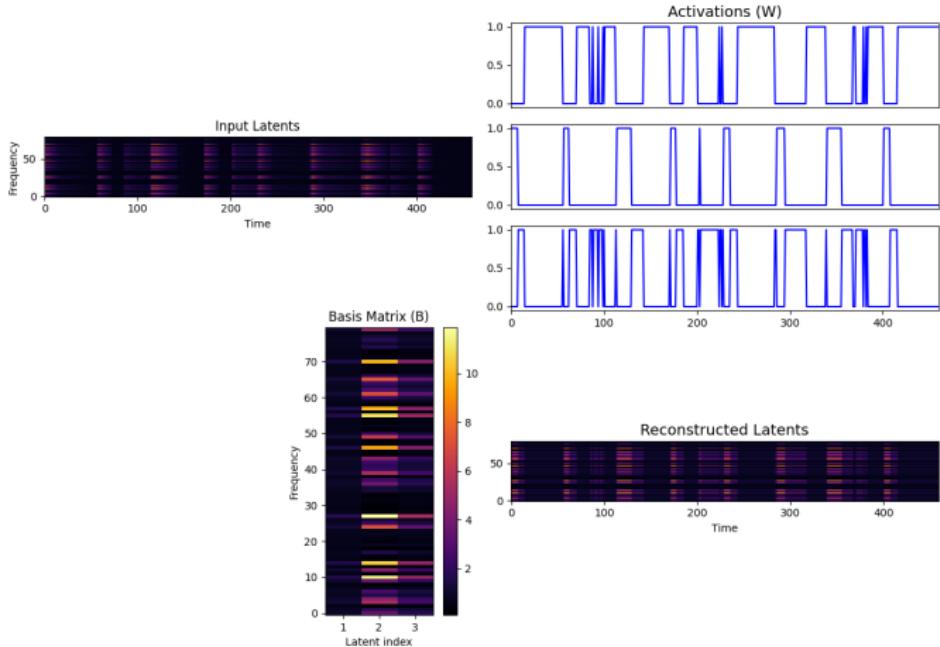


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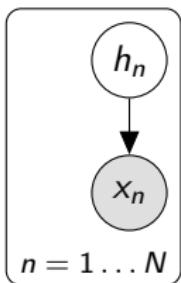
More Advanced GMM Learning Methods

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Extending K-means

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Kmeans ne peut apprendre que des Gaussiennes Isotropiques.

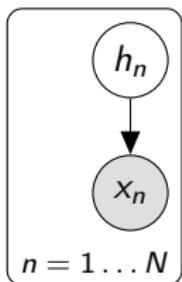


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- $h_n \in \{1, \dots, K\}$, cluster indicators / indicateur de groupes.
- $x_n \in \mathbb{R}^L$, observed data items / des données observées.
- $\theta = \{\mu_1, \mu_2, \dots, \mu_K, \Sigma_1, \Sigma_2, \dots, \Sigma_K, \pi_1, \pi_2, \dots, \pi_K\}$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

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- 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 $\hat{\theta}$ while integrating out hidden variables, such that: / On marginalise sur $h_{1:N}$

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

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- 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 estime des probabilités pour des indicateurs des clusters.
- Find cluster indicator parameters $\hat{\theta}$ while integrating out hidden variables, such that: / On marginalise sur $h_{1:N}$

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

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

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

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- Update $\mu_{k'}$: compute the gradient while $q(h_{1:N})$ is fixed:

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

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

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- Update $\hat{\sigma}_{k'} = \frac{\sum_{n=1}^N \mathbb{E}[h_n=k'] (x_n - \mu_k)^2}{\sum_{n=1}^N \mathbb{E}[h_n=k']}$.
- Update $\hat{\pi}_{k'} = \frac{1}{N} \sum_{n=1}^N \mathbb{E}[h_n = k']$.

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?

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- The derivation.

$$\frac{\partial \mathcal{L}}{\partial q} = \frac{\partial}{\partial q} \left(\int q(h) \log p(x, h | \theta) dh - \int q(h) \log q(h) dh + \lambda \left(\int q(h) dh - 1 \right) \right)$$

$$= \log p(x, h) - \log q(h) - 1 + \lambda = 0$$

$$\rightarrow q(h) = \frac{p(x, h | \theta)}{\exp(1 - \lambda)}$$

$$\rightarrow \exp(1 - \lambda) = p(x | \theta)$$

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- 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**

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

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**

$$\hat{\mu}_{k'} = \frac{\sum_{n=1}^N [h_n=k'] x_n}{\sum_{n=1}^N [h_n=k']}$$

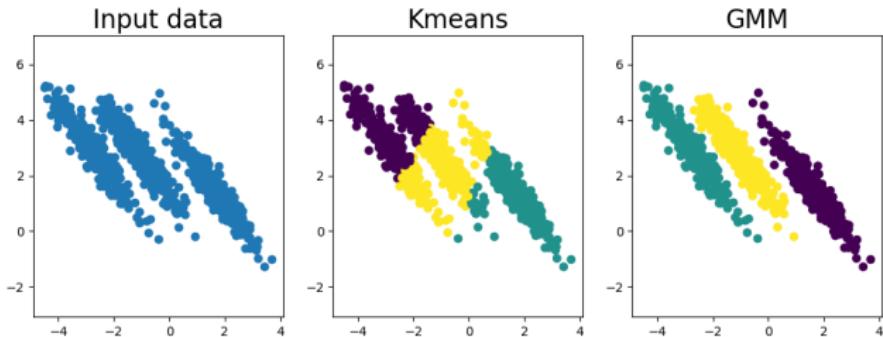
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$$\hat{\mu}_{k'} = \frac{\sum_{n=1}^N \mathbb{E}_q[h_n=k'] x_n}{\sum_{n=1}^N \mathbb{E}_q[h_n=k']}$$

end if

end while

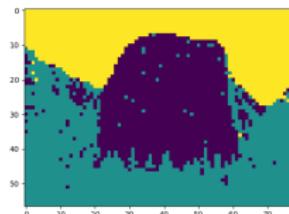
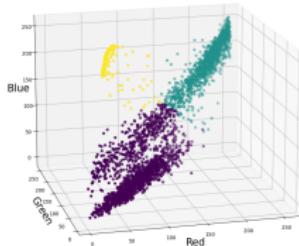
Kmeans vs GMM



GMM on El Capitan

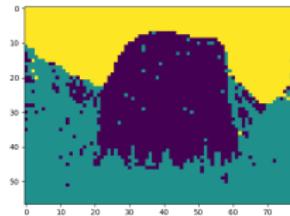
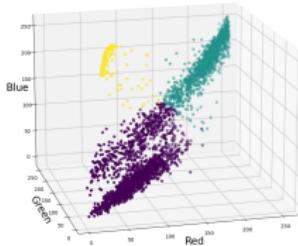


With Kmeans



GMM on El Capitan

With Kmeans



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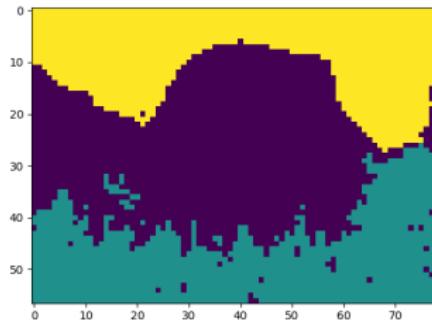
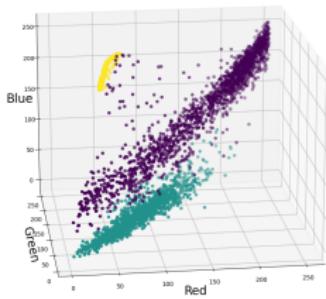


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Gaussian Mixture Model

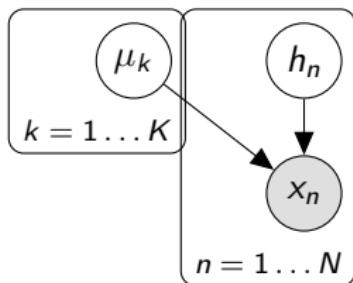
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Learning Variant 3 for GMM - Going Full Bayesian

■ Model:



$$\mu_k \sim \mathcal{N}(\mu_k; 0, \sigma_0^2 I), \text{ for } k \in \{1, \dots, K\}$$

$$h_n \sim \text{Categorical}(\pi)$$

$$x_n | h_n \sim \mathcal{N}(x; \mu_h, \sigma^2 I), \text{ for } n \in \{1, \dots, N\}$$

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

Inference for Variant 3 GMM

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

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

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

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- Algorithm: Fix q_h , update q_θ . We can show that: (via same process as the EM case)

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

where Z is the normalization constant (constant de normalization).
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Inference for Variant 3 GMM - Specifics:

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

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

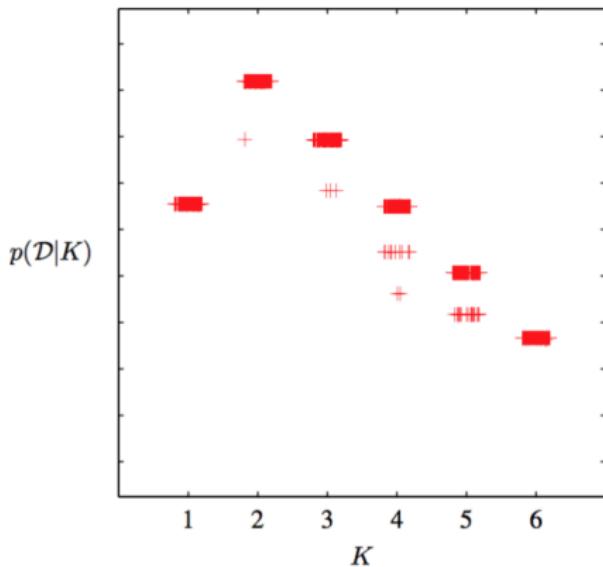
Inference for Variant 3 GMM - Why:

- Variational lower bound:

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

- 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.



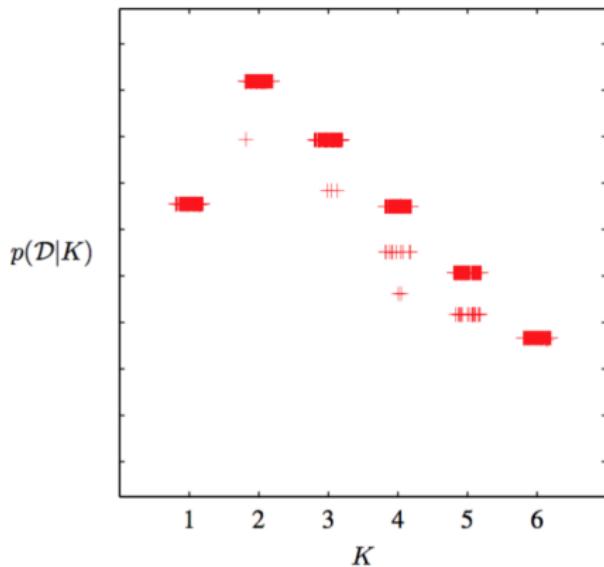
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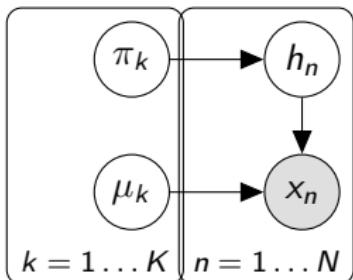
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- But admittedly the algebra gets tiring./C'est évident que les

Variant 4 for GMM - Going Ultra Bayesian

- Model:



$$\pi \sim \text{Dirichlet}(1/K, \dots, 1/K)$$

$$\mu_k \sim \mathcal{N}(\mu_k; 0, \sigma_0^2 I), \text{ for } k \in \{1, \dots, K\}$$

$$h_n \sim \text{Categorical}(\pi)$$

$$x_n | h_n \sim \mathcal{N}(x; \mu_h, \sigma^2 I), \text{ for } n \in \{1, \dots, N\}$$

- $h_n \in \{1, \dots, K\}$, 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 paramètres, et échantillonner 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!

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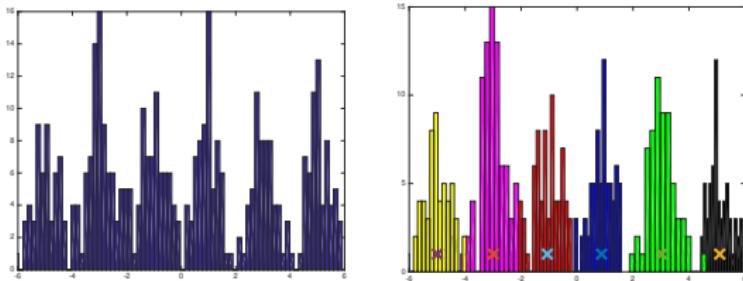
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- Take K to infinity:

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

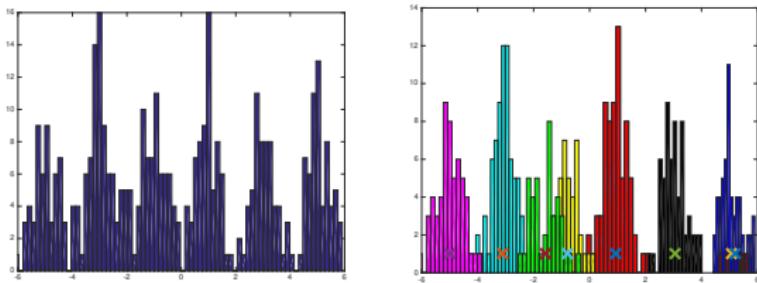
- And, sample from these full conditionals!

Collapsed Gibbs sampling in Infinite GMM



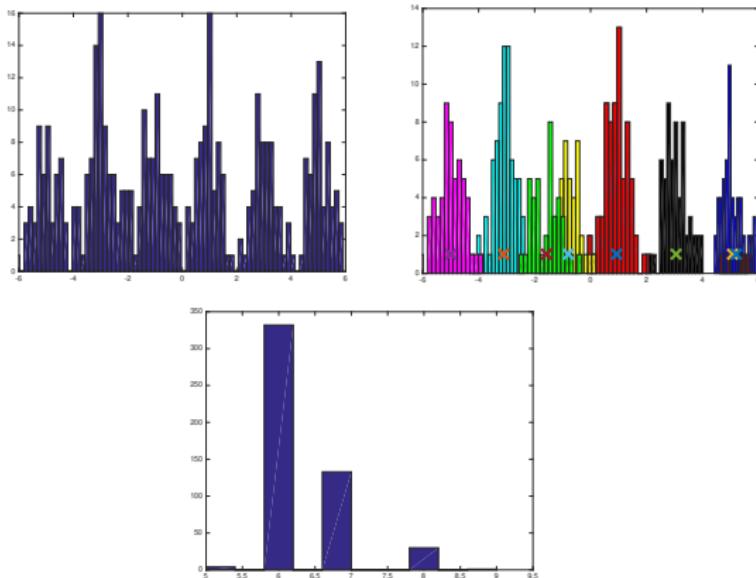
Top left: Histogram of observed data (données observées), Top right: Samples from full conditional of $h_{1:N}$, Bottom: Histogram of K (nombre de clusters)

Collapsed Gibbs sampling in Infinite GMM



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

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- 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.

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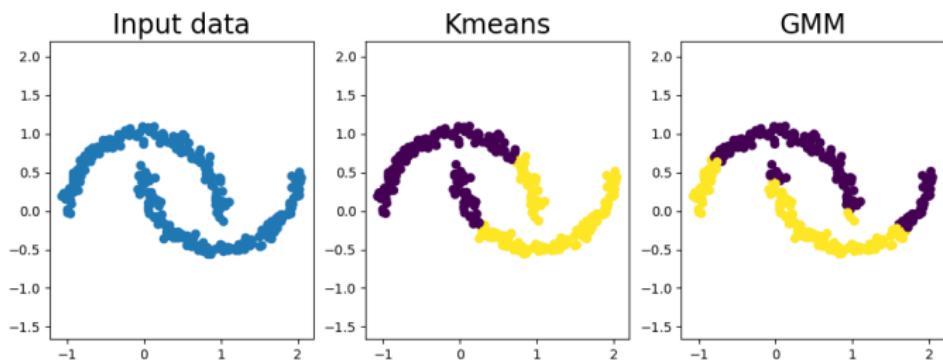
More Advanced GMM Learning Methods

Spectral Clustering

Hierarchical Clustering

Failure case for Centroid Based Methods

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



- Any ideas / Idées?

Remember KPCA?

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

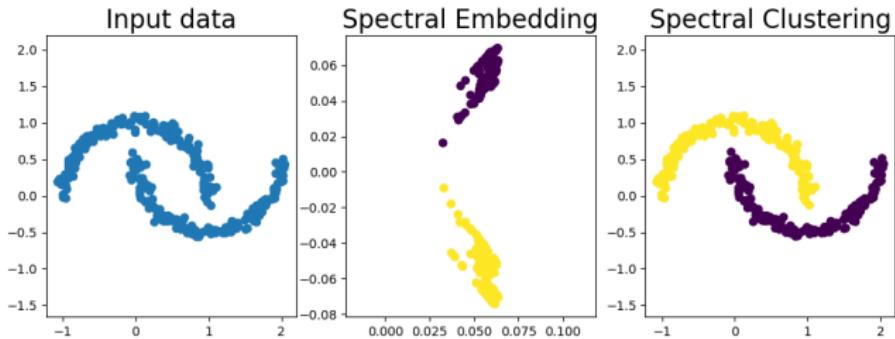
Spectral Clustering

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

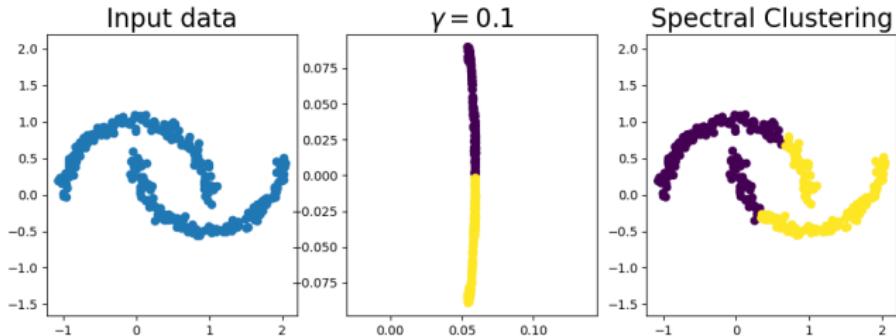
$$L := D^{-1/2} A D^{-1/2}, \quad D_{ii} = \sum_j A_{ij}$$

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

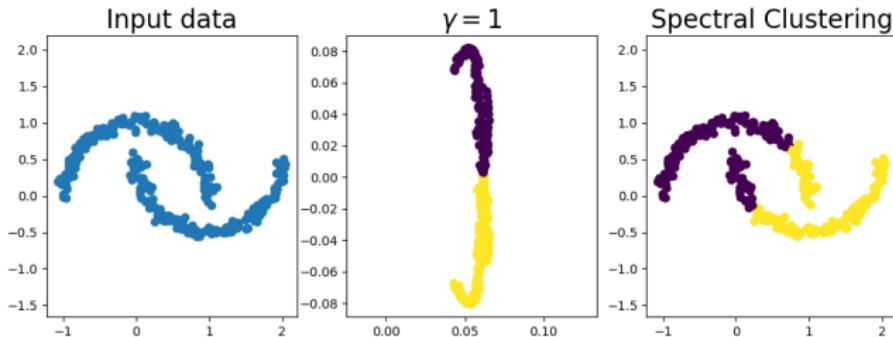
Spectral Clustering in Action



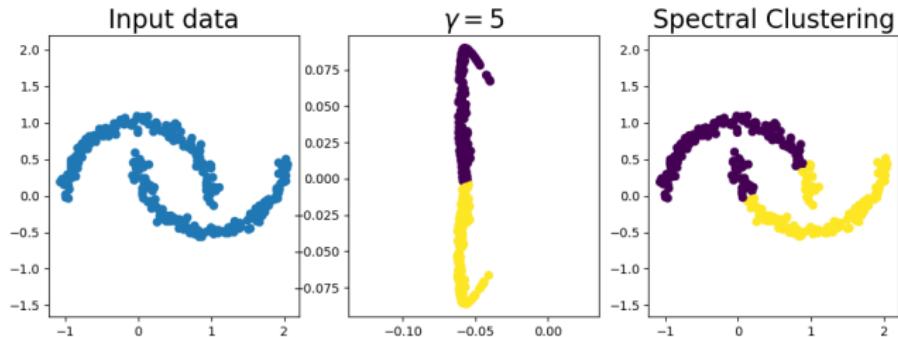
Spectral Clustering, effect of Gamma



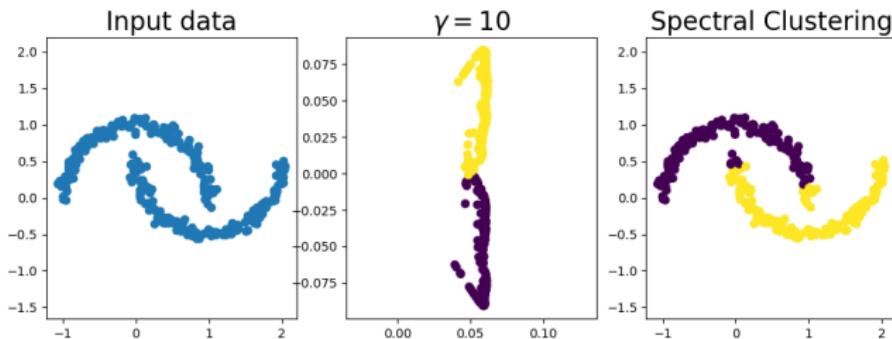
Spectral Clustering, effect of Gamma



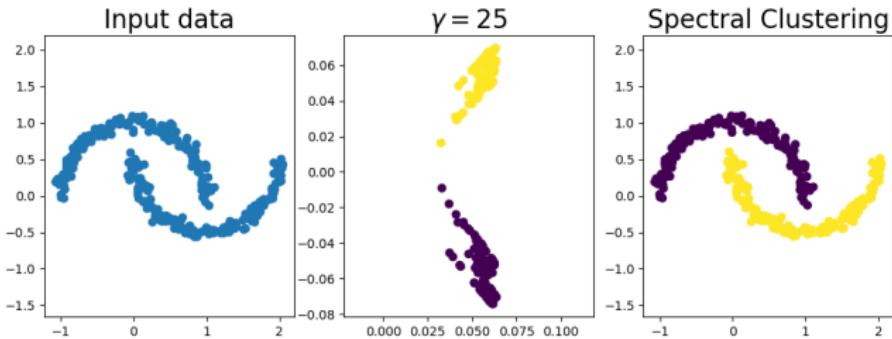
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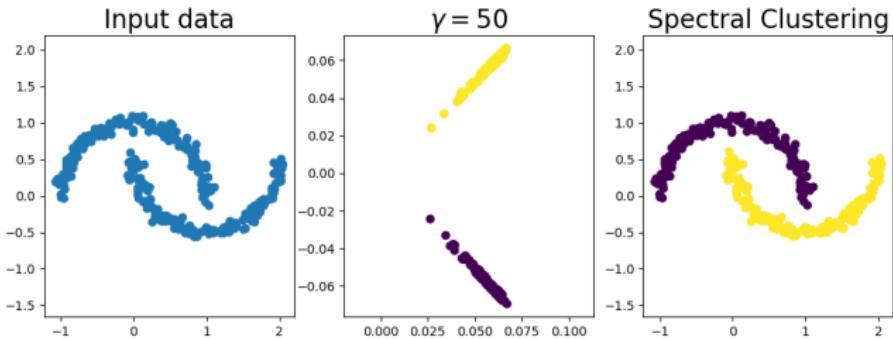


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Agglomerative Clustering

- 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.

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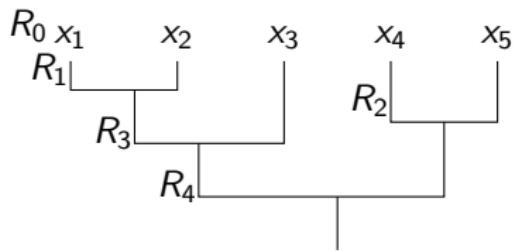
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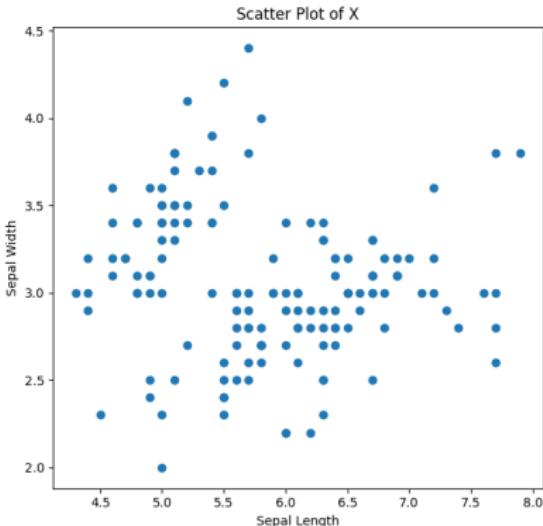
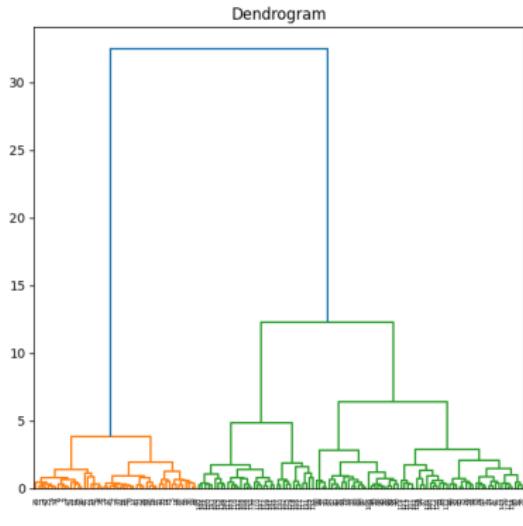
- ▶ Form new cluster pair, remove the pair / Forme un nouvelle paire de clusters, enlève l'ancien,

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

Dendrogram



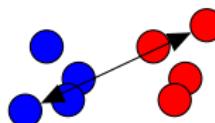
Example Dendrogram on IRIS



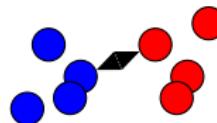
With Ward Linkage

How do we measure distances between clusters

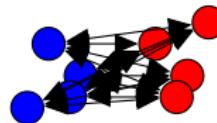
- Linkage functions
 - ▶ Complete linkage



- ▶ Single linkage

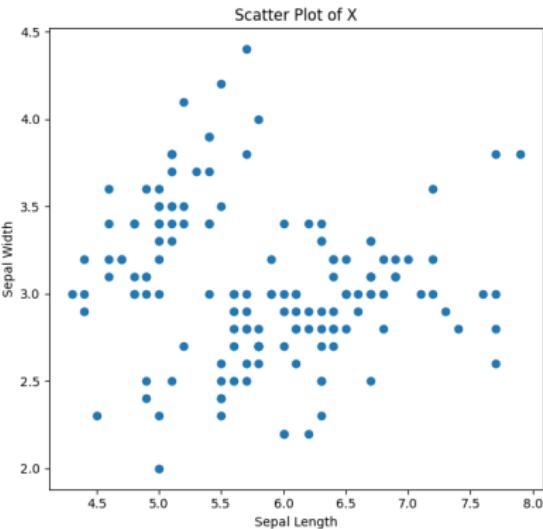
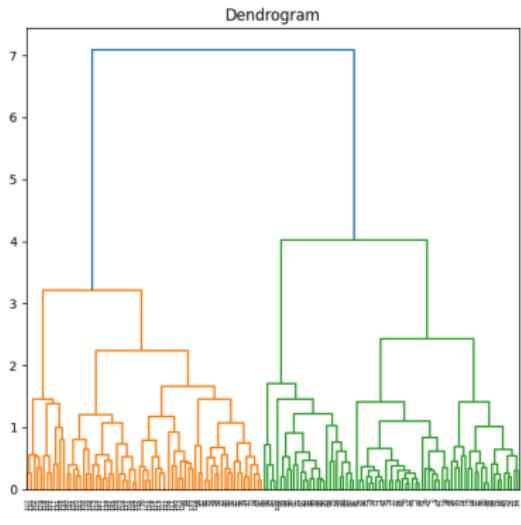


- ▶ Average linkage



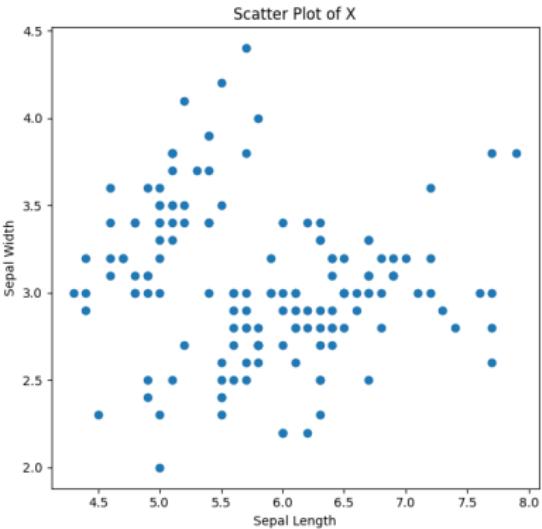
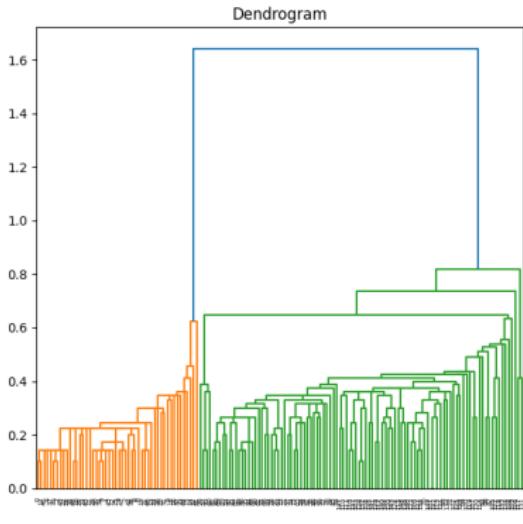
- There's more / Il y en a d'autres.

Example Dendrogram on IRIS



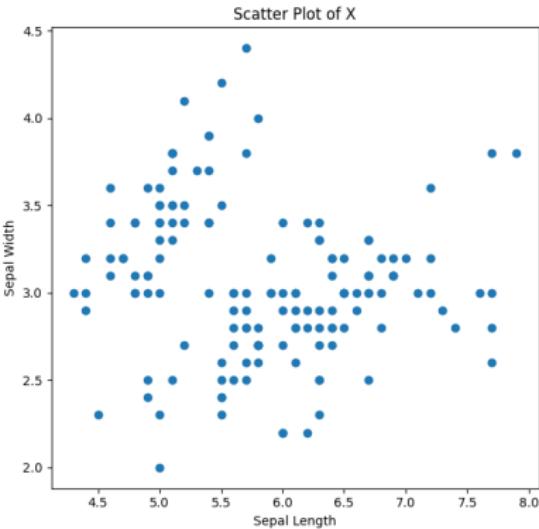
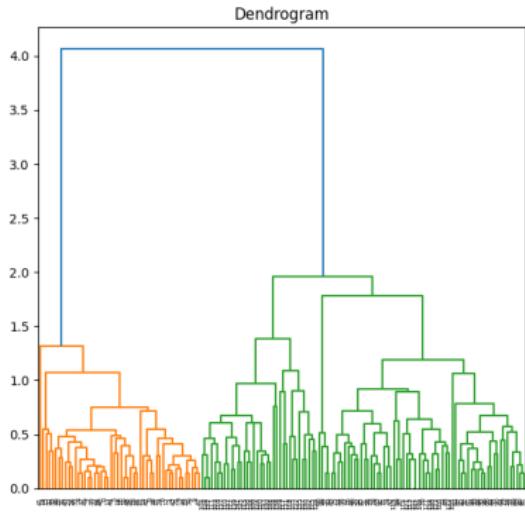
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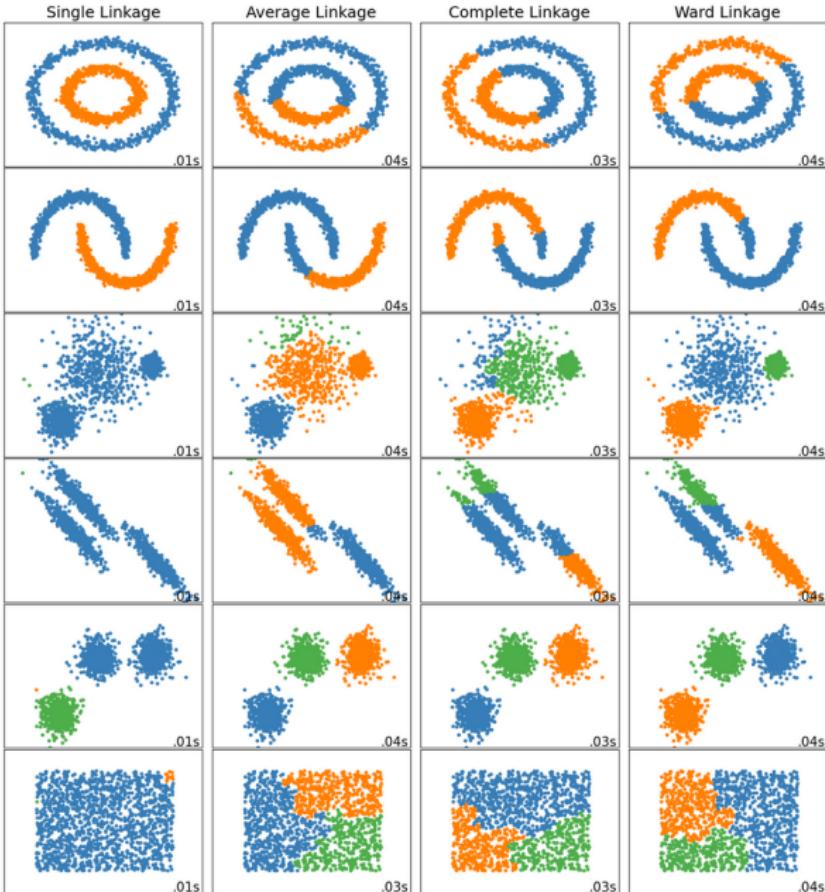
Single Linkage

Example Dendrogram on IRIS



Average Linkage

How does linkage change things



Computational Complexity

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- 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..

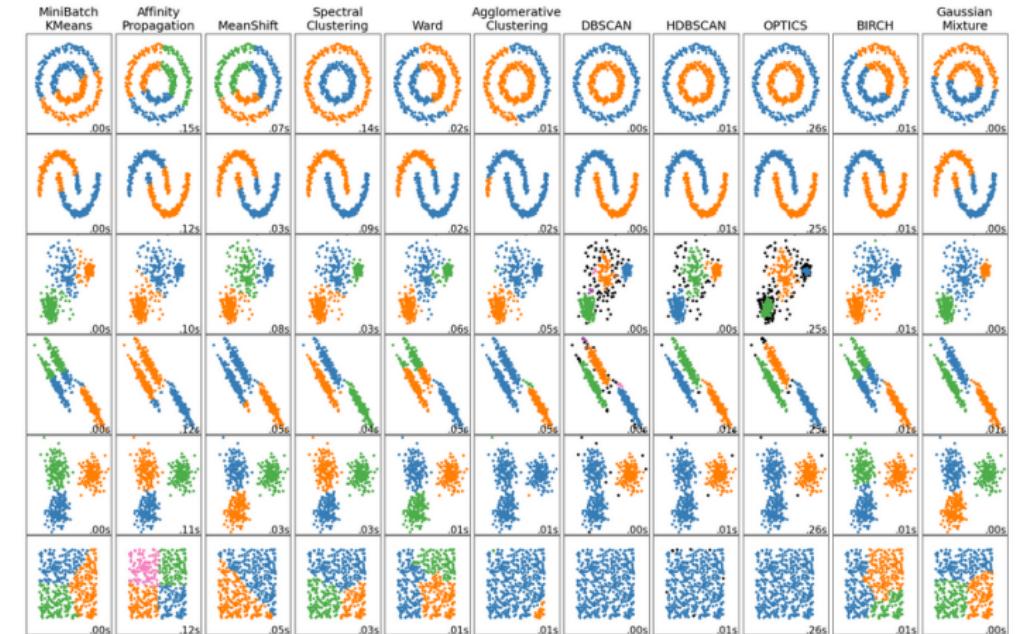
Divisive Clustering

- 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 choisissant 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.
- Hierarchical Clustering
 - ▶ Gives a dendrogram, but expensive! Donne un dendrogram, est un bon utile, mais cher!

There's more!



Suggested reading

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

Next week

- We will add connections between h_n 's!

