



# Bayesian Machine Learning

May 2024 - François HU  
<https://curiousml.github.io/>

# Outline

1

Bayesian statistics

2

**Latent variable models**

- Latent variable models and EM algorithm
- Probabilistic clustering
- Probabilistic dimensionality reduction

3

Variational Inference

4

Markov Chain Monte Carlo

5

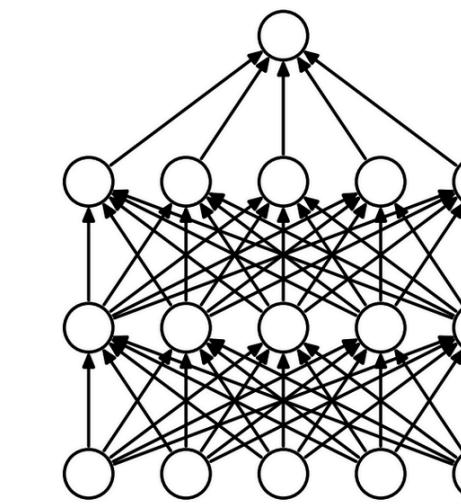
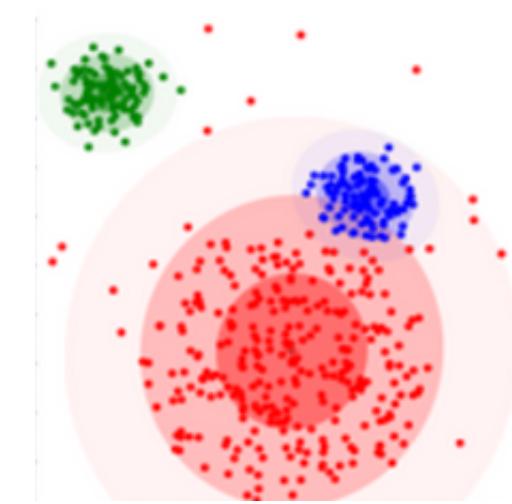
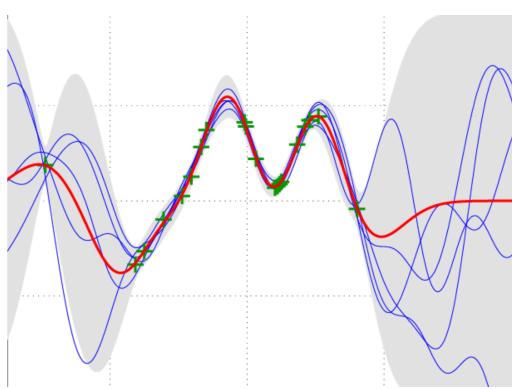
Extensions and oral presentations

0

## Evaluation & conjugate prior

# Evaluation (1/2)

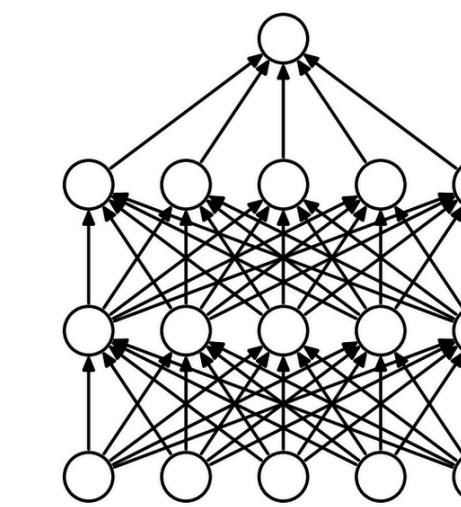
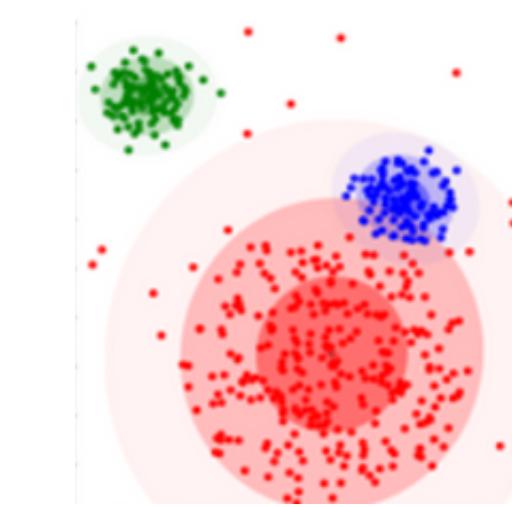
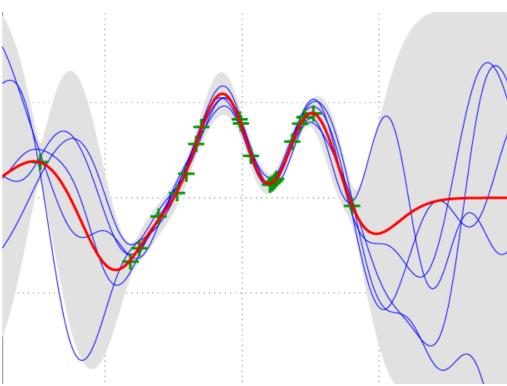
## Group project



- The evaluation will consist of a **group project (4 students max)** based on a research article
- For the last lecture, each student will send me the **codes (only in Python!)** Some of the paper's implementations are in R or Matlab, but you need to adapt them) and give an **oral presentation** in front of the class. Even if the article is mostly theoretical, each presentation should be understandable by other students (The clarity of the speech will be analysed).
- Initiatives like **more experimentations** or identifying the limits of the article will be greatly appreciated. You are welcome to consult other research articles (highly recommended, it should be cited at the end of your presentation) to boost your knowledge.
- The **evaluation** is as follows :
  - **40% on the clarity of the code** (example : many comments, along with understandable variables/functions names. You can use Jupyter Notebook which might have the advantage to be easy to read for the users). When I run your code, it should be easy to run and easy to understand :)
  - **60% on the clarity of the oral presentation.** Less maths but more experimentations and intuitions. At the beginning a big introduction is expected in order to be understandable by other groups.

# Evaluation (2/2)

## Group project



### 1. Project Interpretability:

main paper « **DAG-GNN**: DAG structure learning with graph neural networks »

### 2. Project Fairness:

main paper: « Fair Data Adaptation with Quantile Preservation »

R package: « **fairadapt**: Causal Reasoning for Fair Data Pre-processing »

### 3. Project Uncertainty:

main paper: « Dropout as a bayesian approximation: Representing model uncertainty in deep learning »

### 4. Project Topic modeling:

main paper: « Mixing dirichlet topic models and word embeddings to make **lda2vec** »

open question: Propose a way to automatically generate a topic's title. Implement it.

### 5. Project Missing values:

main paper: « What's a good imputation to predict with missing values? »

# Conjugate priors: Exercices

## Gamma case

**Exercice** (left as an exercice, correction in the next lecture)

$$P(\gamma|x) = \frac{\mathcal{N}(x|\mu, \gamma^{-1}) \times P(\gamma)}{P(x)} \quad \Gamma(\gamma | \alpha_{prior}, \beta_{prior})$$

$$\Gamma(\gamma | \alpha_{prior} + 1/2, \beta_{prior} + (x - \mu)^2/2)$$

### Gamma distribution

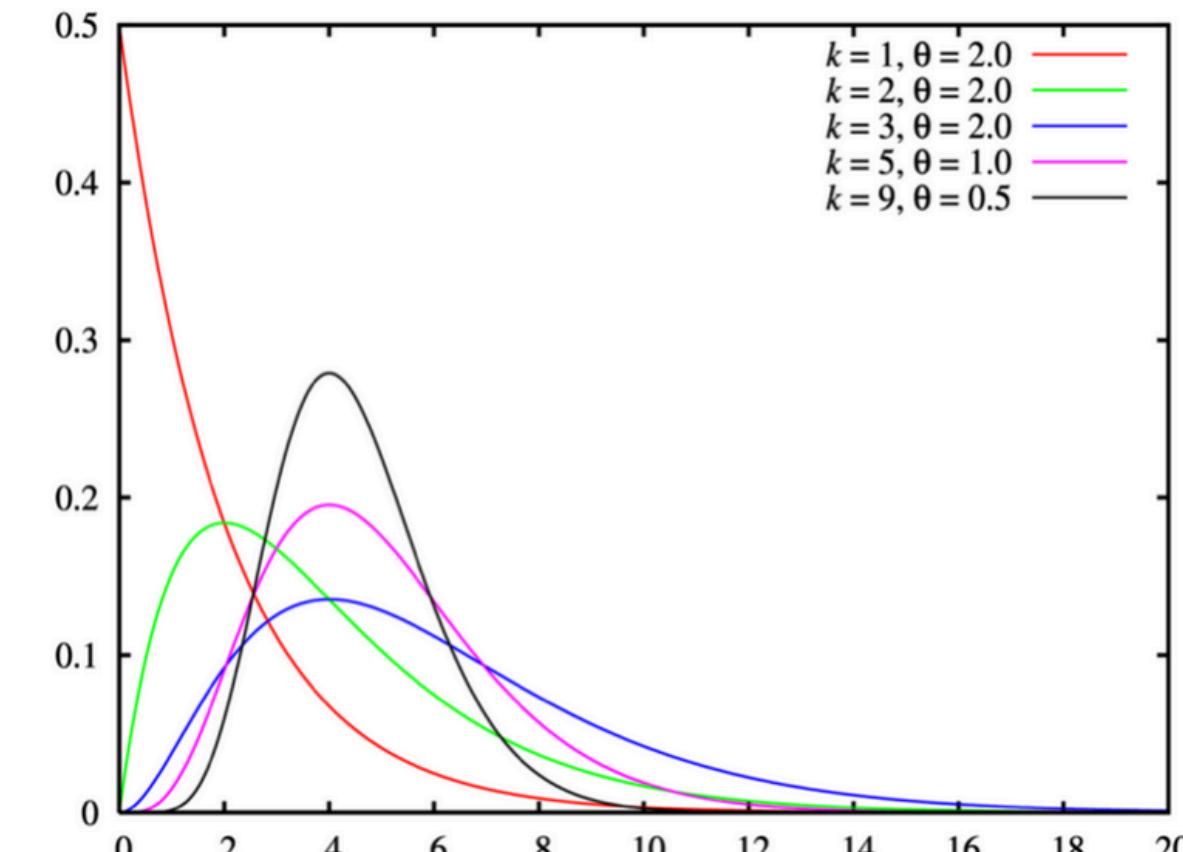
**PDF :**  $\Gamma(x|\alpha, \beta) = \frac{\beta^\alpha}{\Gamma(\alpha)} x^{\alpha-1} e^{-\beta x}$  with  $x, \alpha, \beta > 0$

$$\Gamma(\alpha) = (\alpha - 1)!$$

**mean :**  $\mathbb{E}[x] = \frac{\alpha}{\beta}$

**variance :**  $V(x) = \frac{\alpha}{\beta^2}$

**mode :**  $Mode[x] = \frac{\alpha - 1}{\beta}$



What we want to compute :  $p(\text{parameters} | \text{data}) \propto p(\text{data} | \text{parameters}) \times p(\text{parameters})$

•  $p(\text{data} | \text{parameters}) = \mathcal{N}(x | \mu, \gamma^{-1}) = \frac{\sqrt{\gamma}}{\sqrt{2\pi}} e^{-\gamma \frac{(x-\mu)^2}{2}} \propto \sqrt{\gamma} e^{-\gamma \frac{(x-\mu)^2}{2}}$

•  $p(\text{parameters}) = \prod (\gamma | \alpha_{prior}, \beta_{prior}) = \frac{\beta_{prior}^{\alpha_{prior}}}{\Gamma(\alpha_{prior})} \times \gamma^{\alpha_{prior}-1} e^{-\gamma \beta_{prior}} \propto \gamma^{\alpha_{prior}-1} e^{-\gamma \beta_{prior}}$

So :  $p(\text{parameters} | \text{data}) \propto \gamma^{\alpha_{prior}/2} e^{-\gamma \frac{(x-\mu)^2}{2}} \times \gamma^{\alpha_{prior}-1} e^{-\gamma \beta_{prior}}$   
 $\propto \gamma^{\frac{1}{2} + \alpha_{prior}-1} e^{-\gamma (\beta_{prior} + \frac{(x-\mu)^2}{2})}$

$$p(\text{parameters} | \text{data}) = \boxed{\prod (\gamma | \underbrace{\alpha_{prior} + \frac{1}{2}}_{\alpha_{posterior}}, \underbrace{\beta_{prior} + \frac{(x-\mu)^2}{2}}_{\beta_{posterior}})}$$

# Conjugate priors: Exercices

## Beta case

**Exercice** (left as an exercice, correction in the next lecture)

$$P(\theta|x) = \frac{B(\theta|\alpha_{posterior}, \beta_{posterior})}{P(x)} = \frac{B(\theta|\alpha_{prior} + n_1, \beta_{prior} + n_0) \cdot \theta^{n_1} \cdot (1-\theta)^{n_0}}{B(\theta|\alpha_{prior}, \beta_{prior})}$$

### Beta distribution

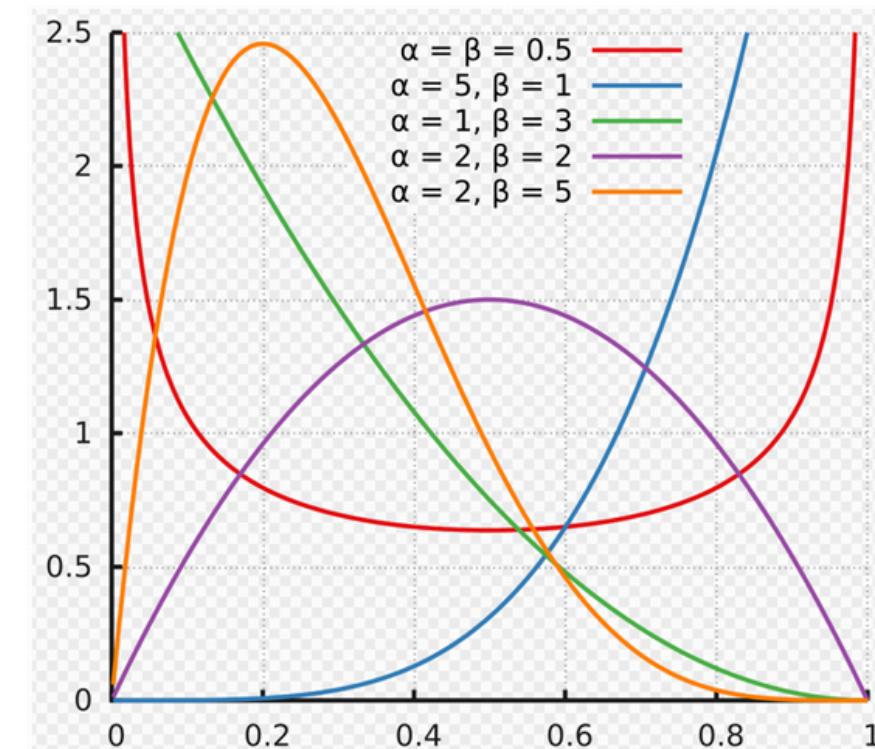
PDF :  $B(x|\alpha, \beta) = \frac{1}{B(\alpha, \beta)} x^{\alpha-1} (1-x)^{\beta-1}$  with  $\alpha, \beta > 0$  and  $x \in [0,1]$

$$B(\alpha, \beta) = \frac{\Gamma(\alpha) \cdot \Gamma(\beta)}{\Gamma(\alpha + \beta)}$$

mean :  $\mathbb{E}[x] = \frac{\alpha}{\alpha + \beta}$

variance :  $V(x) = \frac{\alpha\beta}{(\alpha + \beta)^2 \cdot (\alpha + \beta - 1)}$

mode :  $Mode[x] = \frac{\alpha - 1}{\alpha + \beta - 2}$



What we want to compute :  $p(\text{parameters} | \text{data}) \propto p(\text{data} | \text{parameters}) \times p(\text{parameters})$

•  $p(\text{data} | \text{parameters}) = \text{Ber}(x | \theta) = \binom{n}{x} \theta^x (1-\theta)^{n-x} \propto \theta^x (1-\theta)^{n-x}$

•  $p(\text{parameters}) = B(\theta | \alpha_{prior}, \beta_{prior}) = \frac{\theta^{\alpha_{prior}-1} (1-\theta)^{\beta_{prior}-1}}{B(\alpha_{prior}, \beta_{prior})} \propto \theta^{\alpha_{prior}-1} (1-\theta)^{\beta_{prior}-1}$

So :  $p(\text{parameters} | \text{data}) \propto \theta^{n_1} (1-\theta)^{n_0} \times \theta^{\alpha_{prior}-1} (1-\theta)^{\beta_{prior}-1}$

$$\propto \theta^{n_1 + \alpha_{prior}-1} (1-\theta)^{n_0 + \beta_{prior}-1}$$

$$p(\text{parameters} | \text{data}) = \frac{B(\theta | n_1 + \alpha_{prior}-1, n_0 + \beta_{prior}-1)}{\underbrace{\alpha_{posterior}}_{\alpha_{prior}} \underbrace{\beta_{posterior}}_{\beta_{prior}}}$$

1

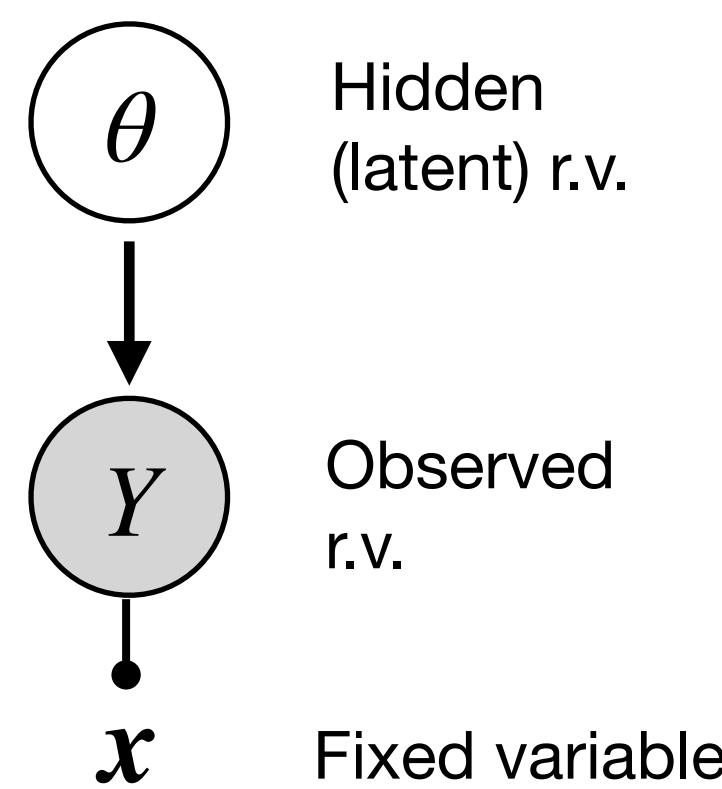
# **Latent variable models and mixture models**

# 1. Latent Variable Models

## Spoilers

**Latent variable models** : a statistical model that links a set of **observable** variables to a set of **unobservable (latent)** variables

**Example** : Bayesian Linear regression



**Other latent variable models** : unsupervised methods

- **Clustering** models
- **Dimensionality reduction** models

**Questions** :

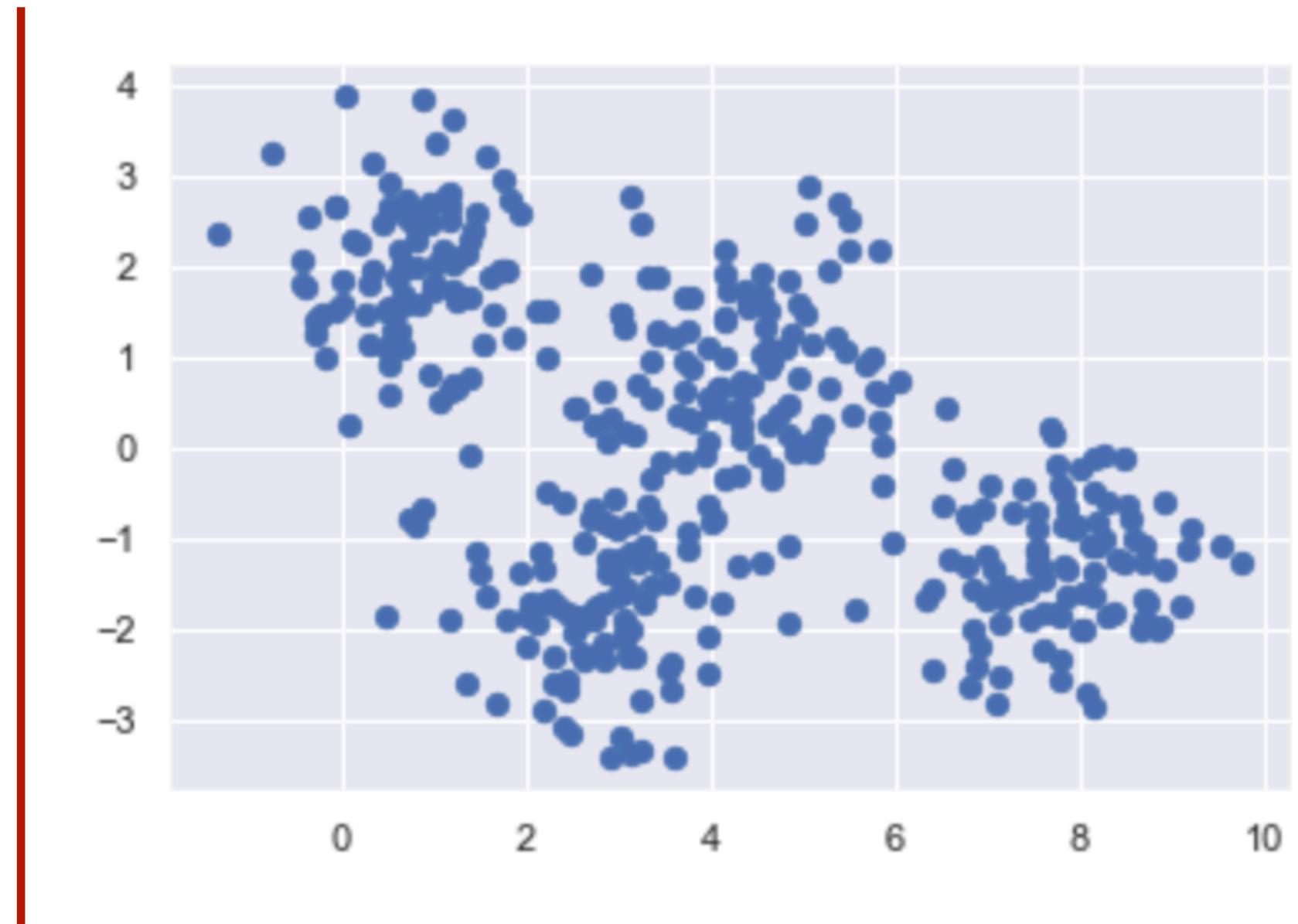
- **Why do we need latent variable models ?** simpler models (so fewer parameters) without reducing its flexibility
- **How to train these models ?** next section

# 1. Latent Variable Models

## Mixture models : Definition

**Mixture models** : a probabilistic model representing a **linear combination** of different distributions

**Example** : synthetic data



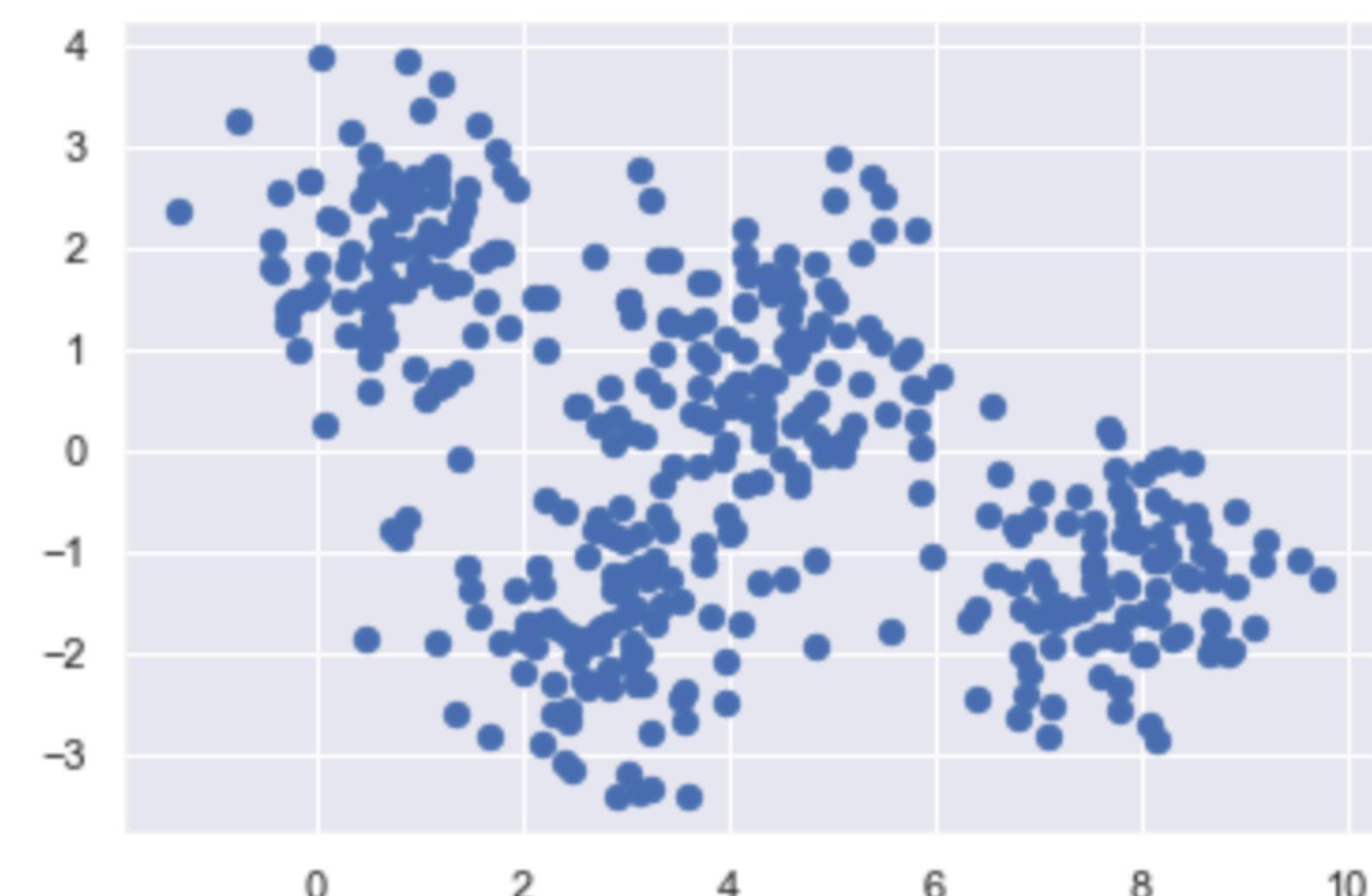
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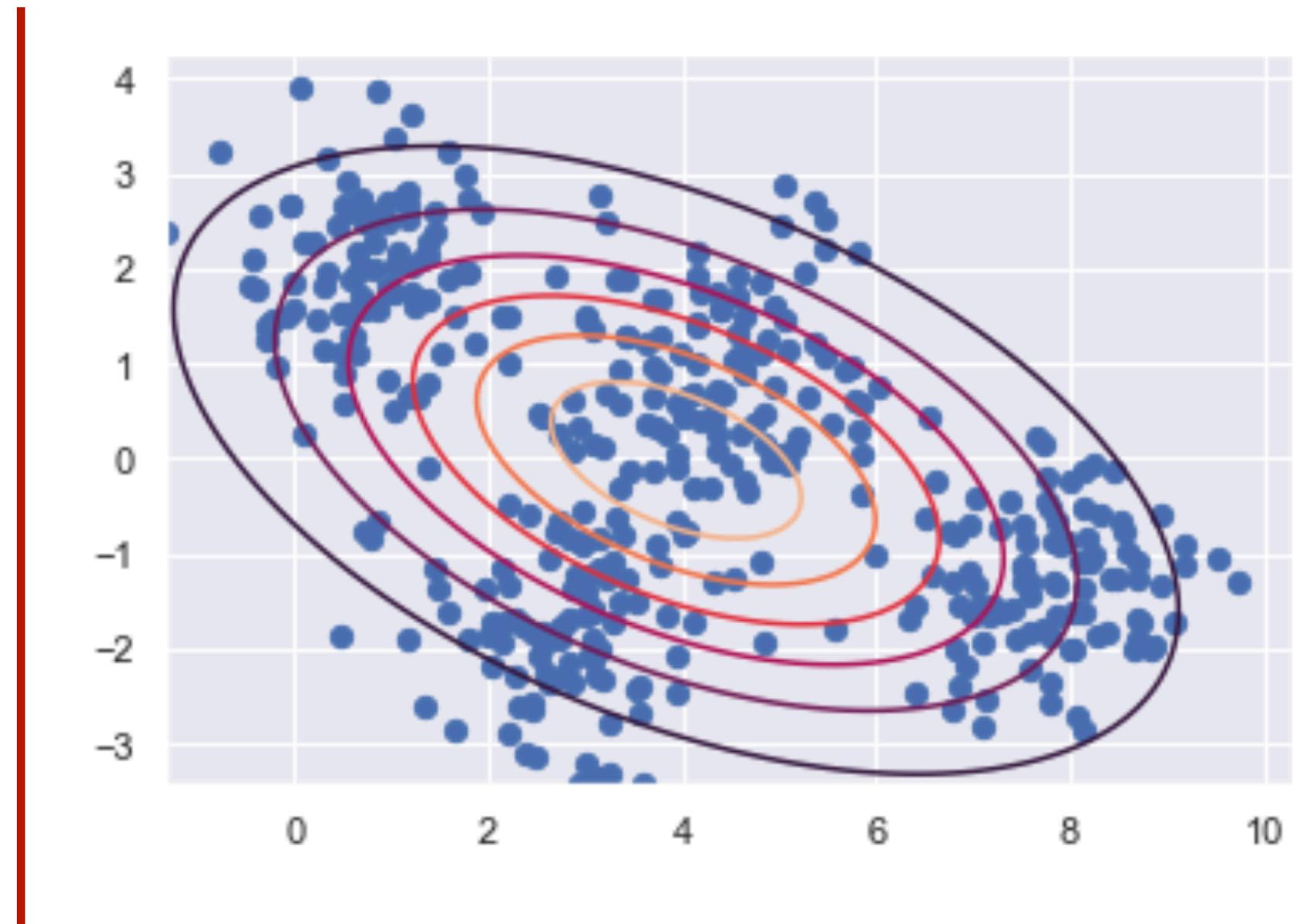
$$\mathcal{N}(\mu, \Sigma)$$

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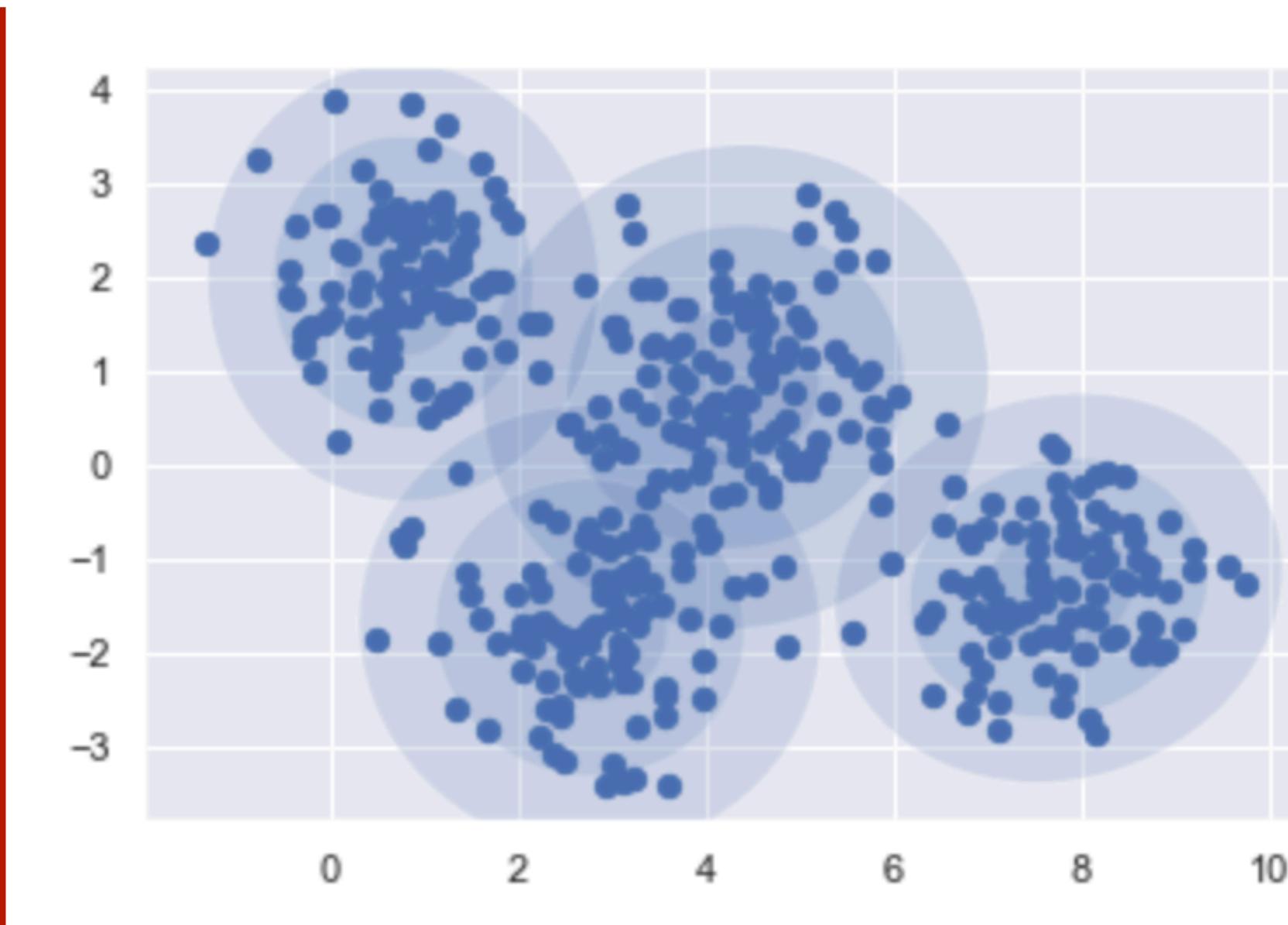


# 1. Latent Variable Models

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We want to fit a **Gaussian Mixture Model (GMM) !**

$$\sum_{k=1}^4 \pi_k \cdot \mathcal{N}(\mu_k, \Sigma_k)$$



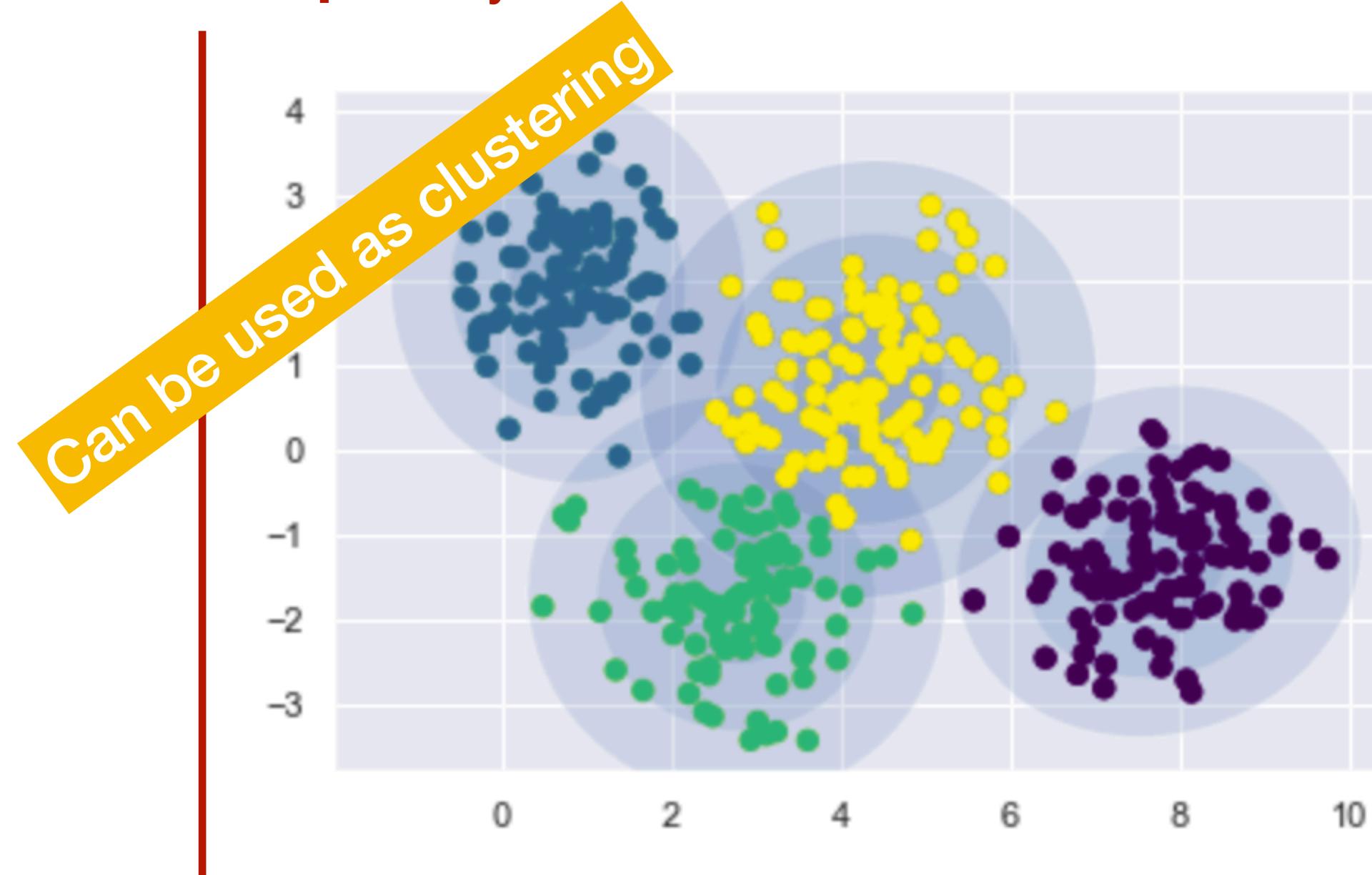
parameters :  $\{\pi_k, \mu_k, \Sigma_k\}_{k \in \{1, \dots, 4\}} =: \theta$

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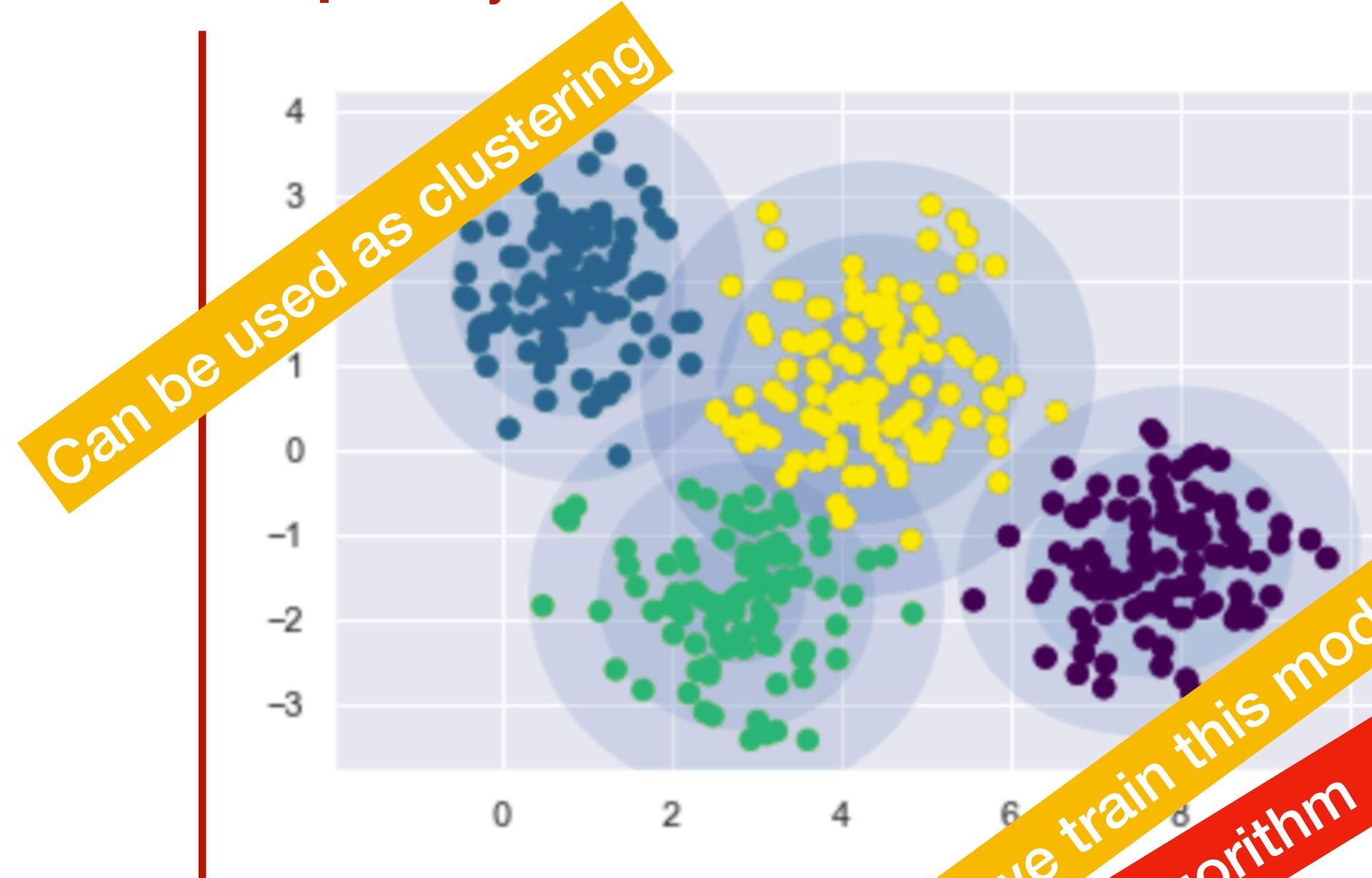
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# 1. Latent Variable Models

## Gaussian Mixture Model : Definition

**Mixture models** : a probabilistic model representing a **linear combination** of different distributions

**Example** : synthetic data



How do we train this model ?  
EM algorithm

Mixture modeling provides the **freedom / flexibility** to model the unknown pdf. Downside : more parameters

Let's fit a gaussian !

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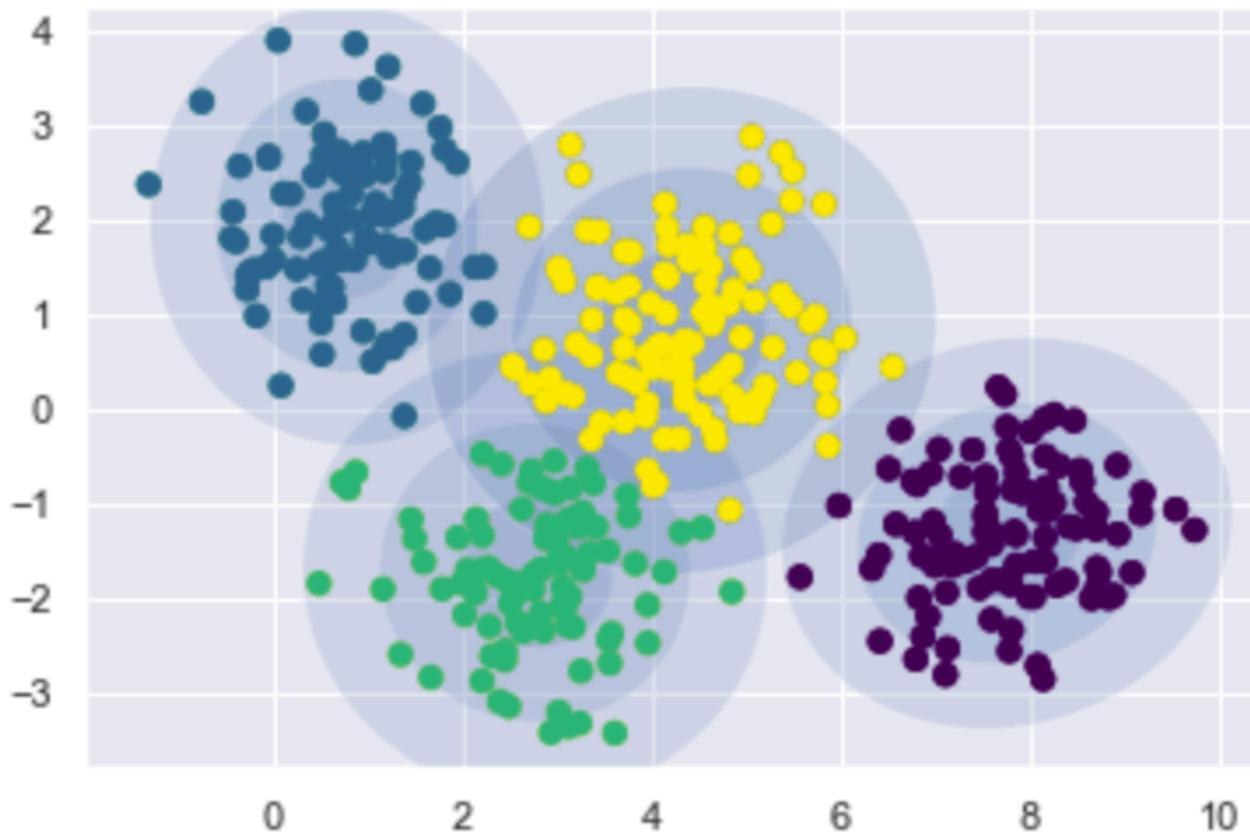


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## Probabilistic clustering and EM-algorithm

## 2. Probabilistic clustering

### Gaussian Mixture Model as a Latent variable model



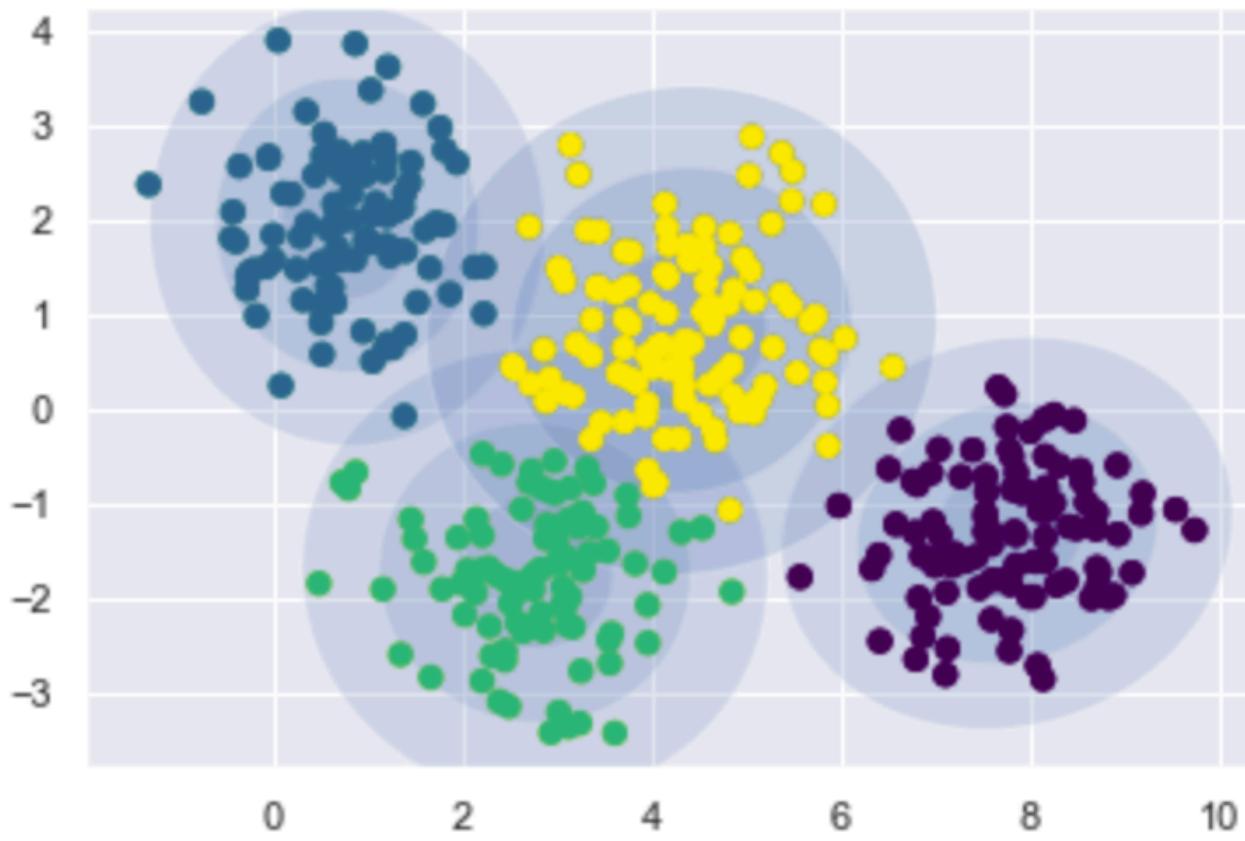
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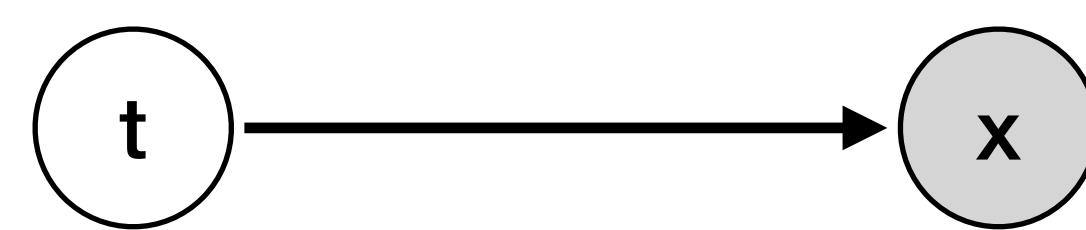


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**Latent variable model for GMM :**



the source :  
from **which gaussian**  
 $\{1, 2, 3, 4\}$   
this data came from ?

Gaussian  
distribution

$$p(t = k | \theta) =$$

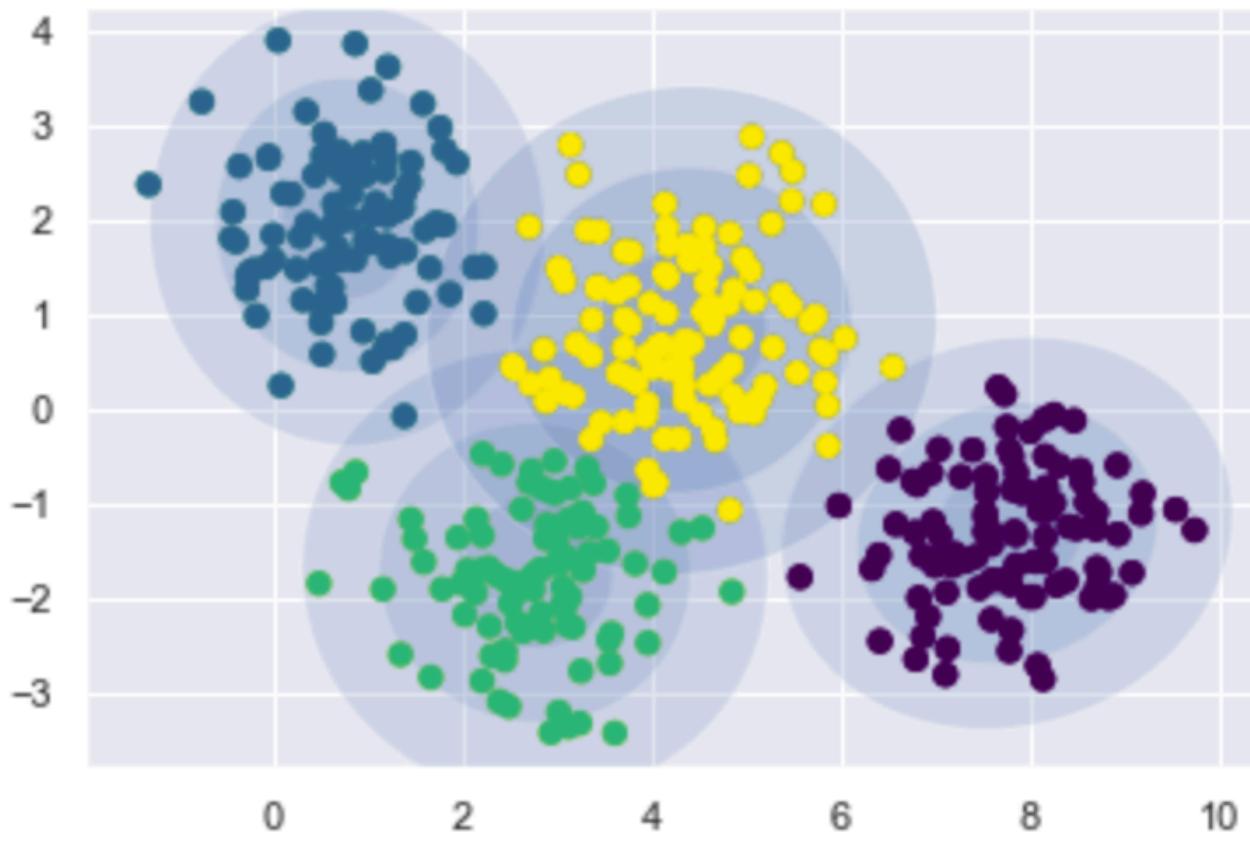
$$p(x | t = k, \theta) =$$

$$p(x | \theta) =$$

**Reminder :** a PGM models how an observation is generated

## 2. Probabilistic clustering

### Gaussian Mixture Model as a Latent variable model

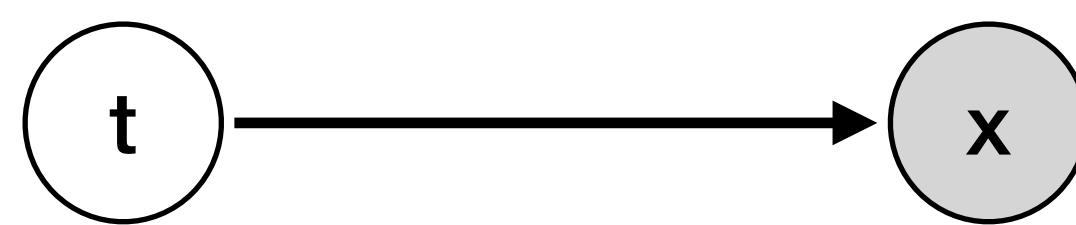


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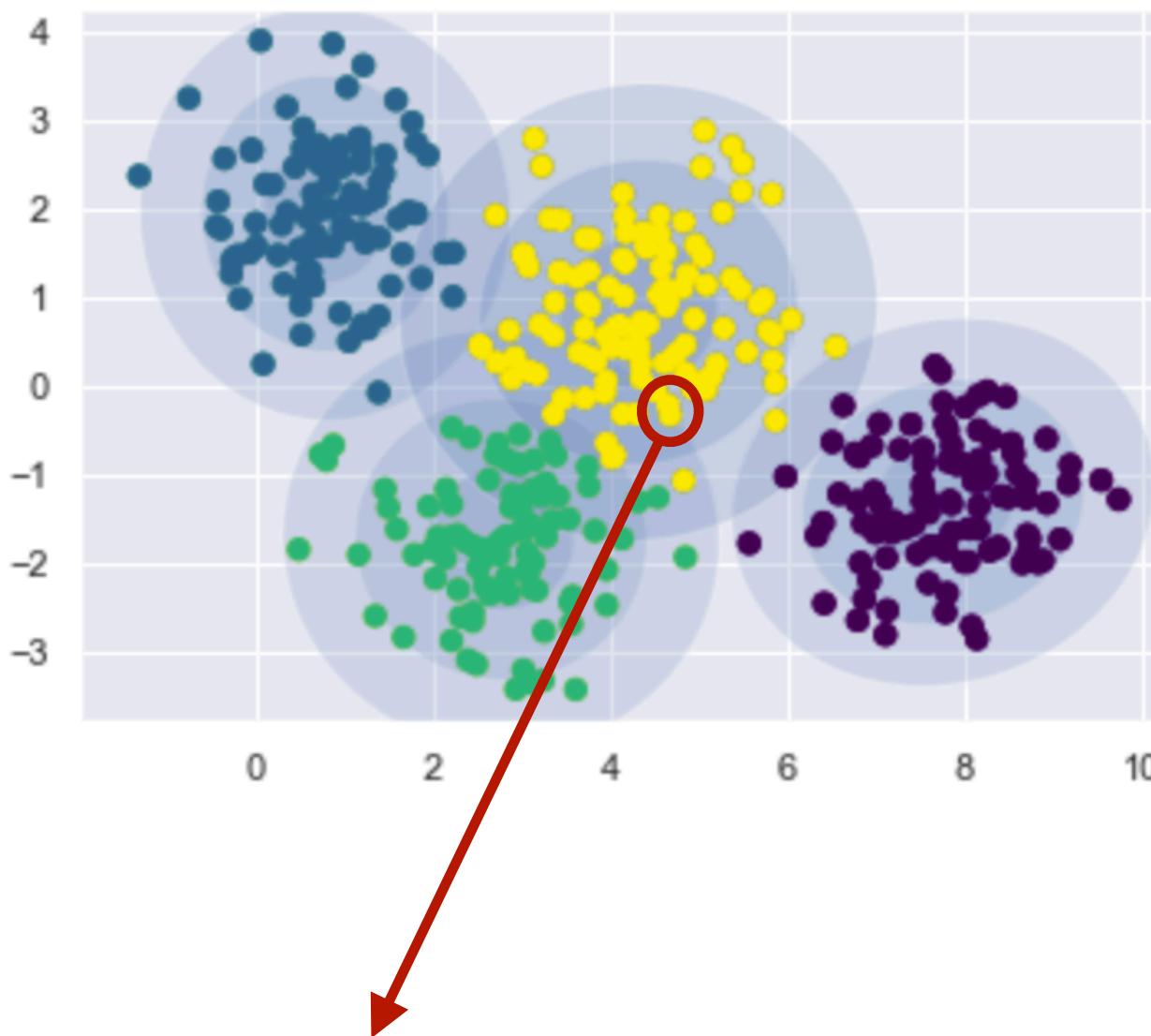
$$p(x | t = k, \theta) = \mathcal{N}(x | \mu_k, \Sigma_k)$$

$$p(x | \theta) = \sum_{k=1}^4 p(x | t = k, \theta)p(t = k | \theta)$$

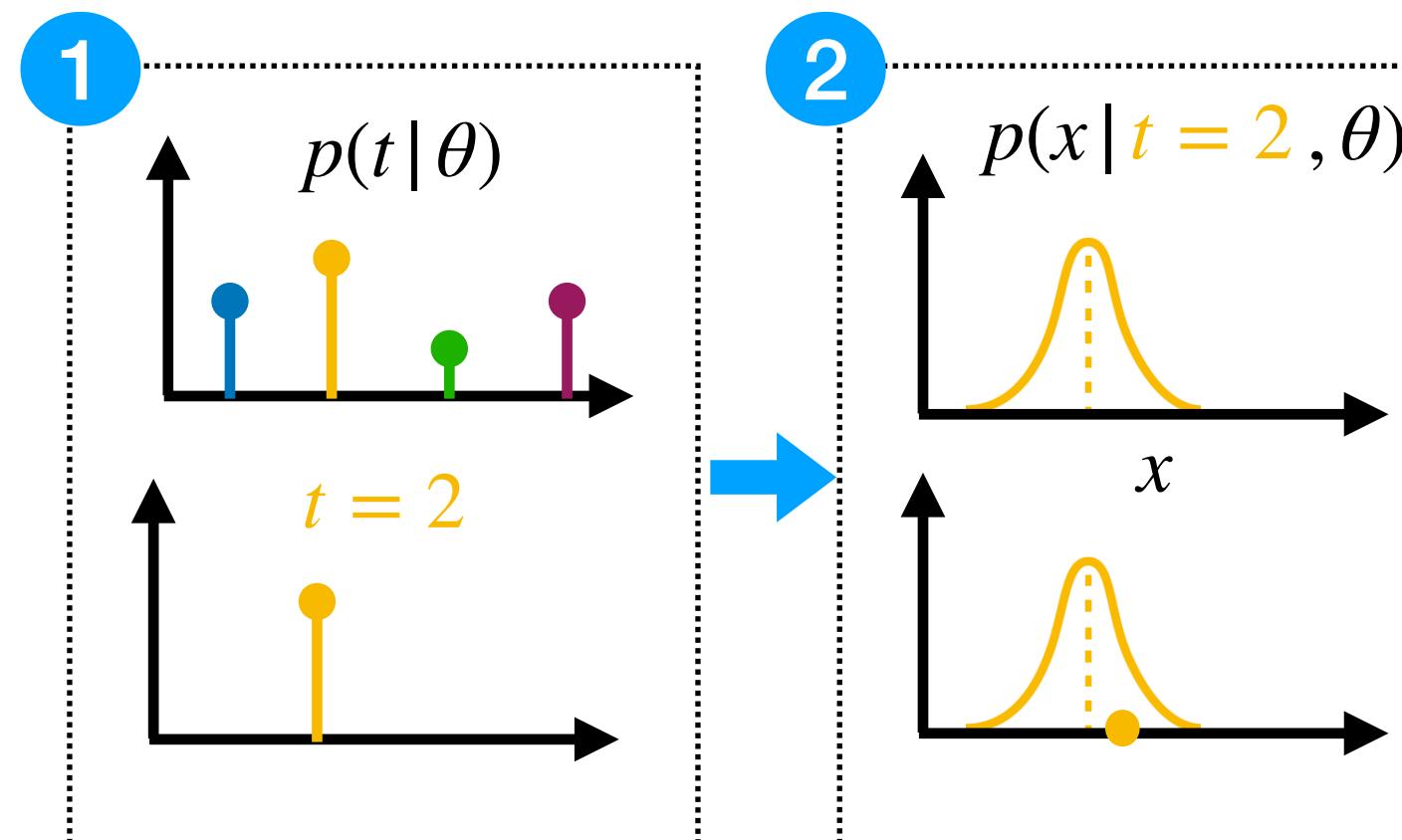
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## 2. Probabilistic clustering

### Gaussian Mixture Model as a Latent variable model



We assume that this  $x$  is generated as follows :

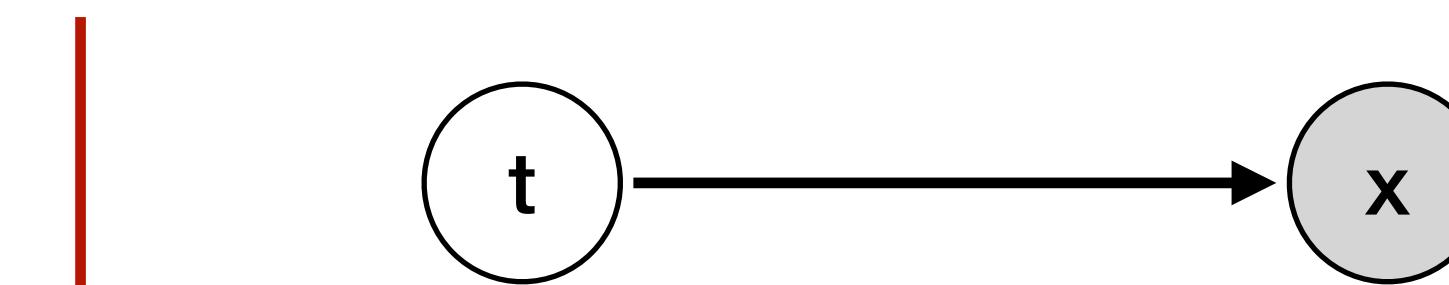


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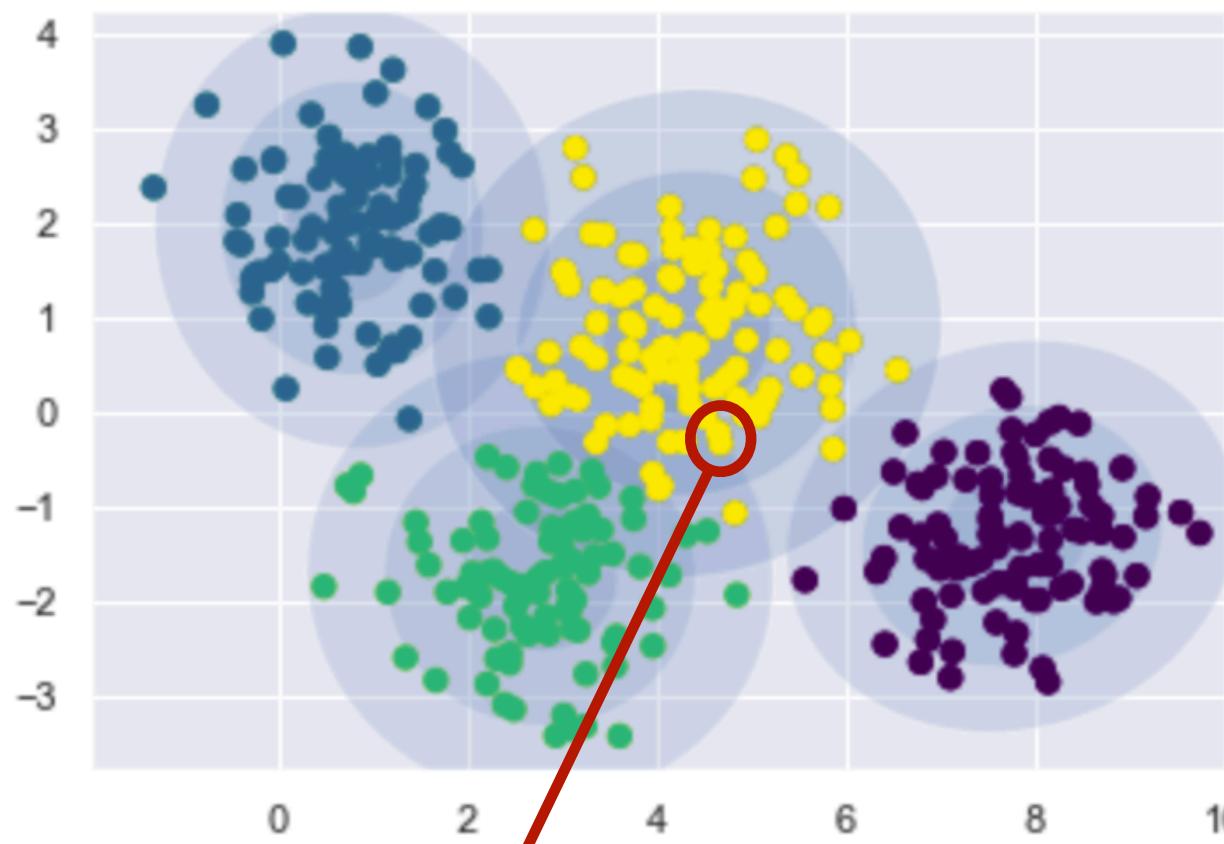
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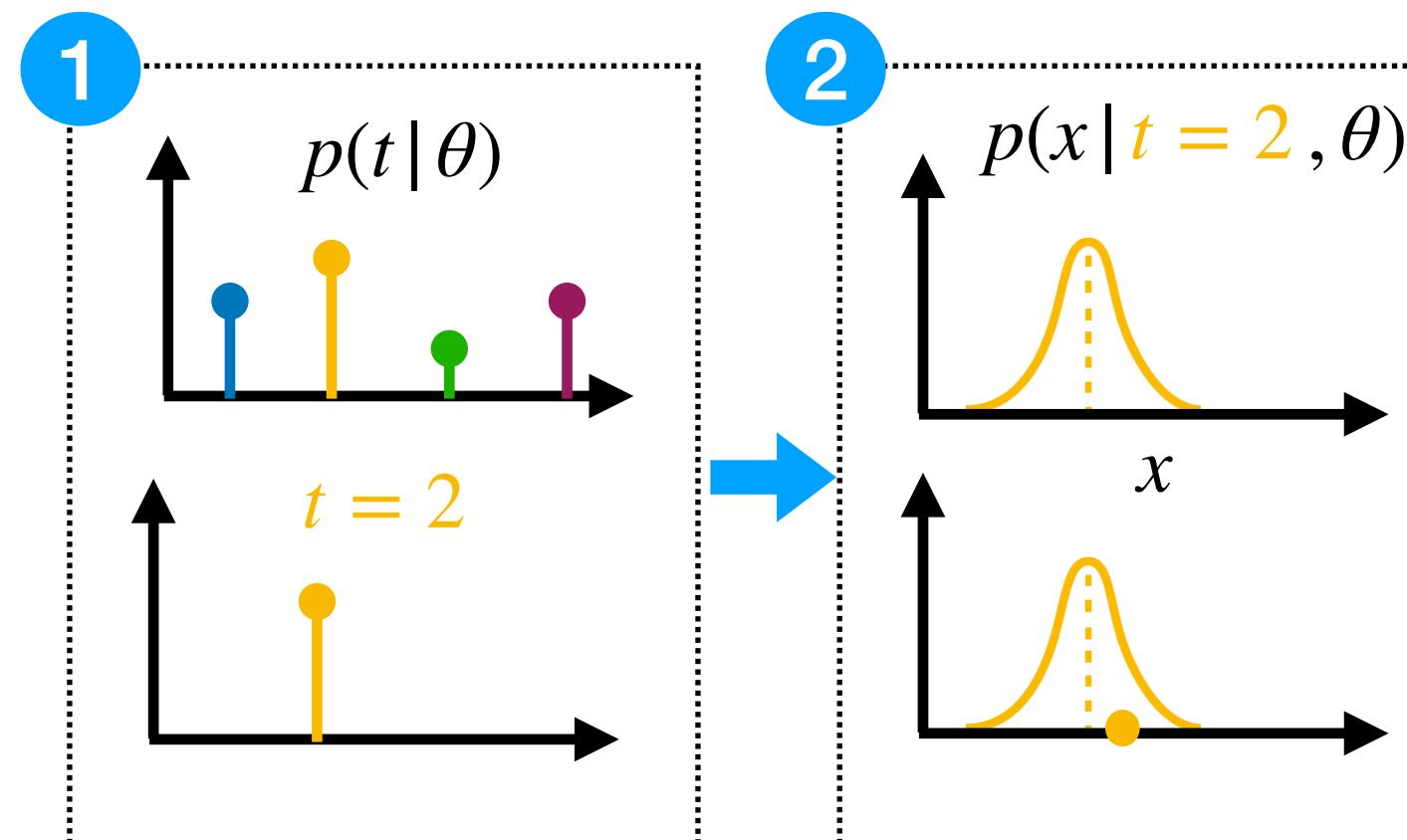
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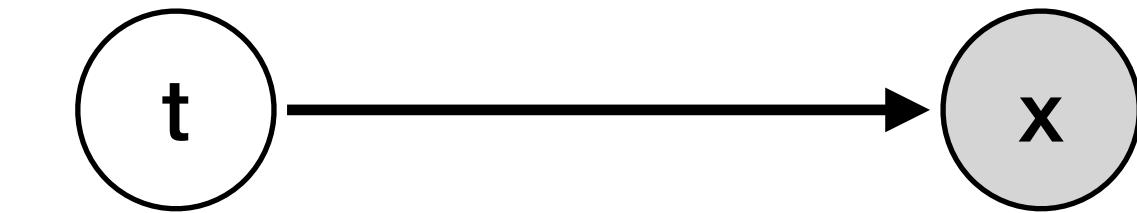
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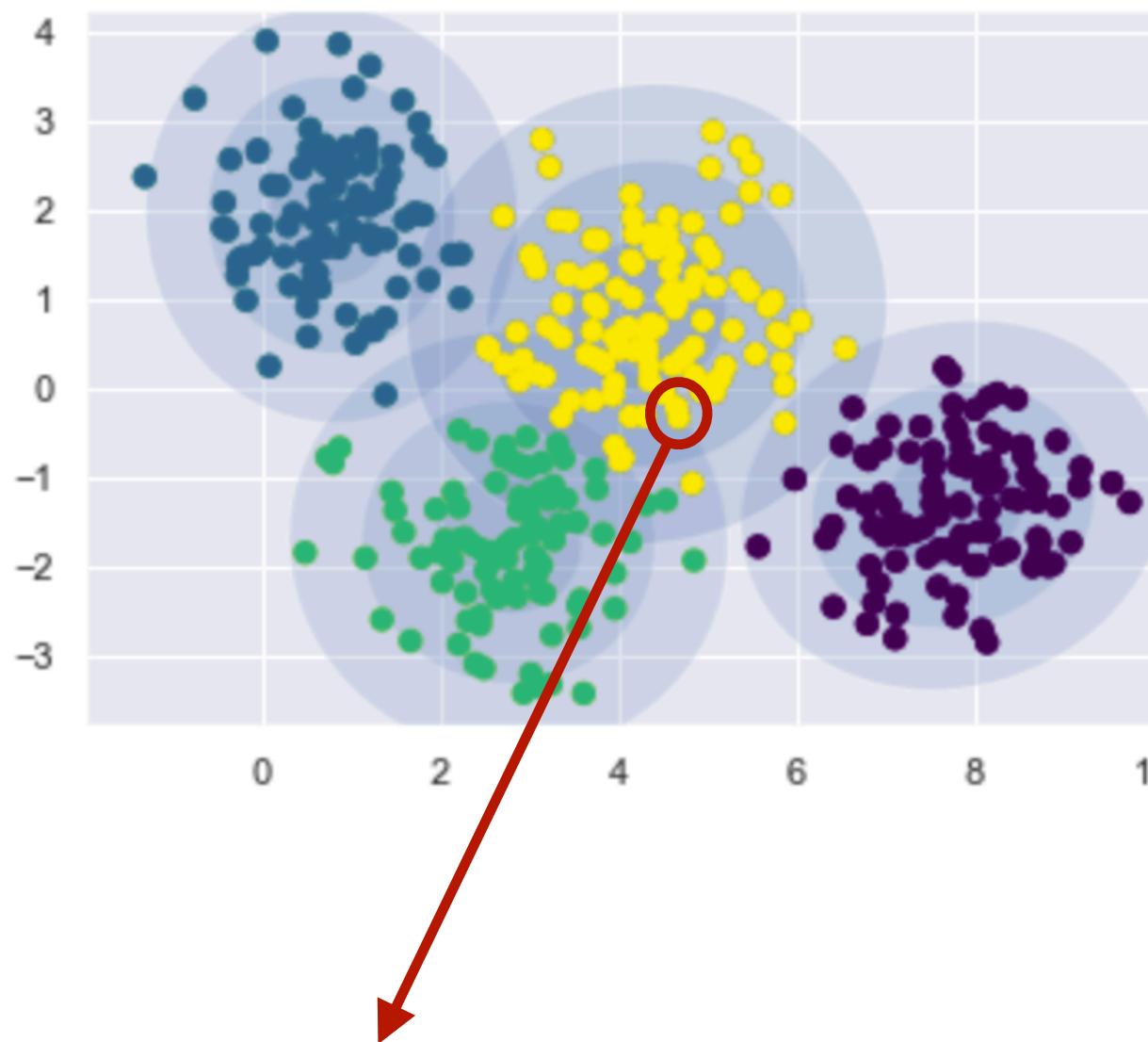


**Hard clustering** : if we **know the source** of each instances then,

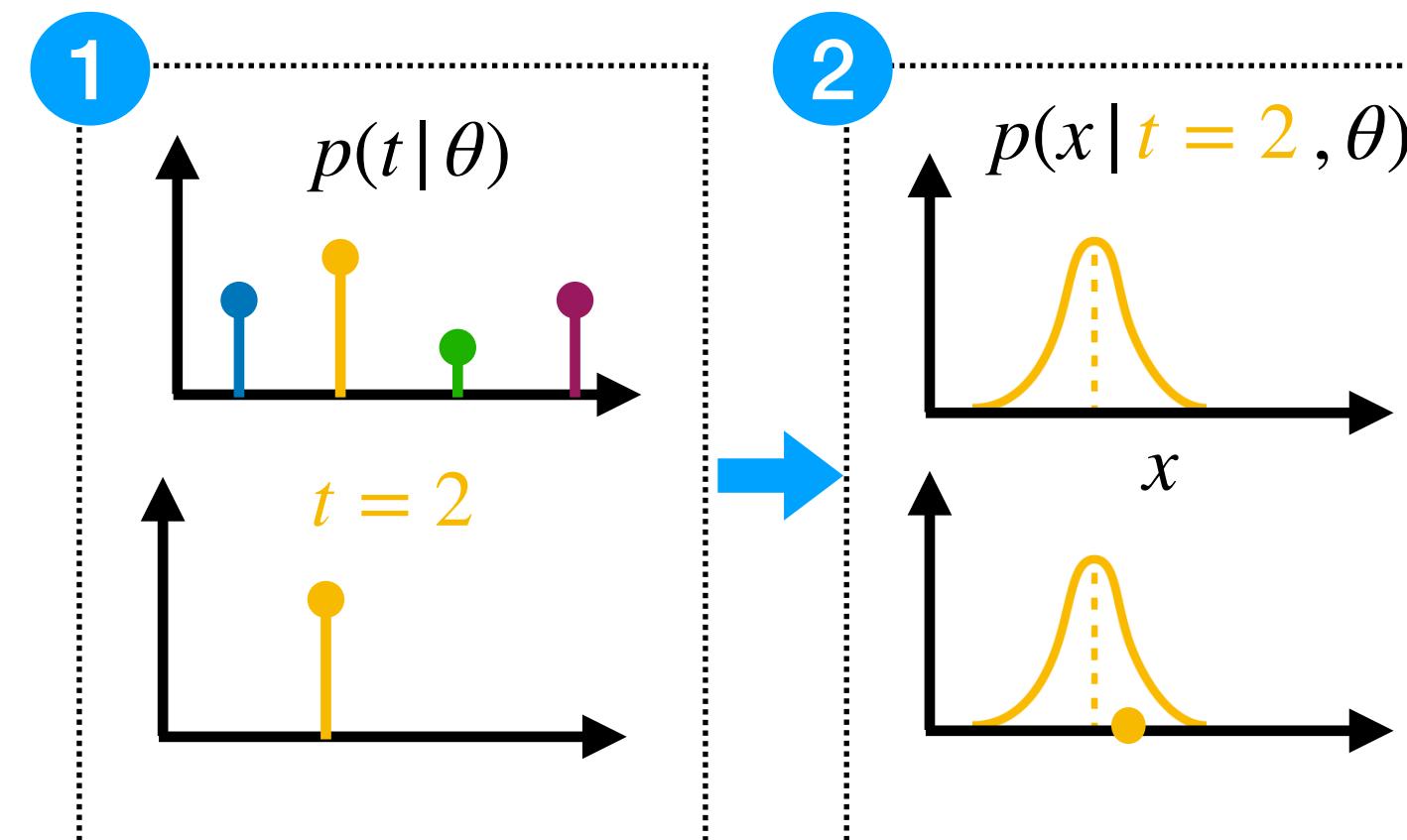
**Soft / probabilistic clustering** : if we **know the source** of each instances then,

## 2. Probabilistic clustering

### Gaussian Mixture Model as a Latent variable model



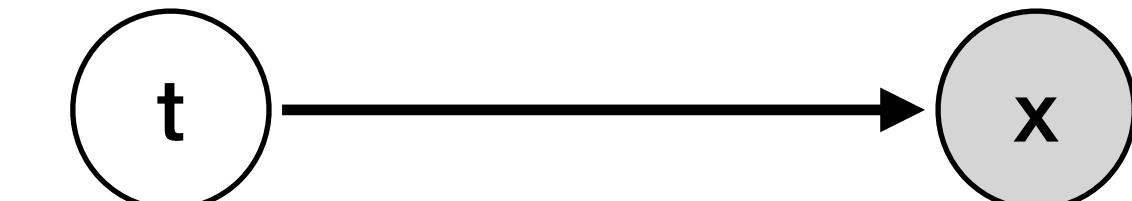
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**Hard clustering** : if we **know the source** of each instances then,

$$p(x | t = 2, \theta) = \mathcal{N}(x | \mu_{hard}^{MLE}, \Sigma_{hard}^{MLE})$$

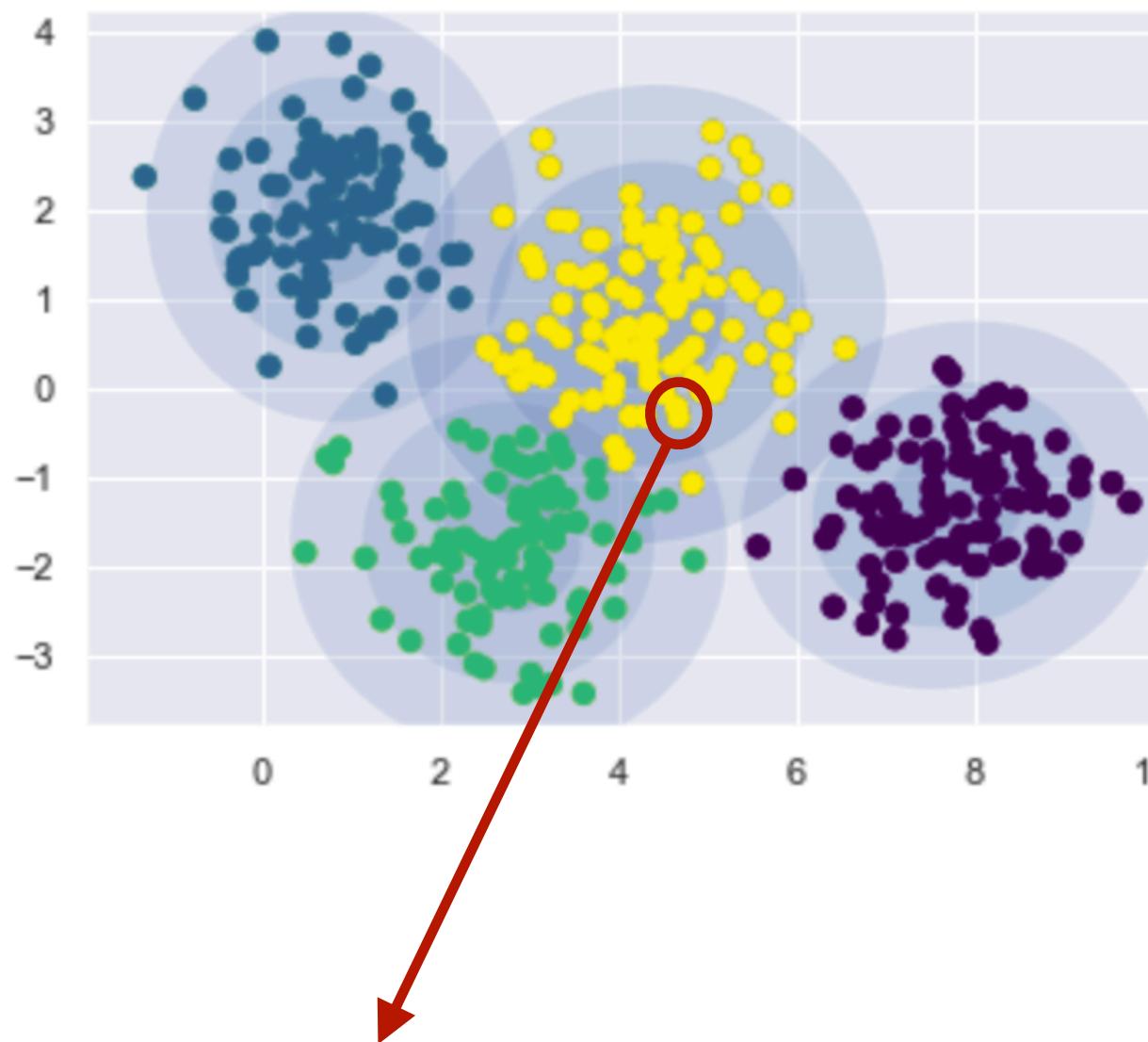
$$\mu_{hard}^{MLE} = \frac{\sum_{i \in \text{cluster 2}} x_i}{\text{Number of points in cluster 2}}$$

$$\Sigma_{hard}^{MLE} = \frac{\sum_{i \in \text{cluster 2}} (x_i - \mu_{hard}^{MLE}) \times (x_i - \mu_{hard}^{MLE})^T}{\text{Number of points in cluster 2}}$$

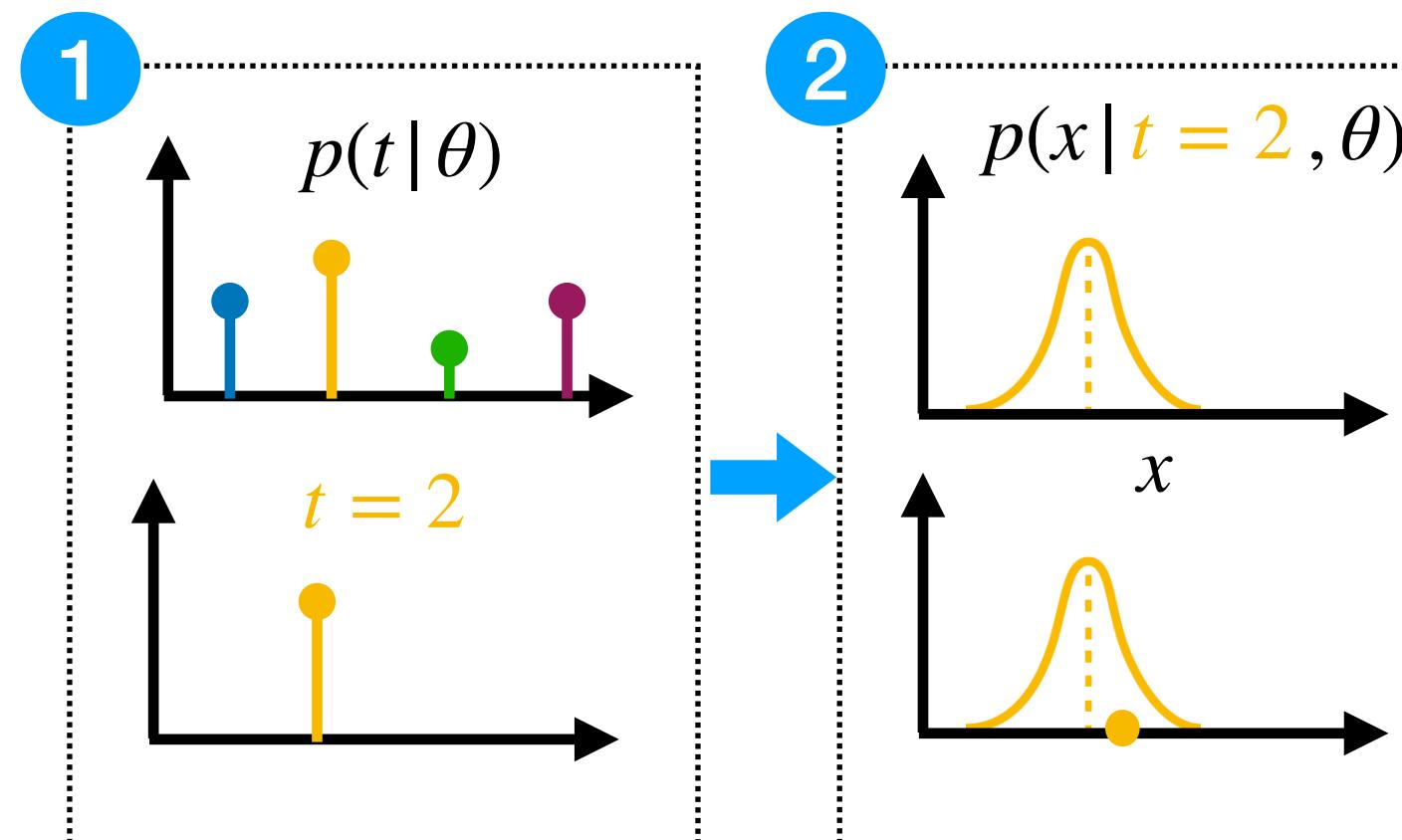
**Soft / probabilistic clustering** : if we **know the source** of each instances then,

## 2. Probabilistic clustering

### Gaussian Mixture Model as a Latent variable model



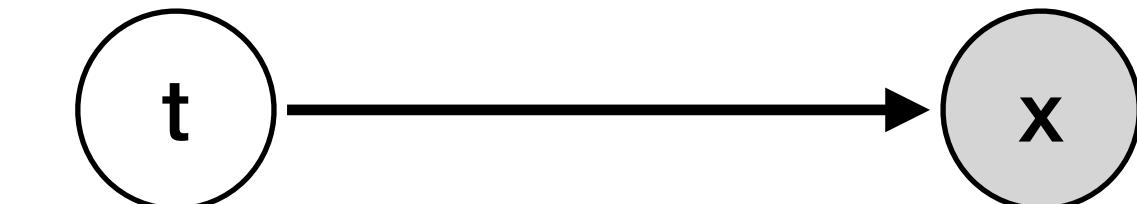
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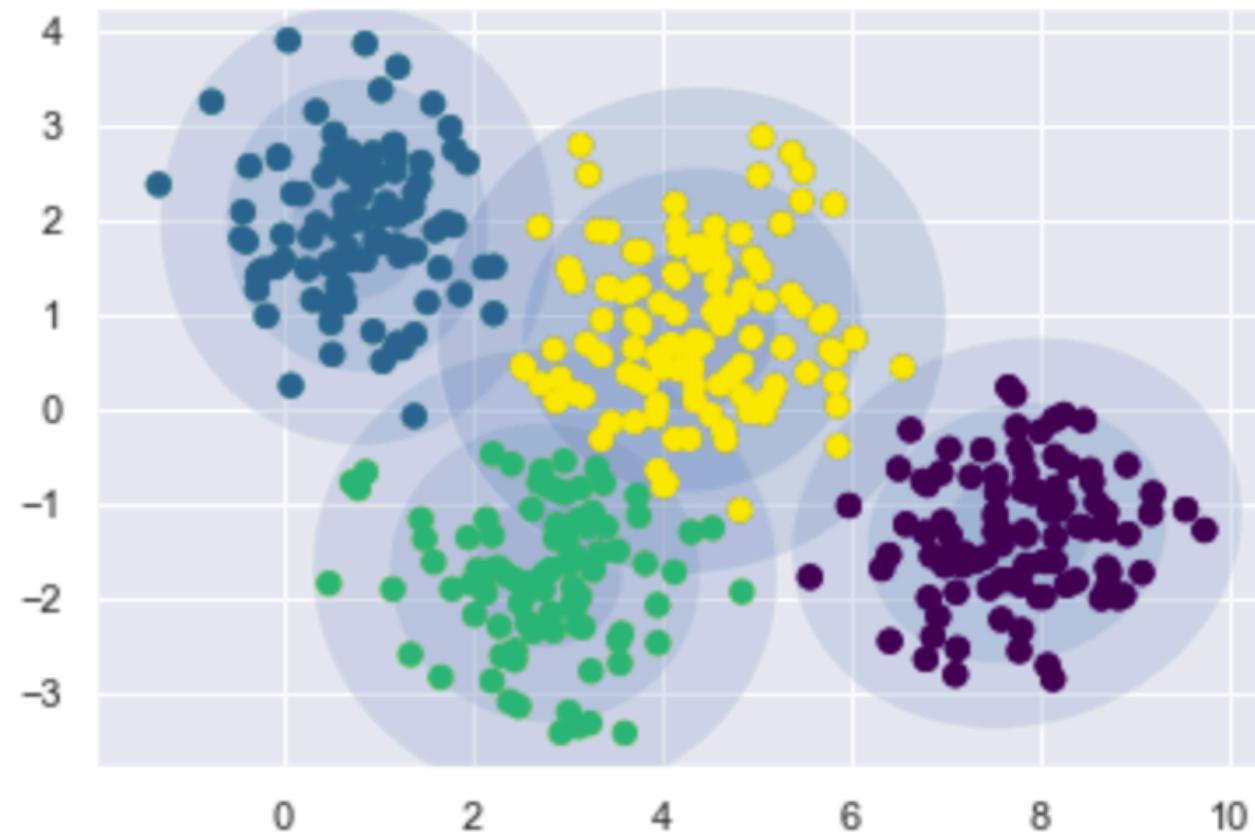
$$p(x | t = 2, \theta) = \mathcal{N}(x | \mu_{soft}^{MLE}, \Sigma_{soft}^{MLE})$$

$$\mu_{soft}^{MLE} = \frac{\sum_i p(t = 2 | x, \theta) x_i}{\sum_i p(t = 2 | x, \theta)}$$

$$\Sigma_{soft}^{MLE} = \frac{\sum_i p(t = 2 | x_i, \theta) (x_i - \mu_{soft}^{MLE}) \times (x_i - \mu_{soft}^{MLE})^T}{\sum_i p(t = 2 | x_i, \theta)}$$

## 2. Probabilistic clustering

### Gaussian Mixture Model : some intuitions for training this model [0/6]



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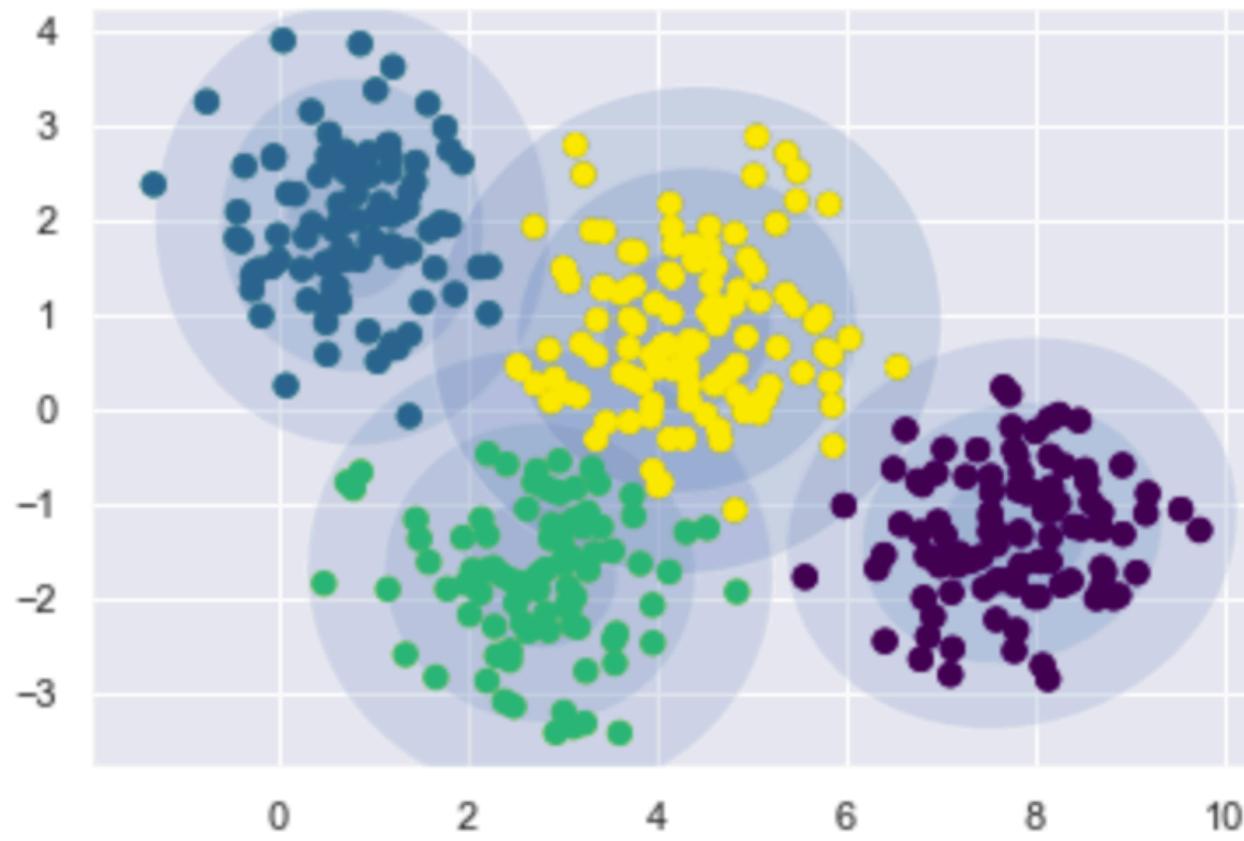
$$p(x | t = 2, \theta) = \mathcal{N}(x | \mu_{soft}^{MLE}, \Sigma_{soft}^{MLE})$$

$$\mu_{soft}^{MLE} = \frac{\sum_i p(t = 2 | x_i, \theta) x_i}{\sum_i p(t = 2 | x_i, \theta)}$$

$$\Sigma_{soft}^{MLE} = \frac{\sum_i p(t = 2 | x_i, \theta) (x_i - \mu_{soft}^{MLE}) \times (x_i - \mu_{soft}^{MLE})^T}{\sum_i p(t = 2 | x_i, \theta)}$$

## 2. Probabilistic clustering

### Gaussian Mixture Model : some intuitions for training this model [0/6]



**Soft / probabilistic clustering :** if we **know the source** of each instances then,

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**Remarks:** If we **know the parameters** of each instances then,

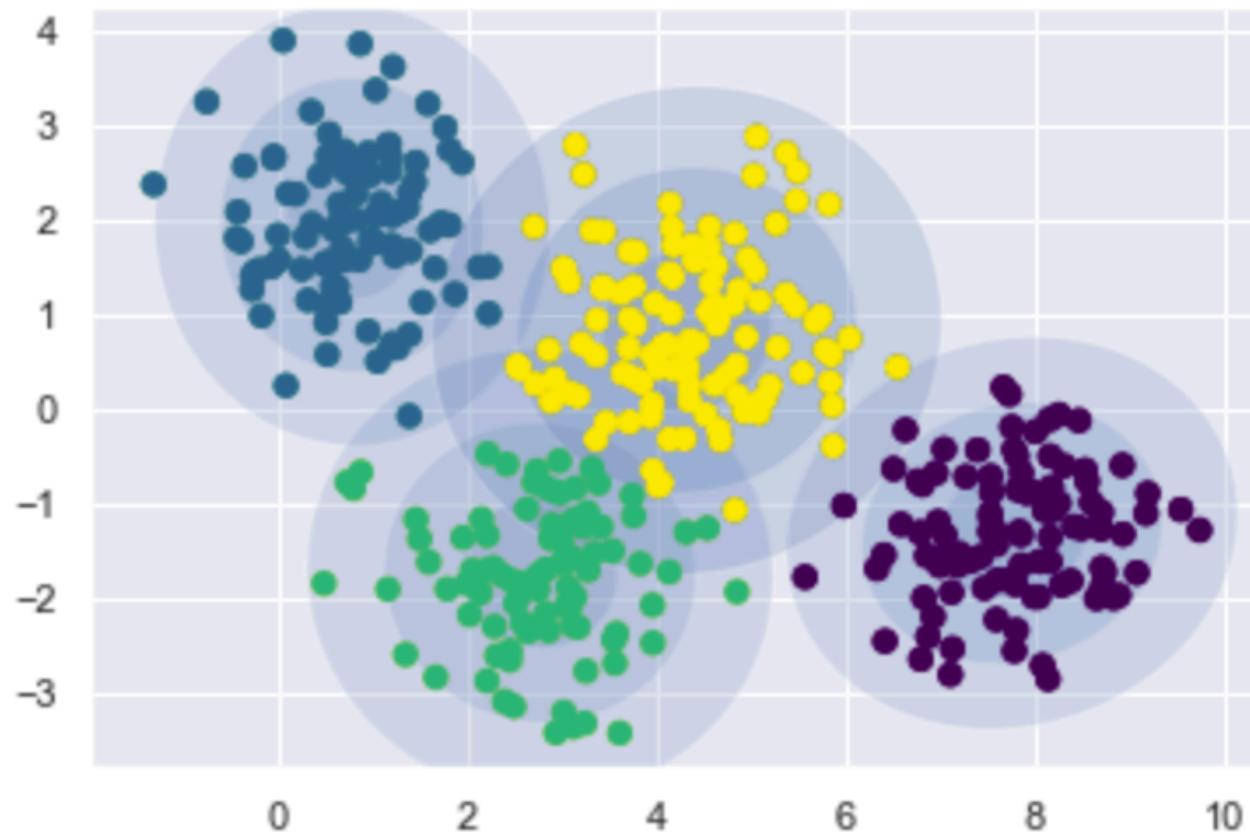
$$p(t = 2 | x, \theta) = \frac{p(x | t = 2, \theta) \times p(t = 2 | \theta)}{\text{Const}}$$

We are now in the following situation :

- **ESTIMATION:**  
If we **knew the parameters**, we could compute the posteriors
- **MAXIMIZATION:**  
If we **knew the posteriors/ sources**, we could easily compute the parameters

## 2. Probabilistic clustering

### Gaussian Mixture Model : some intuitions for training this model [0/6]



**Soft / probabilistic clustering :** if we **know the source** of each instances then,

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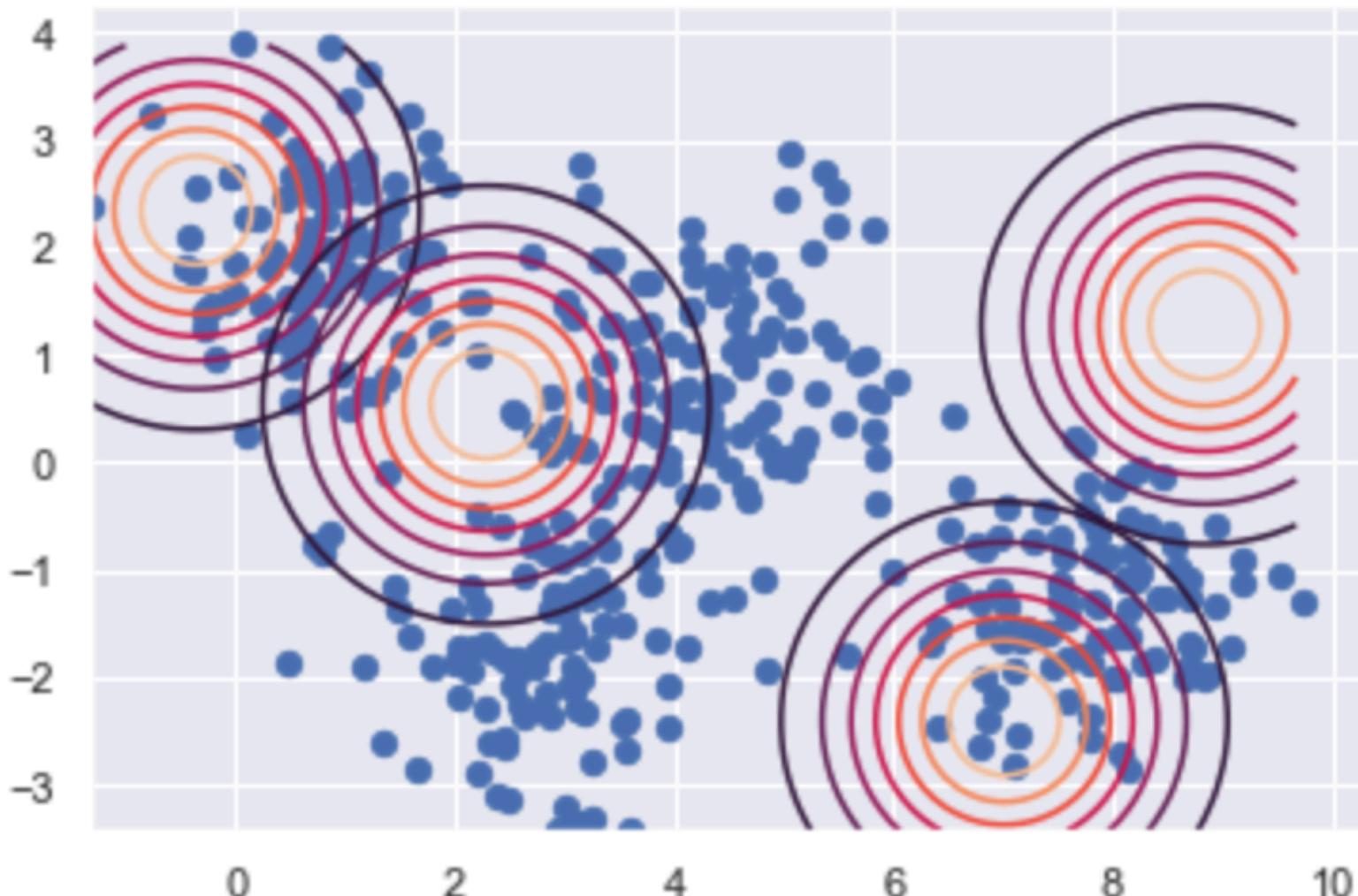
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**Remarks:** If we **know the parameters** of each instances then,

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**INITIALISATION : first estimation**

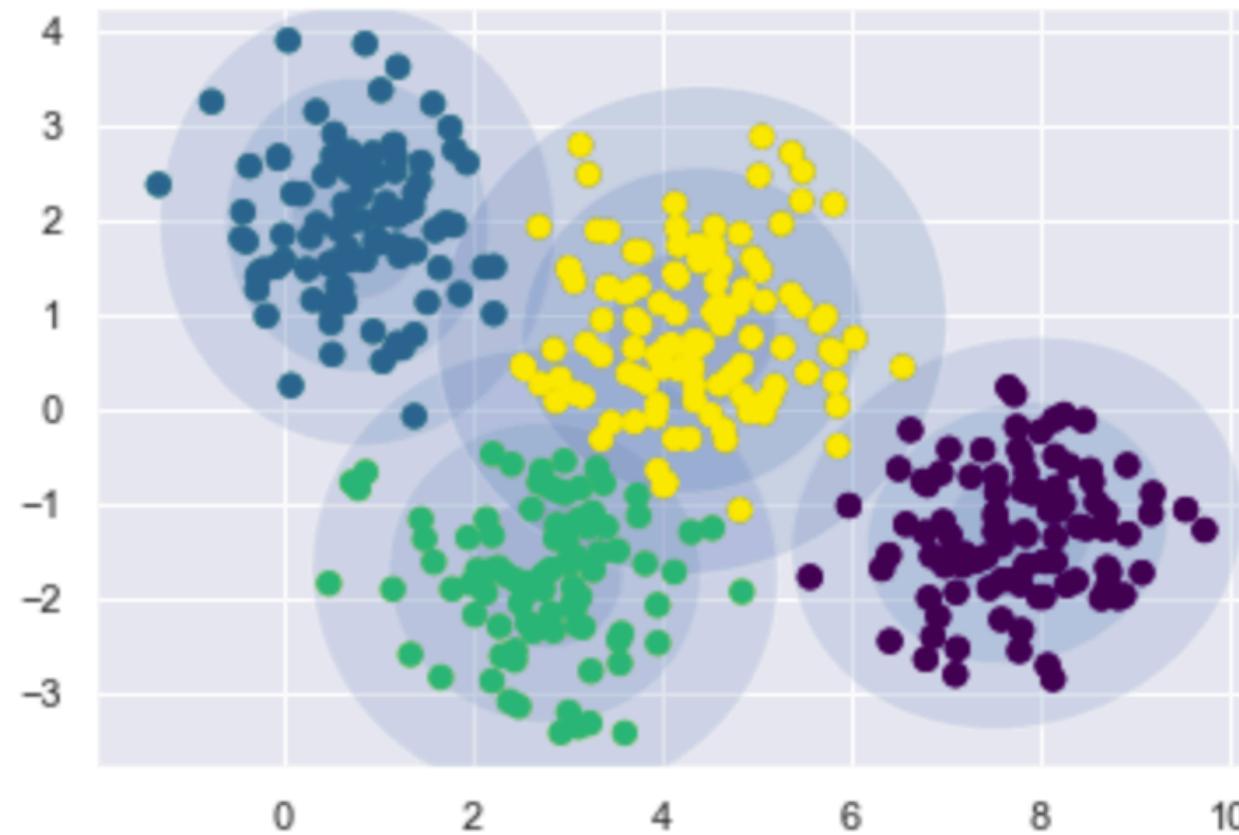


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## 2. Probabilistic clustering

### Gaussian Mixture Model : some intuitions for training this model [1/6]



**Soft / probabilistic clustering :** if we **know the source** of each instances then,

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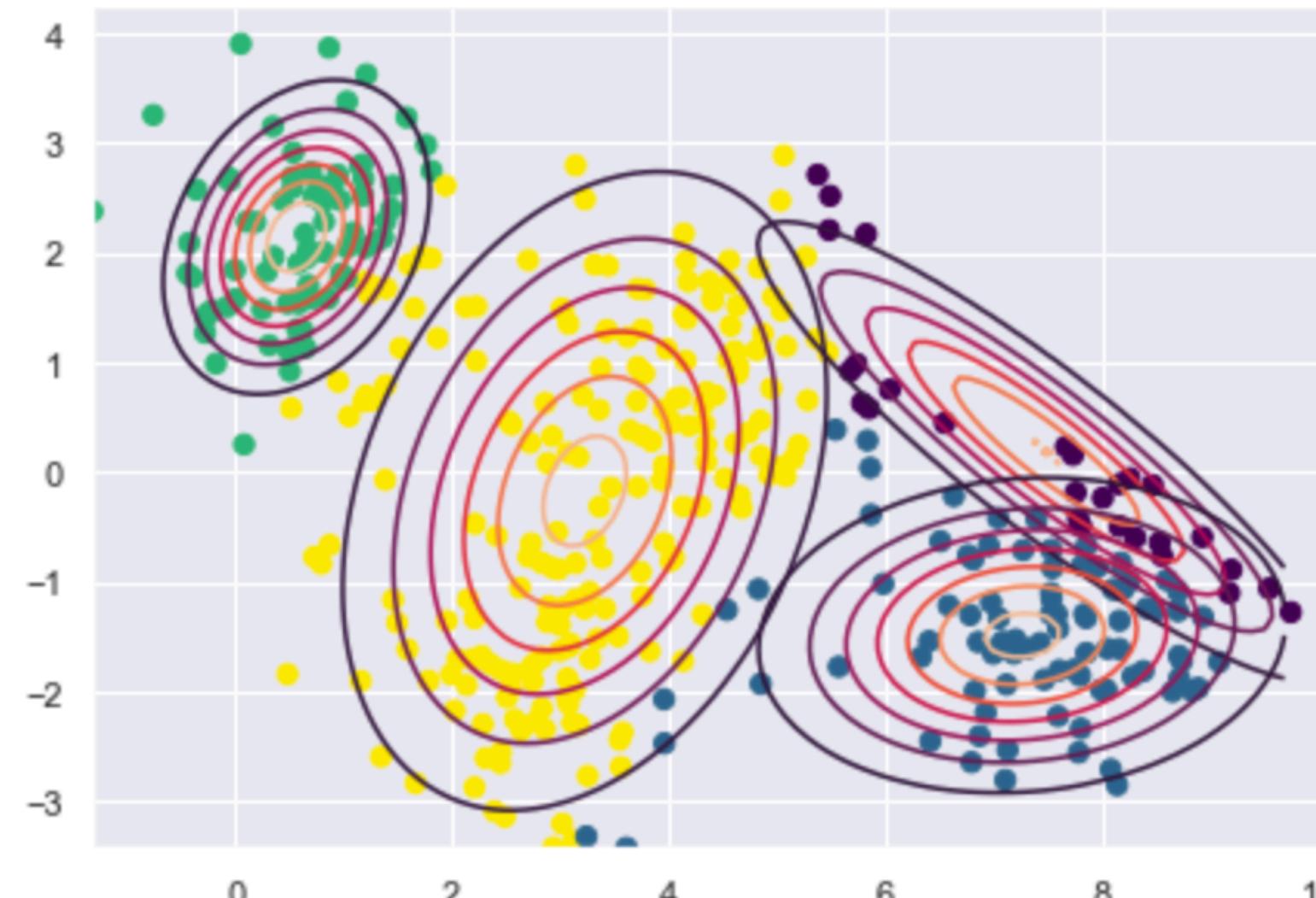
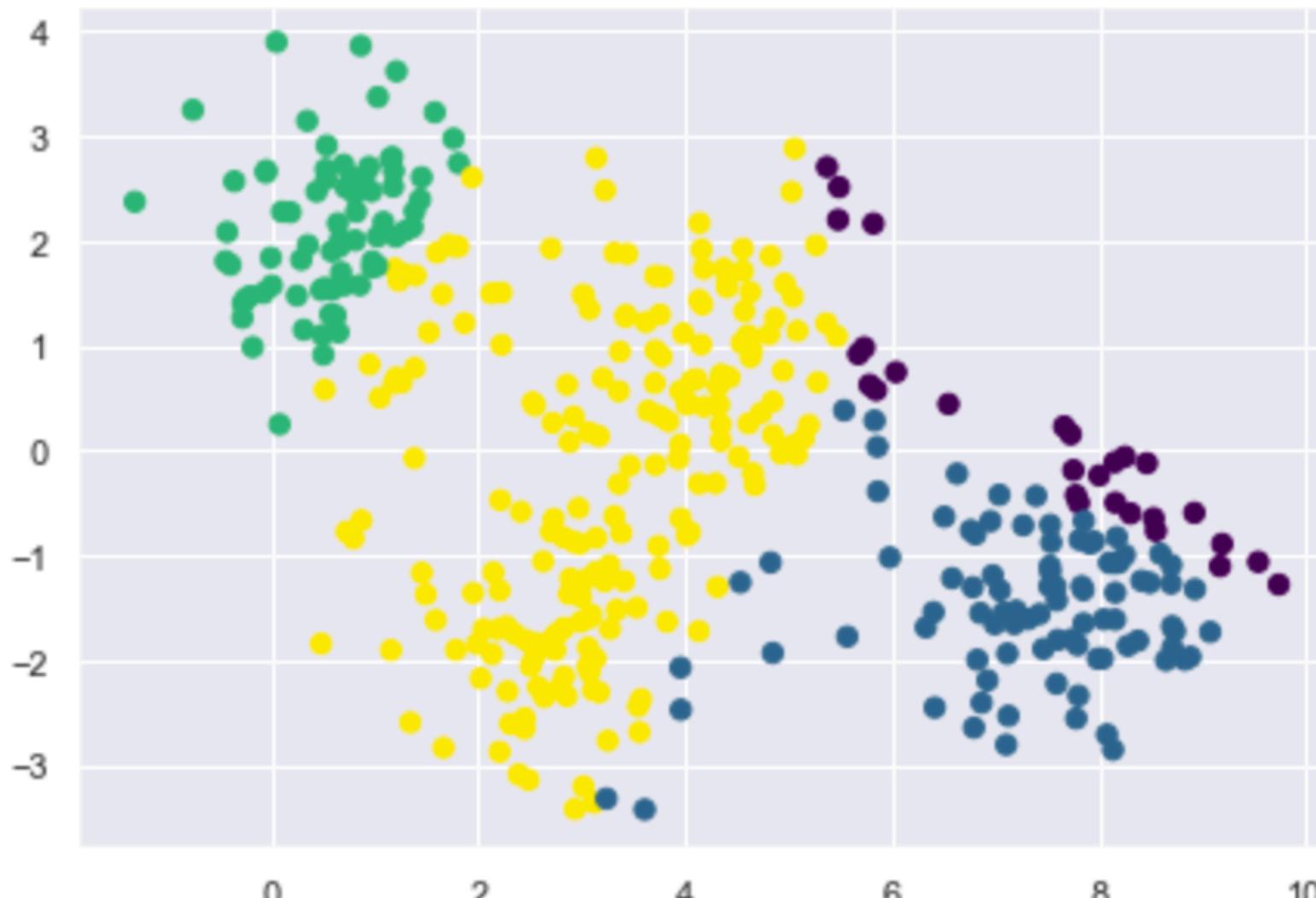
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#### STEP 1

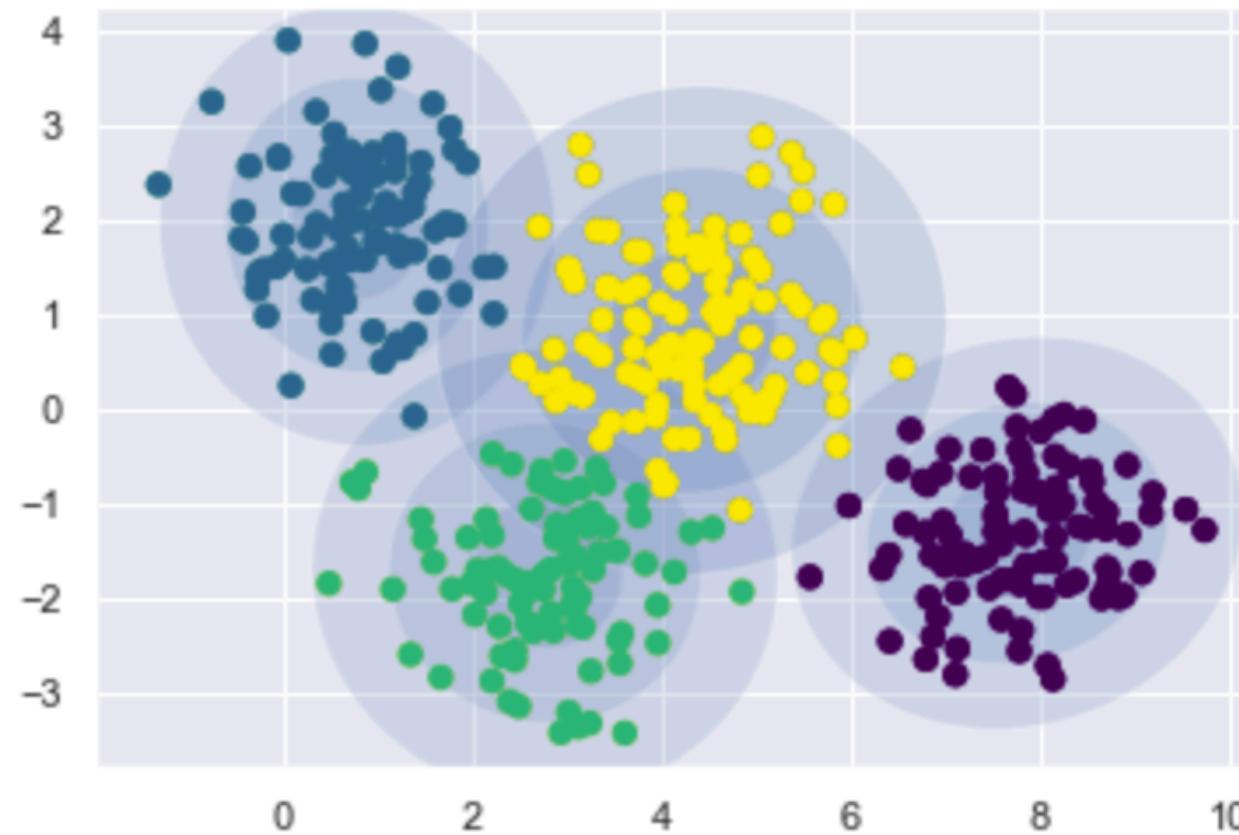


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## 2. Probabilistic clustering

### Gaussian Mixture Model : some intuitions for training this model [2/6]



**Soft / probabilistic clustering :** if we **know the source** of each instances then,

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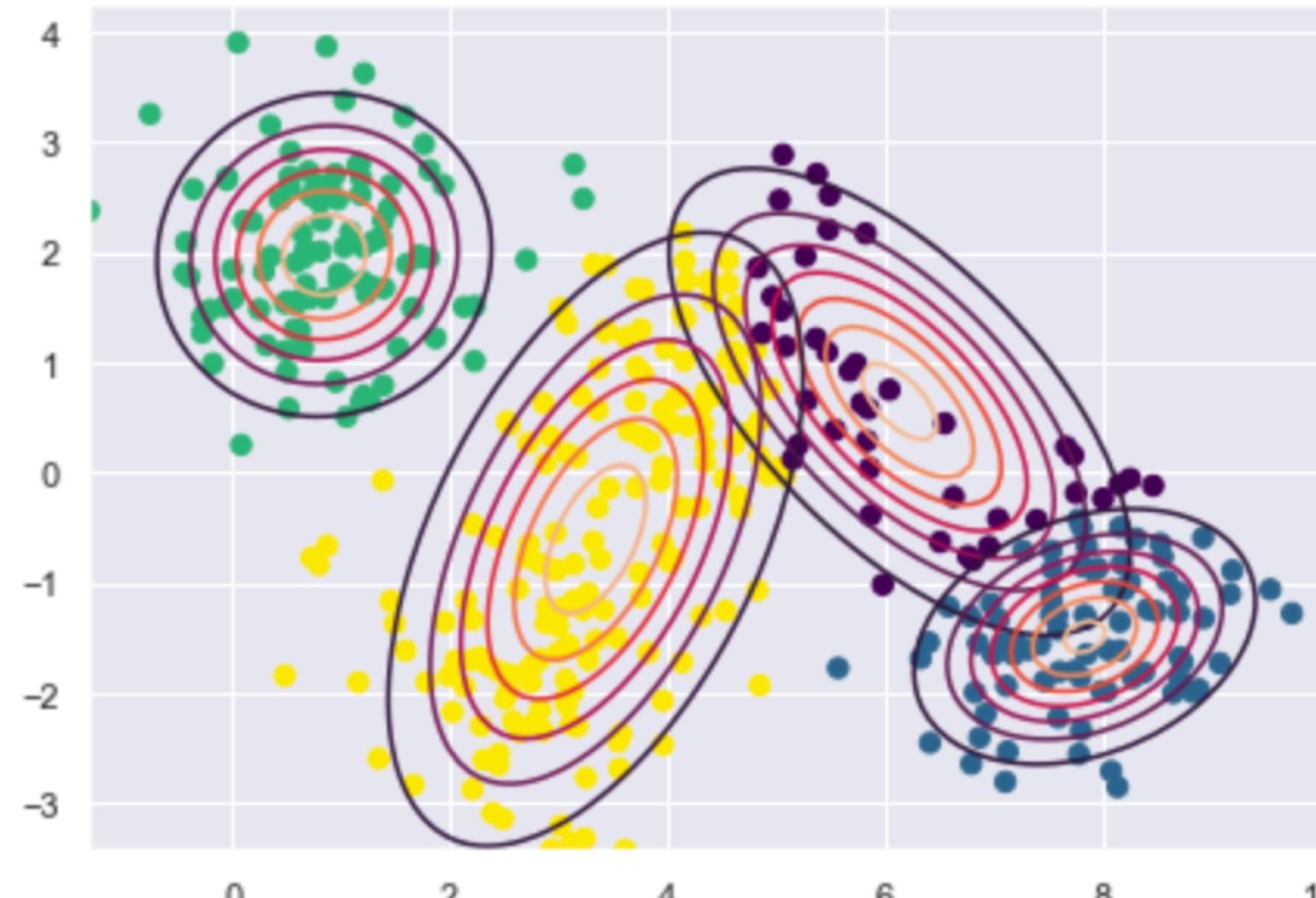
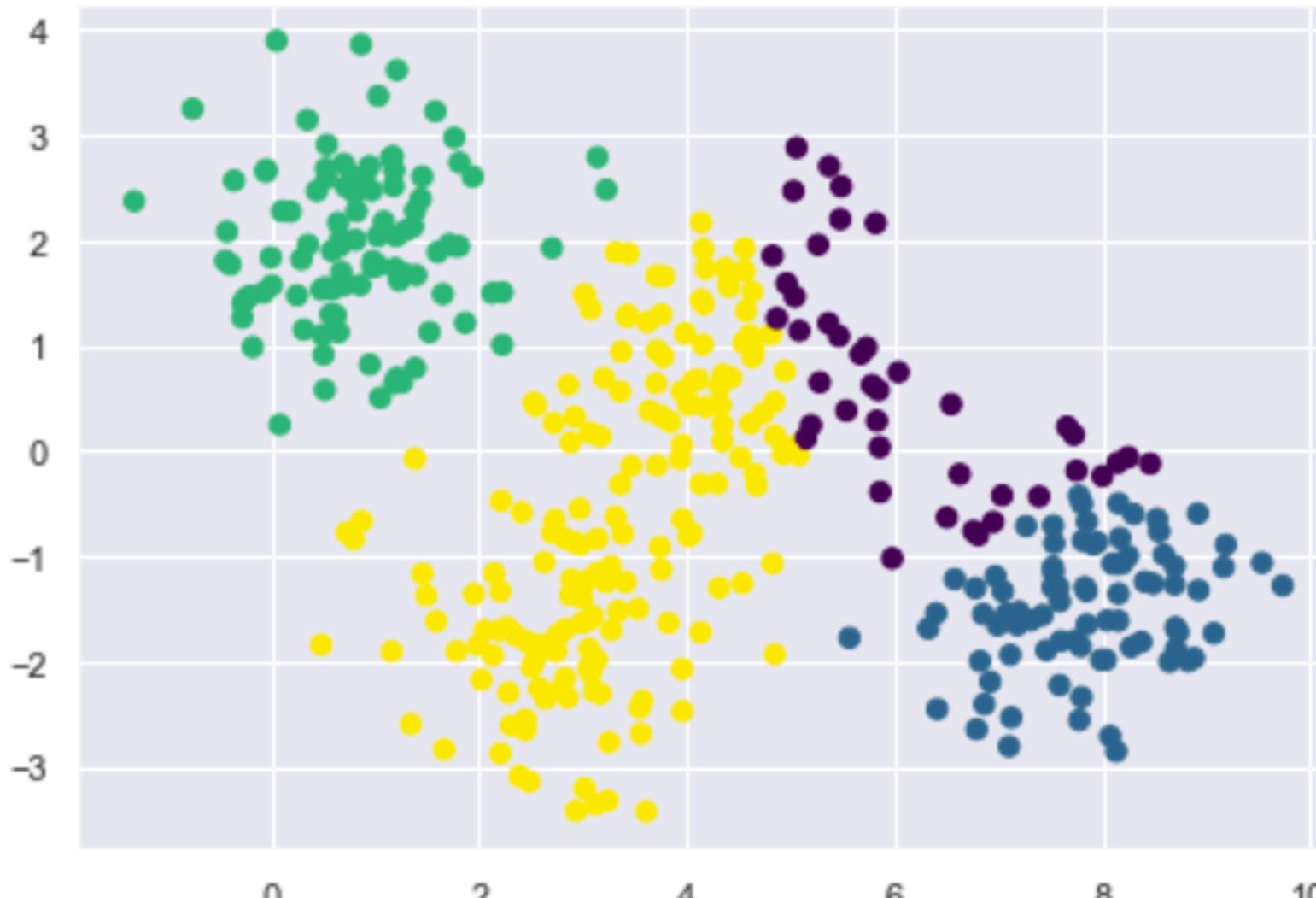
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**Remarks:** If we **know the parameters** of each instances then,

$$p(t = 2 | x, \theta) = \frac{p(x | t = 2, \theta) \times p(t = 2 | \theta)}{\text{Const}}$$

### STEP 2

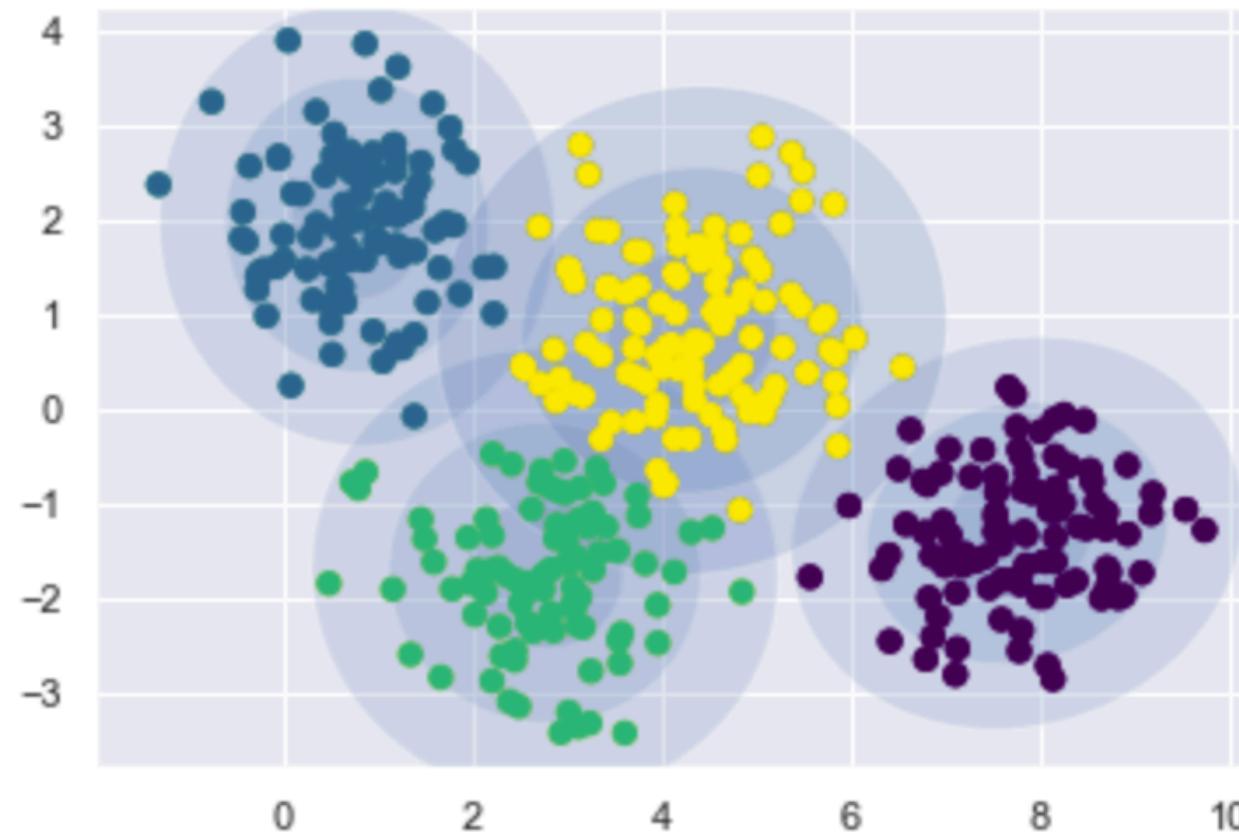


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## 2. Probabilistic clustering

### Gaussian Mixture Model : some intuitions for training this model [3/6]



**Soft / probabilistic clustering :** if we **know the source** of each instances then,

$$p(x | t = 2, \theta) = \mathcal{N}(x | \mu_{soft}^{MLE}, \Sigma_{soft}^{MLE})$$

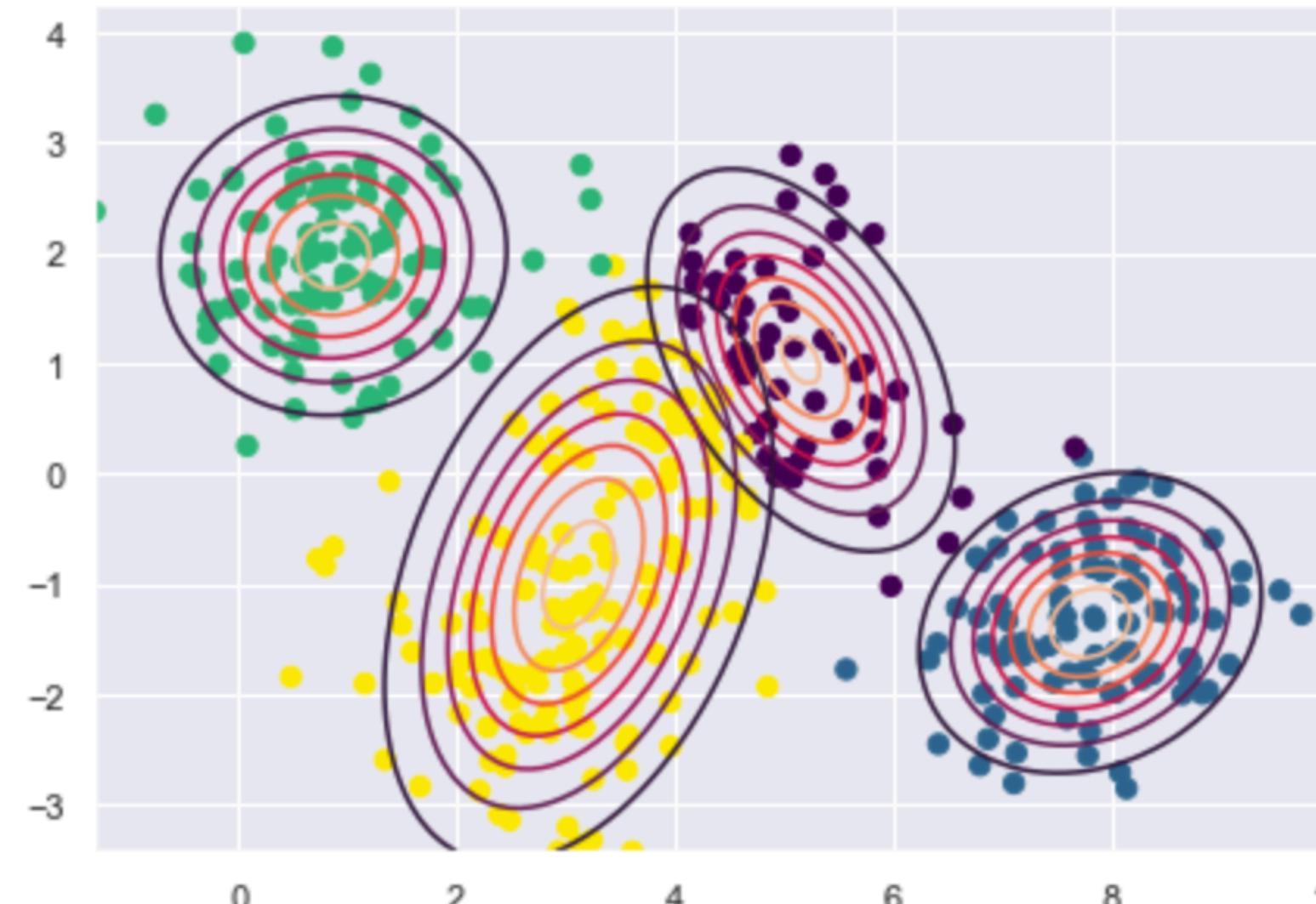
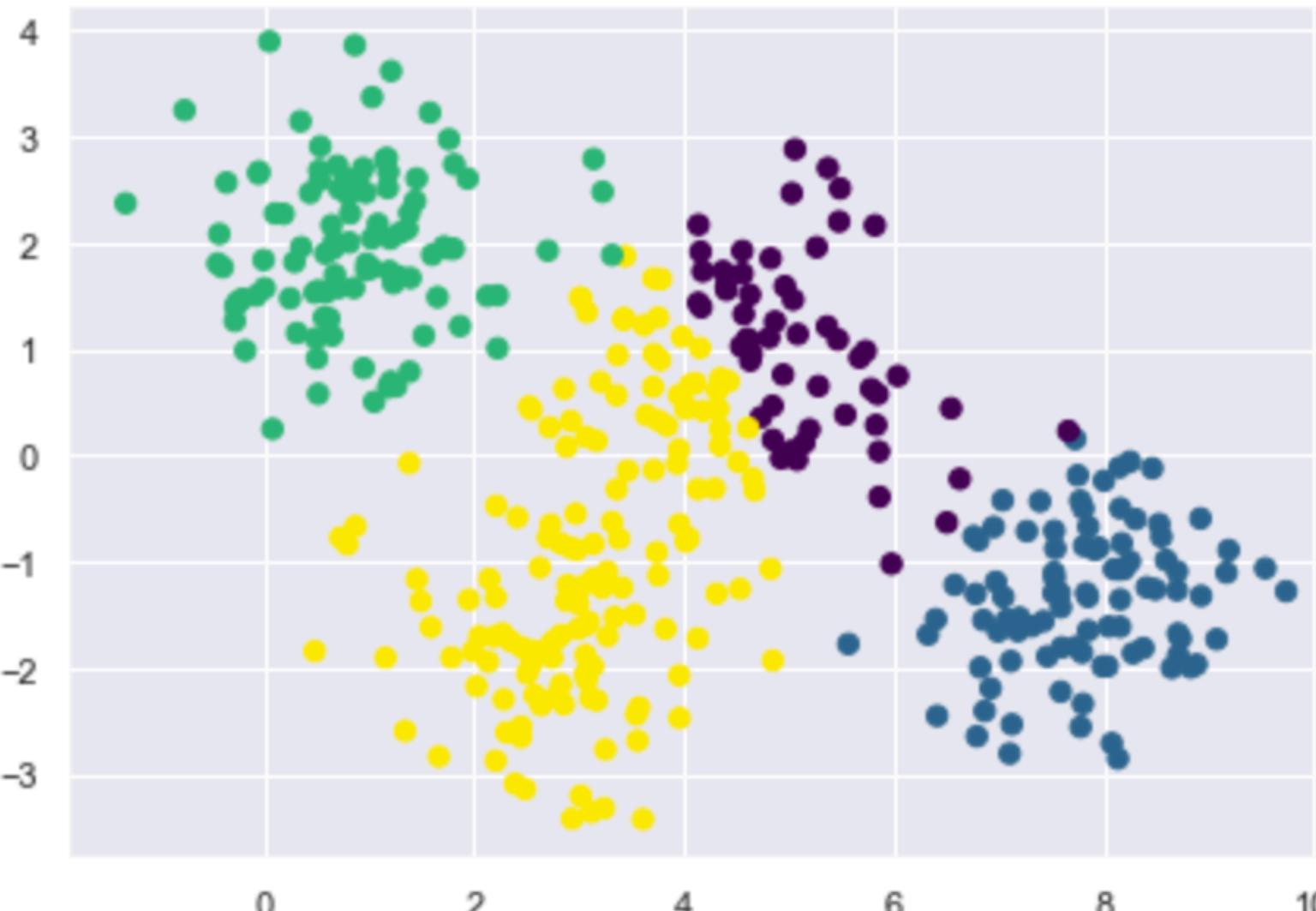
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**Remarks:** If we **know the parameters** of each instances then,

$$p(t = 2 | x, \theta) = \frac{p(x | t = 2, \theta) \times p(t = 2 | \theta)}{\text{Const}}$$

### STEP 3

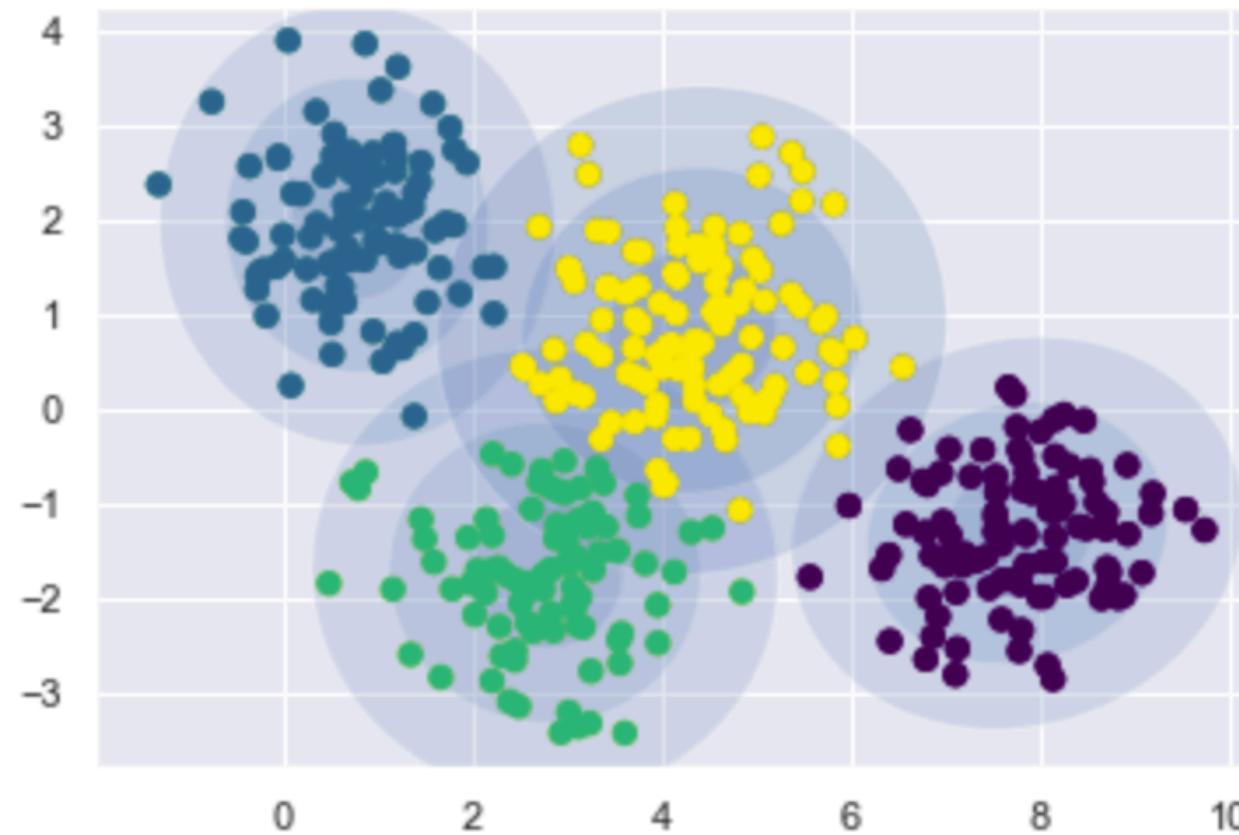


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## 2. Probabilistic clustering

### Gaussian Mixture Model : some intuitions for training this model [4/6]



**Soft / probabilistic clustering :** if we **know the source** of each instances then,

$$p(x | t = 2, \theta) = \mathcal{N}(x | \mu_{soft}^{MLE}, \Sigma_{soft}^{MLE})$$

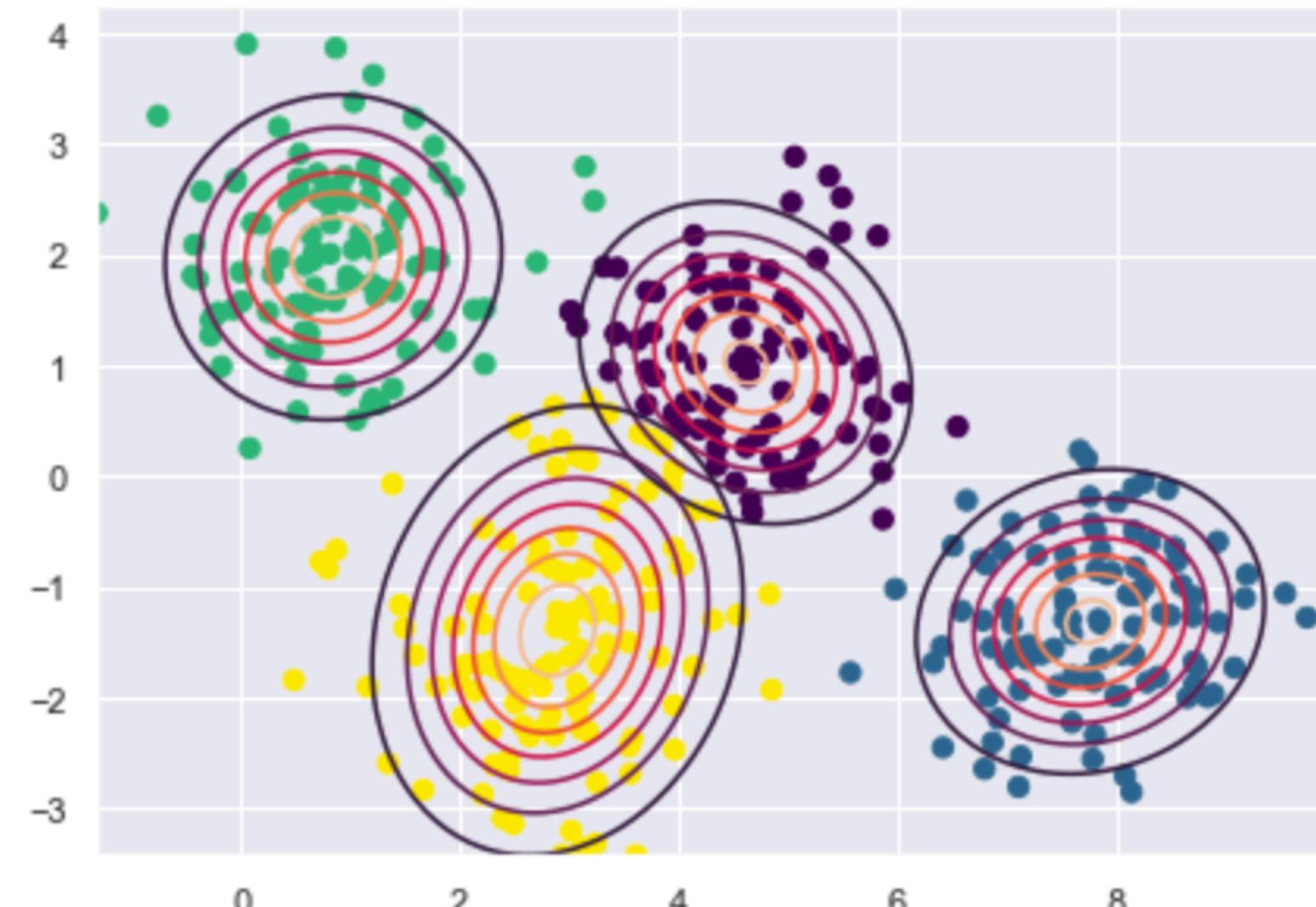
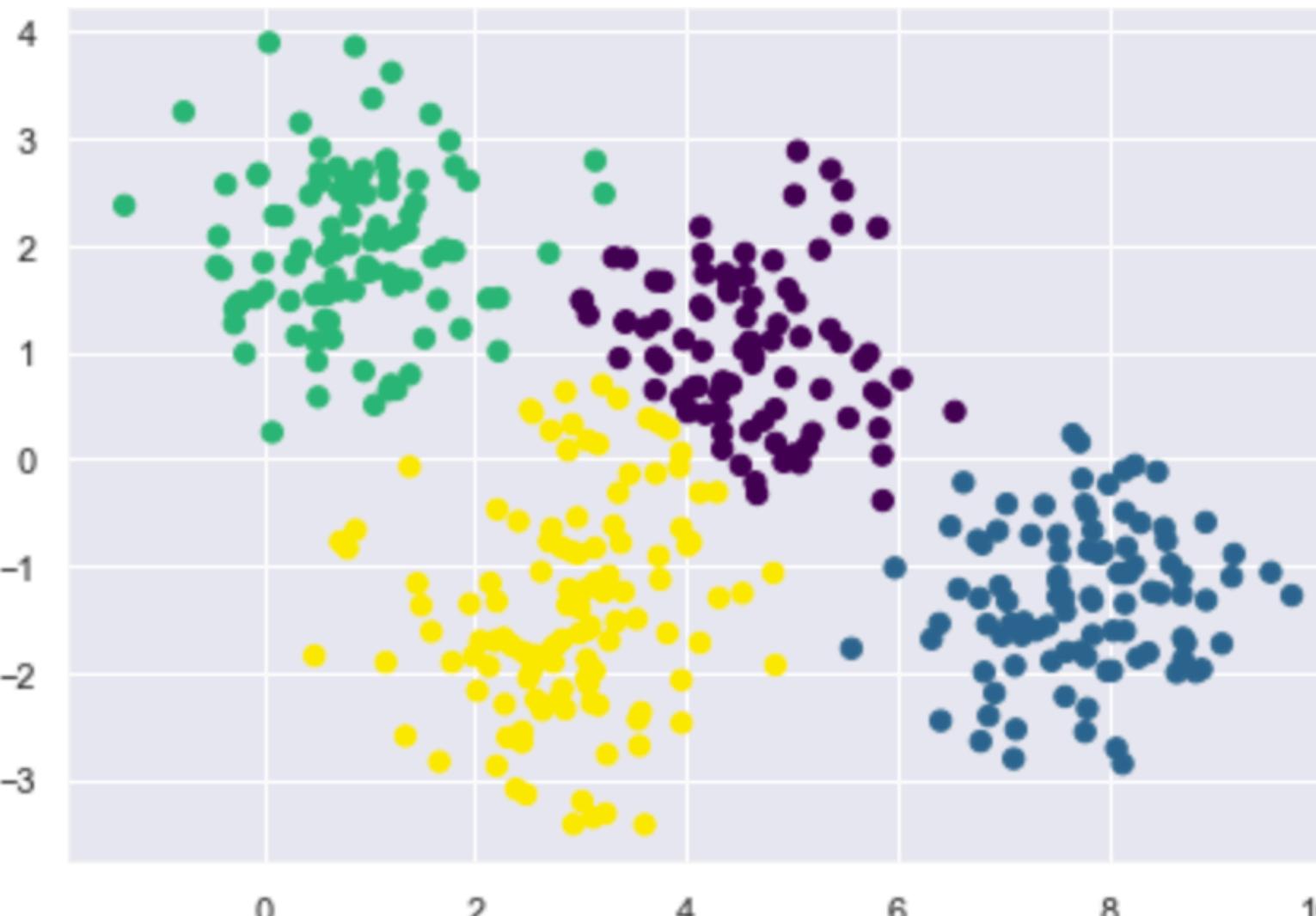
$$\mu_{soft}^{MLE} = \frac{\sum_i p(t = 2 | x, \theta) x_i}{\sum_i p(t = 2 | x, \theta)}$$

$$\Sigma_{soft}^{MLE} = \frac{\sum_i p(t = 2 | x_i, \theta) (x_i - \mu_{soft}^{MLE}) \times (x_i - \mu_{soft}^{MLE})^T}{\sum_i p(t = 2 | x_i, \theta)}$$

**Remarks:** If we **know the parameters** of each instances then,

$$p(t = 2 | x, \theta) = \frac{p(x | t = 2, \theta) \times p(t = 2 | \theta)}{\text{Const}}$$

#### STEP 4

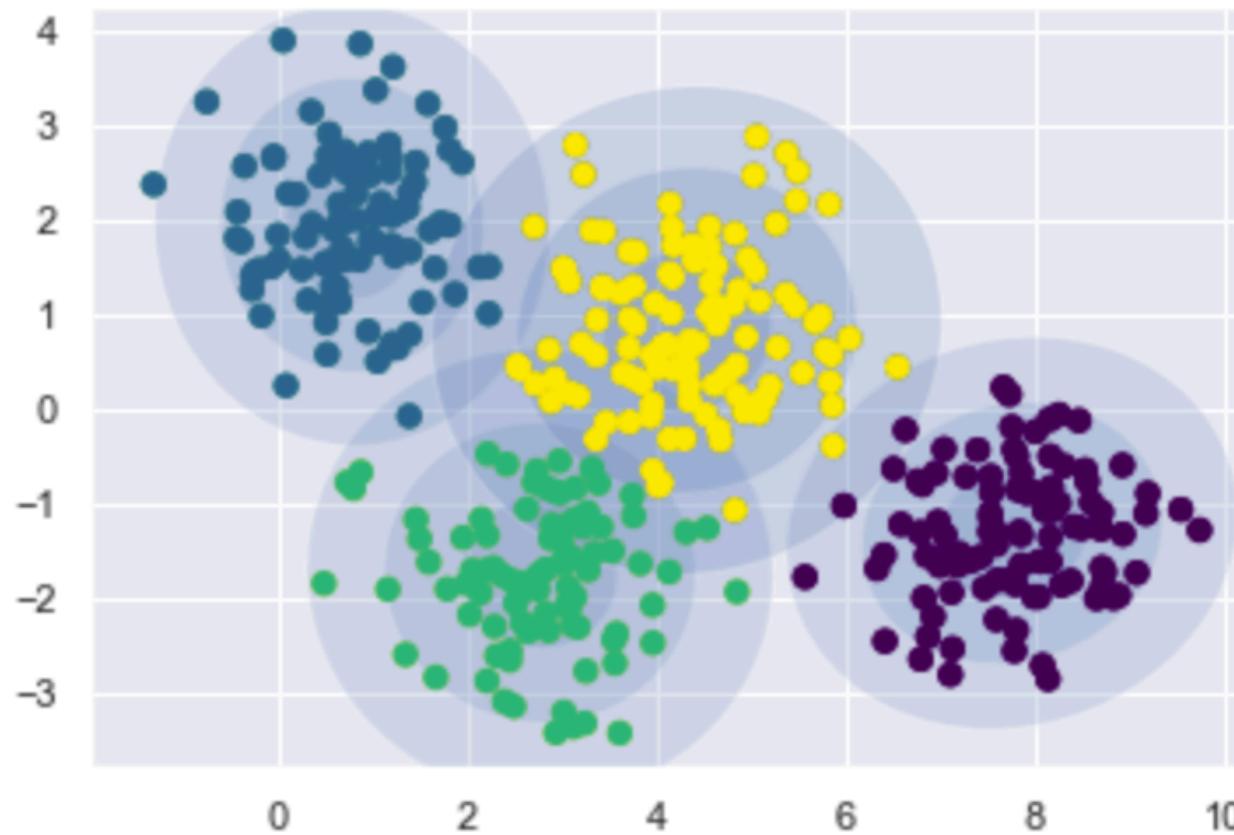


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## 2. Probabilistic clustering

### Gaussian Mixture Model : some intuitions for training this model [5/6]



**Soft / probabilistic clustering :** if we **know the source** of each instances then,

$$p(x | t = 2, \theta) = \mathcal{N}(x | \mu_{soft}^{MLE}, \Sigma_{soft}^{MLE})$$

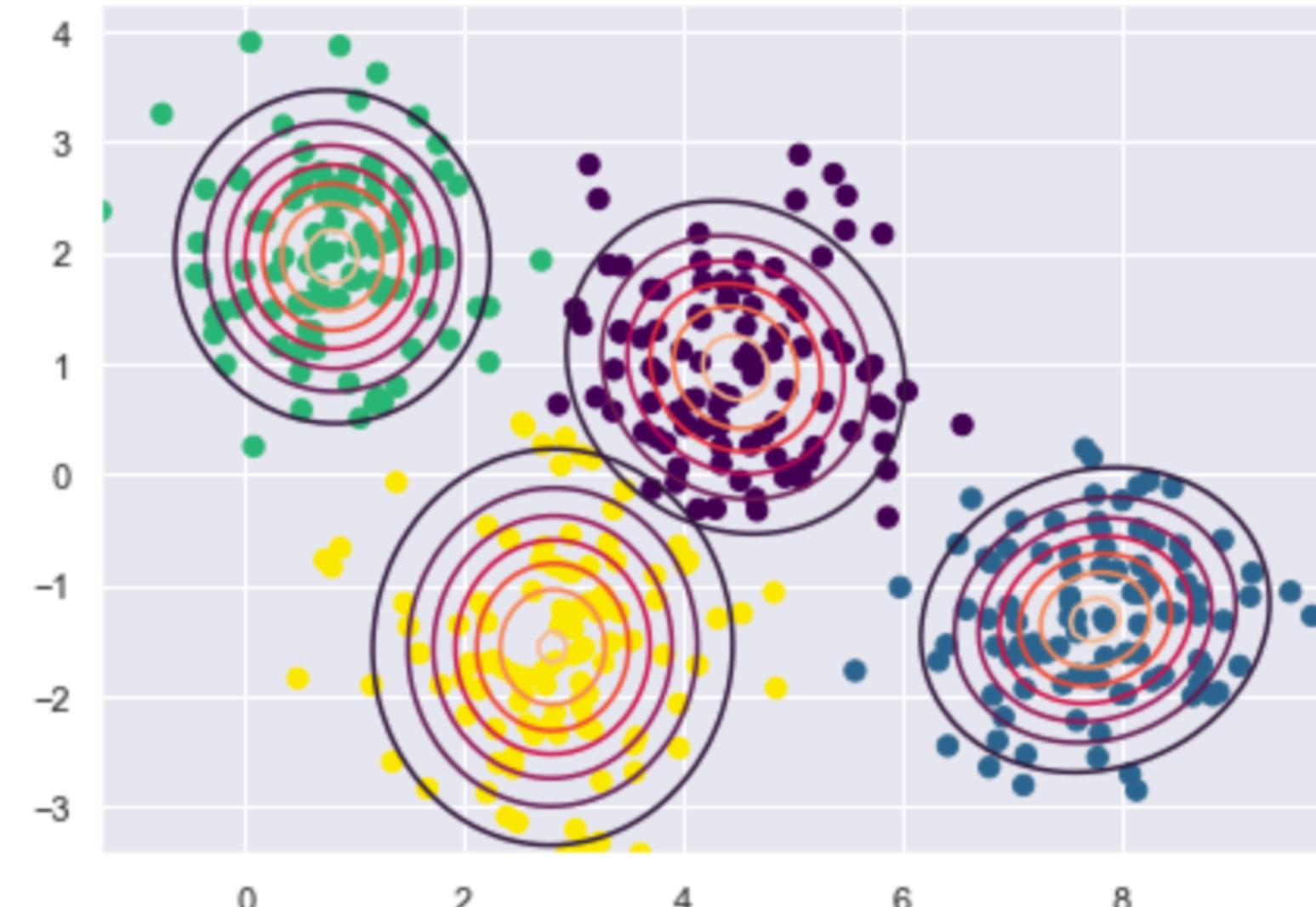
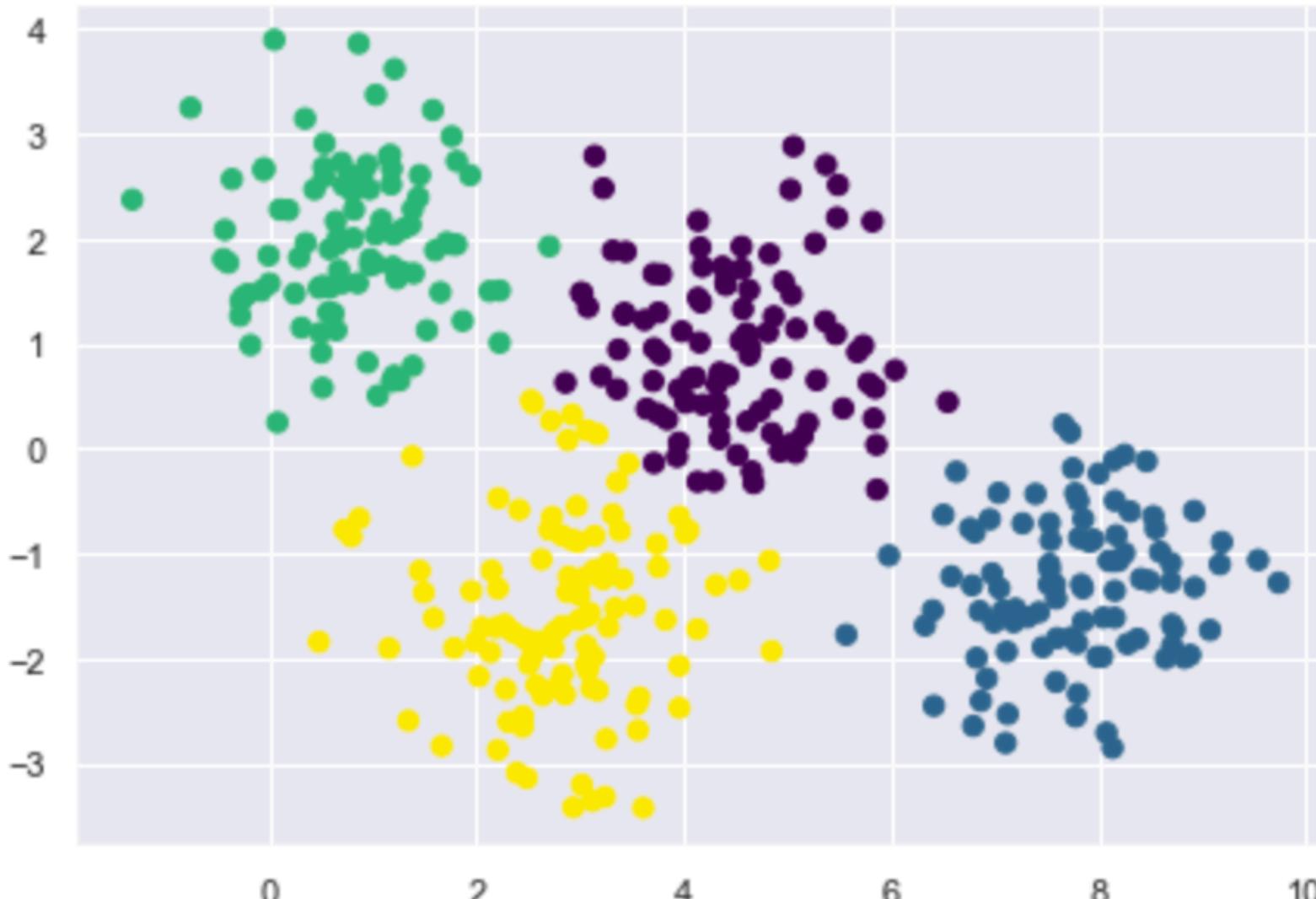
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**Remarks:** If we **know the parameters** of each instances then,

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### STEP 5

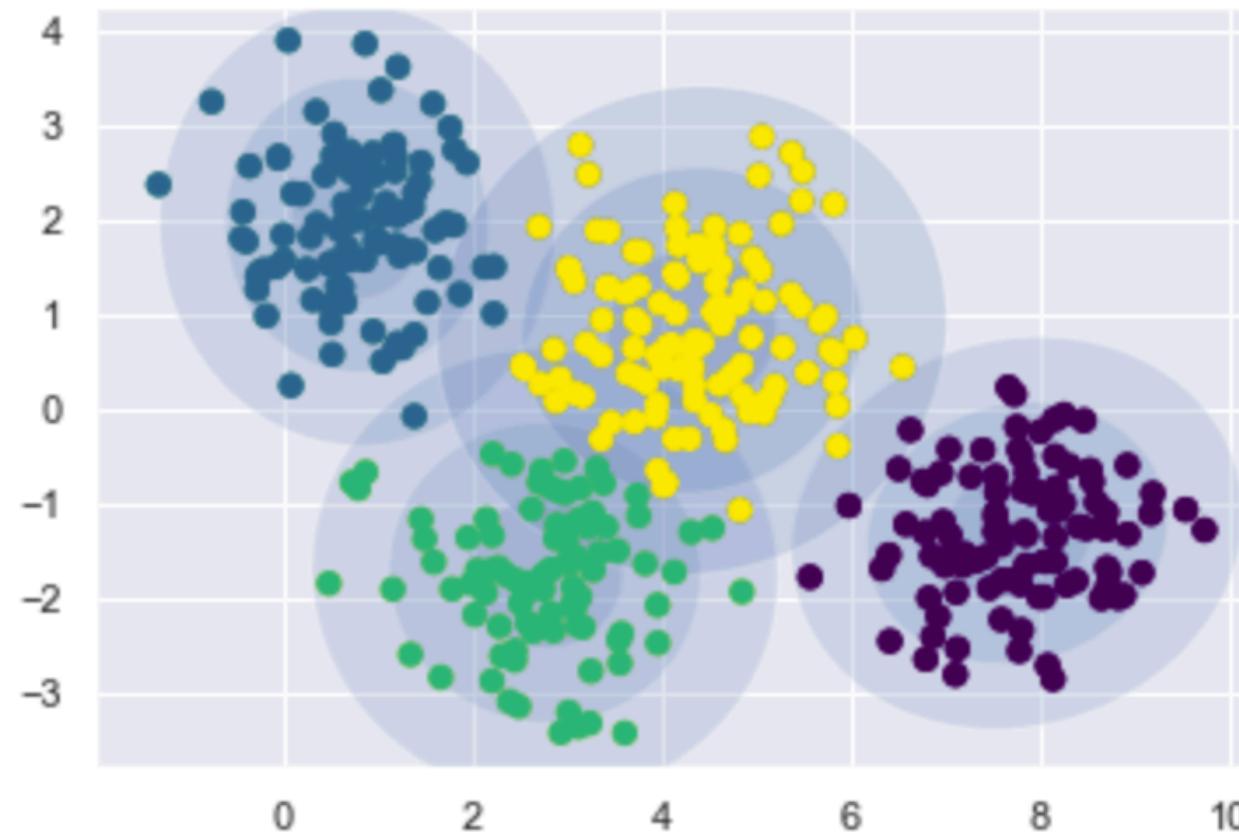


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## 2. Probabilistic clustering

### Gaussian Mixture Model : some intuitions for training this model [6/6]



**Soft / probabilistic clustering :** if we **know the source** of each instances then,

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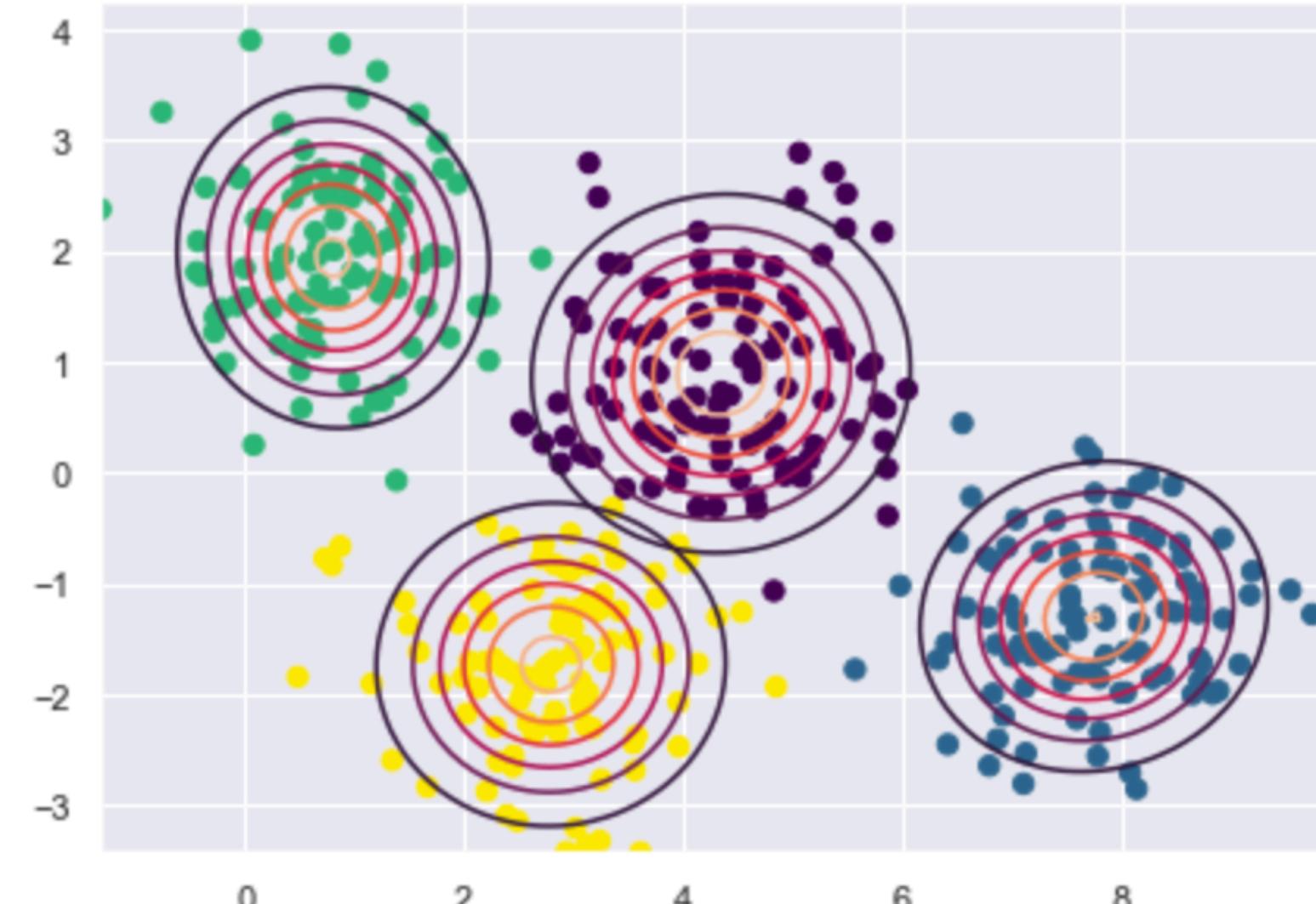
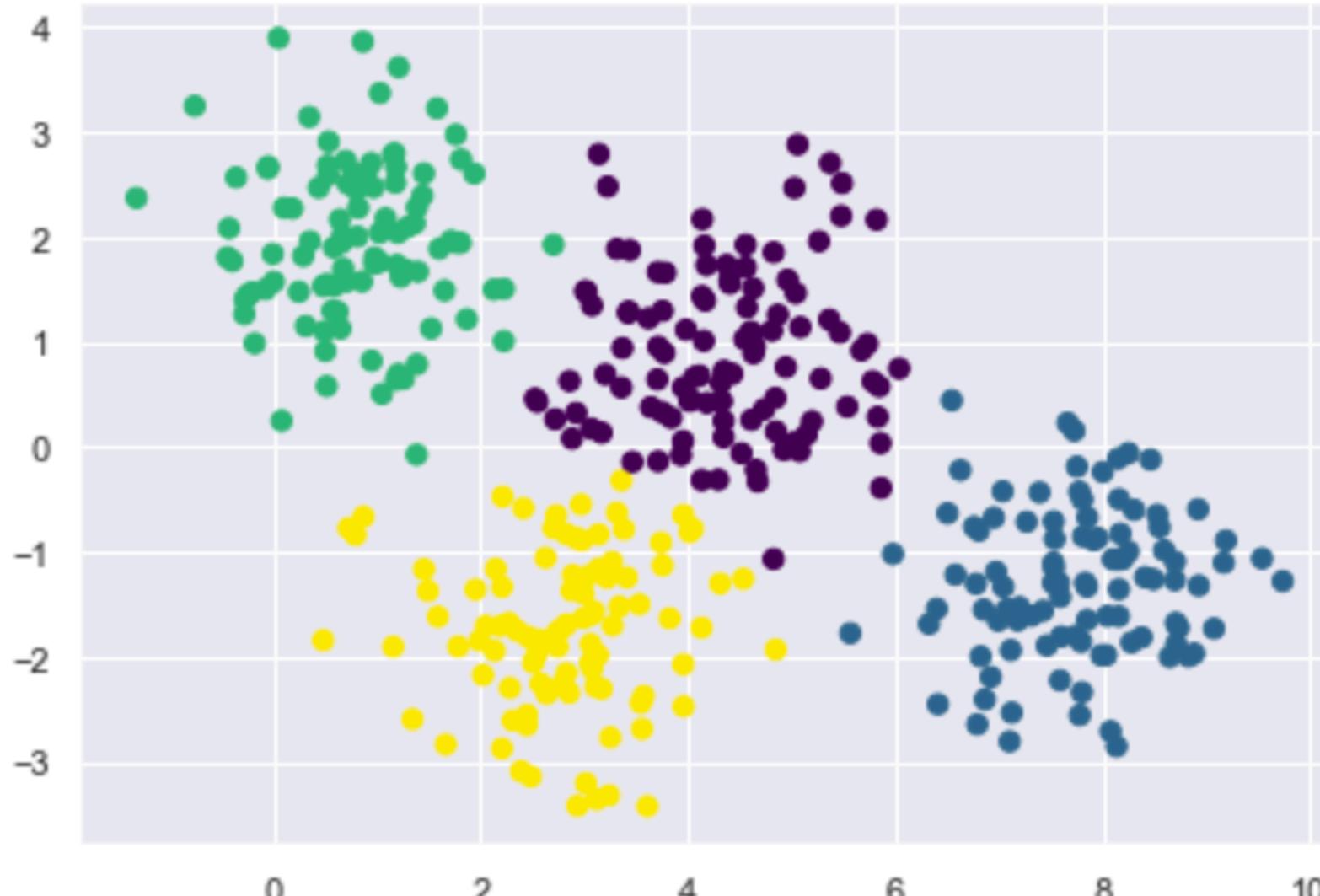
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**Remarks:** If we **know the parameters** of each instances then,

$$p(t = 2 | x, \theta) = \frac{p(x | t = 2, \theta) \times p(t = 2 | \theta)}{\text{Const}}$$

#### STEP 6

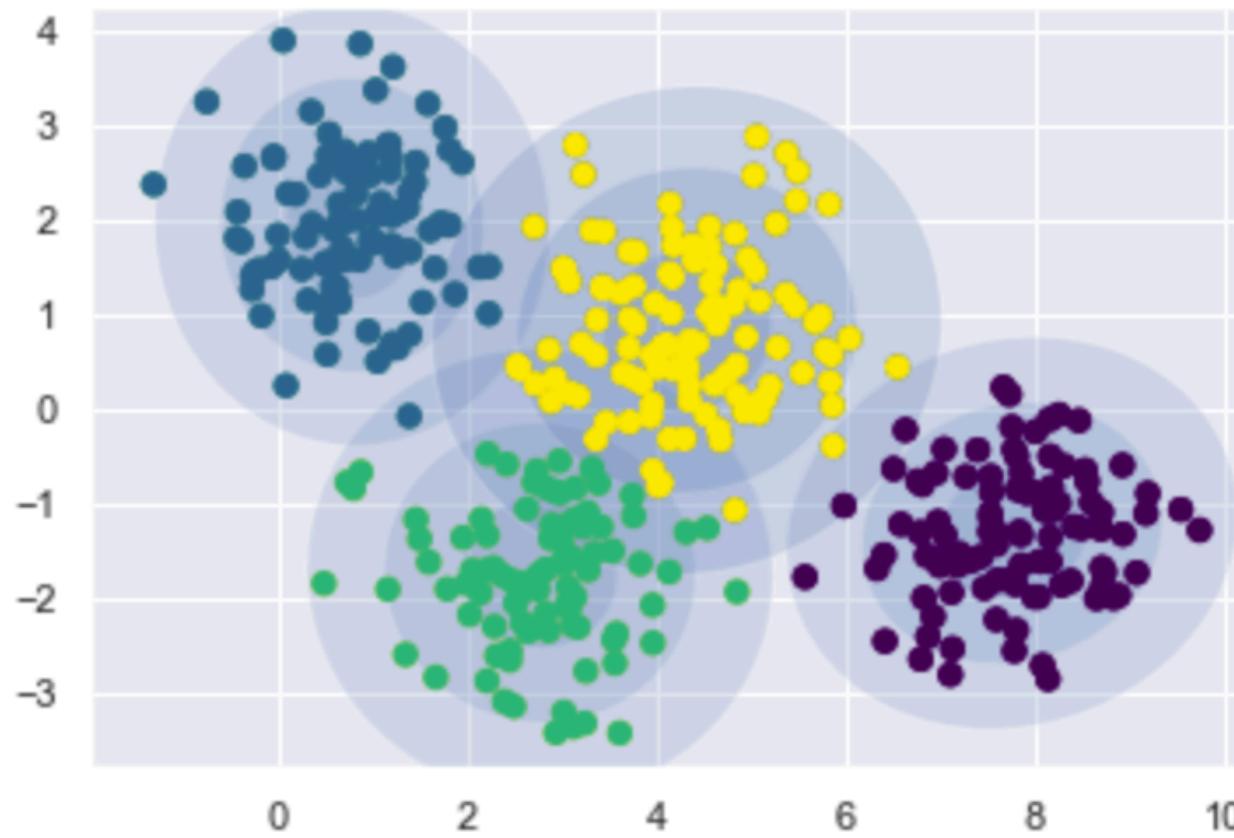


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## 2. Probabilistic clustering

### Gaussian Mixture Model : some intuitions for training this model [6/6]



**Soft / probabilistic clustering :** if we **know the source** of each instances then,

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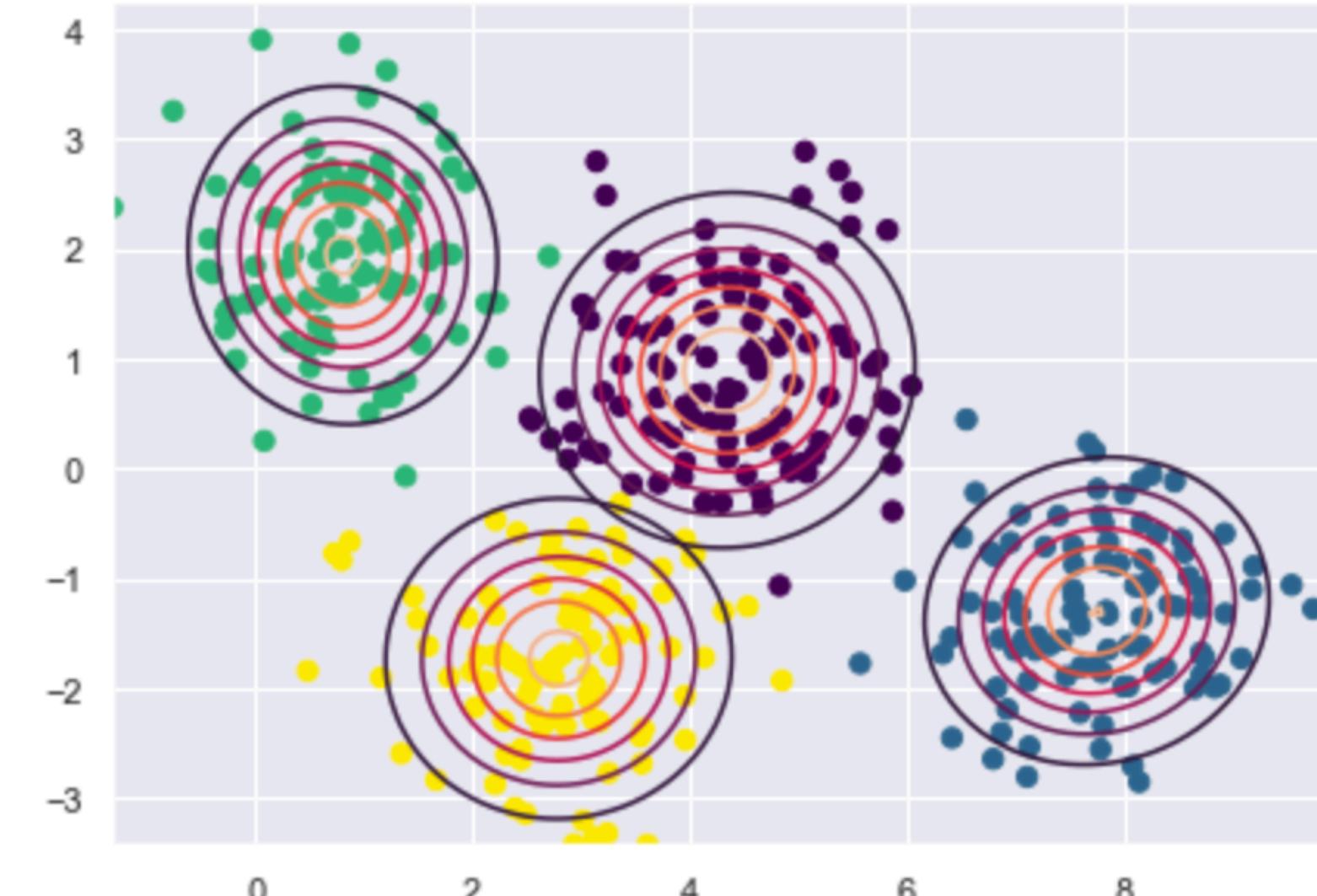
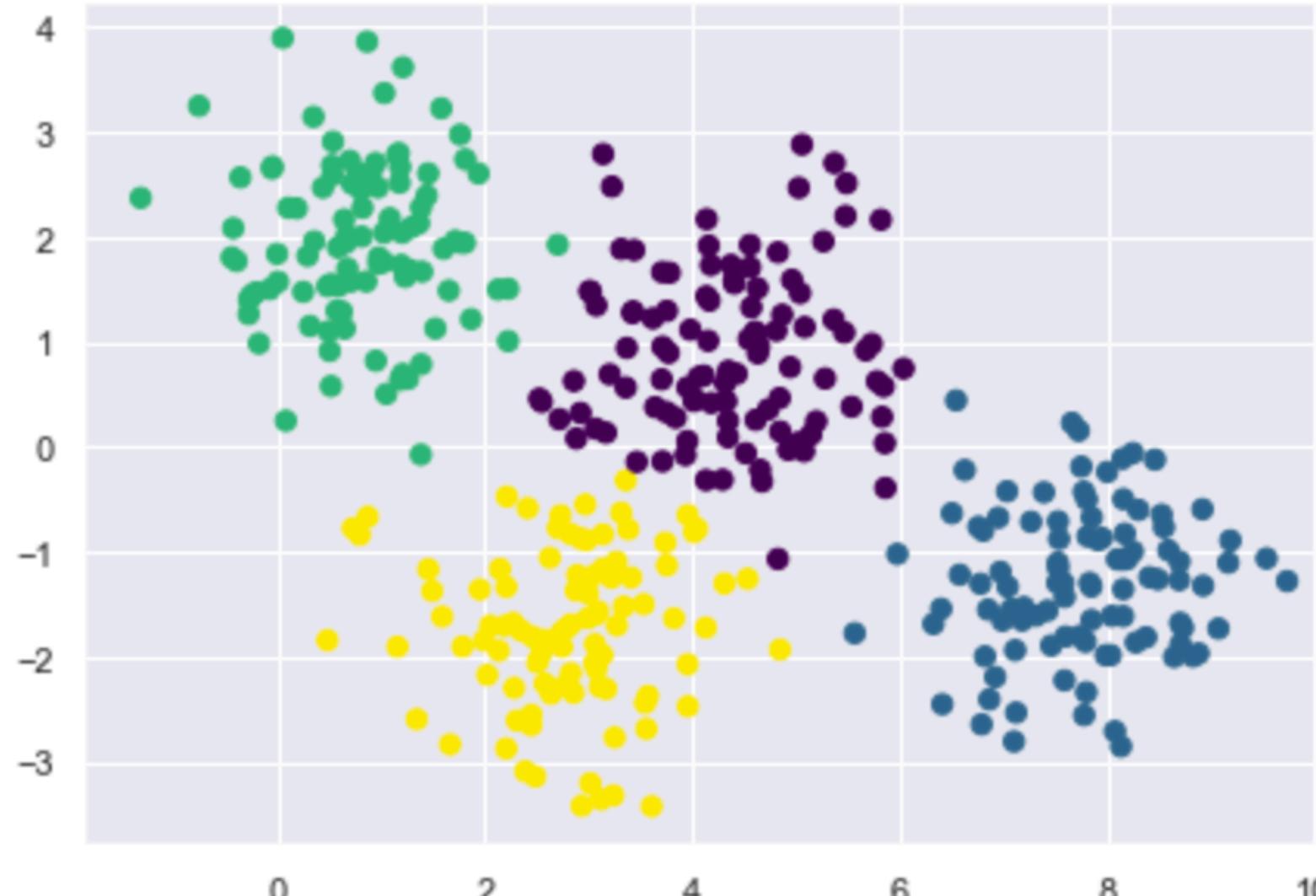
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**Remarks:** If we **know the parameters** of each instances then,

$$p(t = 2 | x, \theta) = \frac{p(x | t = 2, \theta) \times p(t = 2 | \theta)}{\text{Const}}$$

### STEP 6



**flexible  
probabilistic  
approach to  
clustering  
problem**

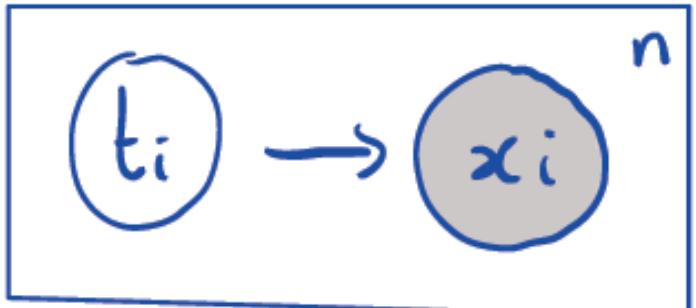
2.b

## EM-algorithm

## 2.b. Expectation-Maximization algorithm

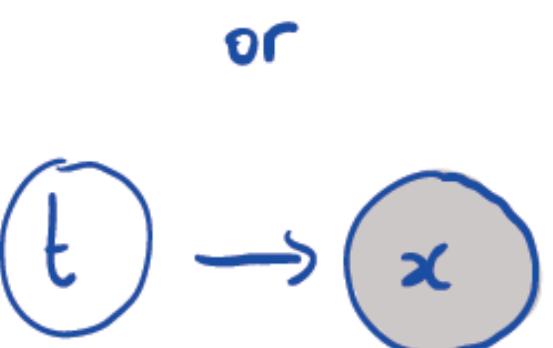
### Reminder : Maximum Likelihood Estimation (MLE)

Our aim is to find :  $\hat{\theta}^{MLE} = \arg \max_{\theta} p(\mathbf{x} | \theta) = \arg \max_{\theta} \log p(\mathbf{x} | \theta)$



$$p(x_i | \theta) = \sum_{k=1}^4 p(x_i, t_i=k | \theta)$$

$$\log P(\mathbf{x} | \theta) = \log \prod_{i=1}^n p(x_i | \theta) = \sum_{i=1}^n \log p(x_i | \theta)$$



$$\hat{\theta} = \arg \max_{\theta} \{ \log P(\mathbf{x} | \theta) \}$$

$$= \sum_{i=1}^n \log \sum_{k=1}^4 p(x_i, t_i=k | \theta)$$

$$= \sum_{i=1}^n \log \sum_{k=1}^4 \frac{q(t_i=k)}{q(t_i=R)} p(x_i, t_i=k | \theta) \text{ for any distribution } q$$

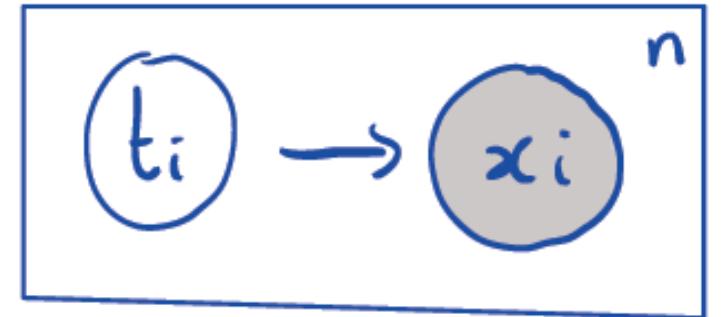
$$\underset{\text{Jensen}}{\geq} \sum_{i=1}^n \sum_{k=1}^4 q(t_i=k) \log \frac{p(x_i, t_i=k | \theta)}{q(t_i=k)} \text{ for any } q$$

$$= \mathcal{L}(\theta, q) \text{ for any } \theta \text{ and } q$$

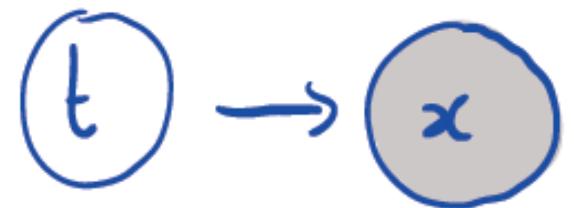
## 2.b. Expectation-Maximization algorithm variational lower bound

Our aim is to find :  $\hat{\theta}^{MLE} = \arg \max_{\theta} p(\mathbf{x} | \theta) = \arg \max_{\theta} \log p(\mathbf{x} | \theta)$

$$\log P(\mathbf{x} | \theta) \underset{\text{Jensen}}{\geq} \mathcal{L}(\theta, q)$$



or

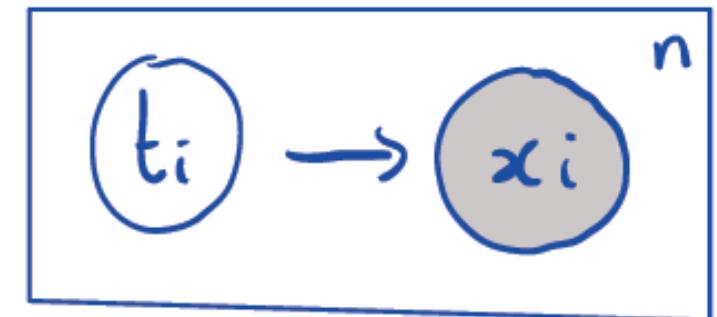


$$p(x_i | \theta) = \sum_{k=1}^4 p(x_i, t_i=k | \theta)$$

$$\hat{\theta} = \arg \max_{\theta} \left\{ \log P(\mathbf{x} | \theta) \right\}$$

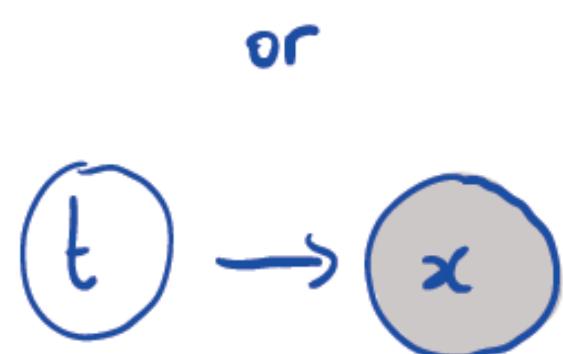
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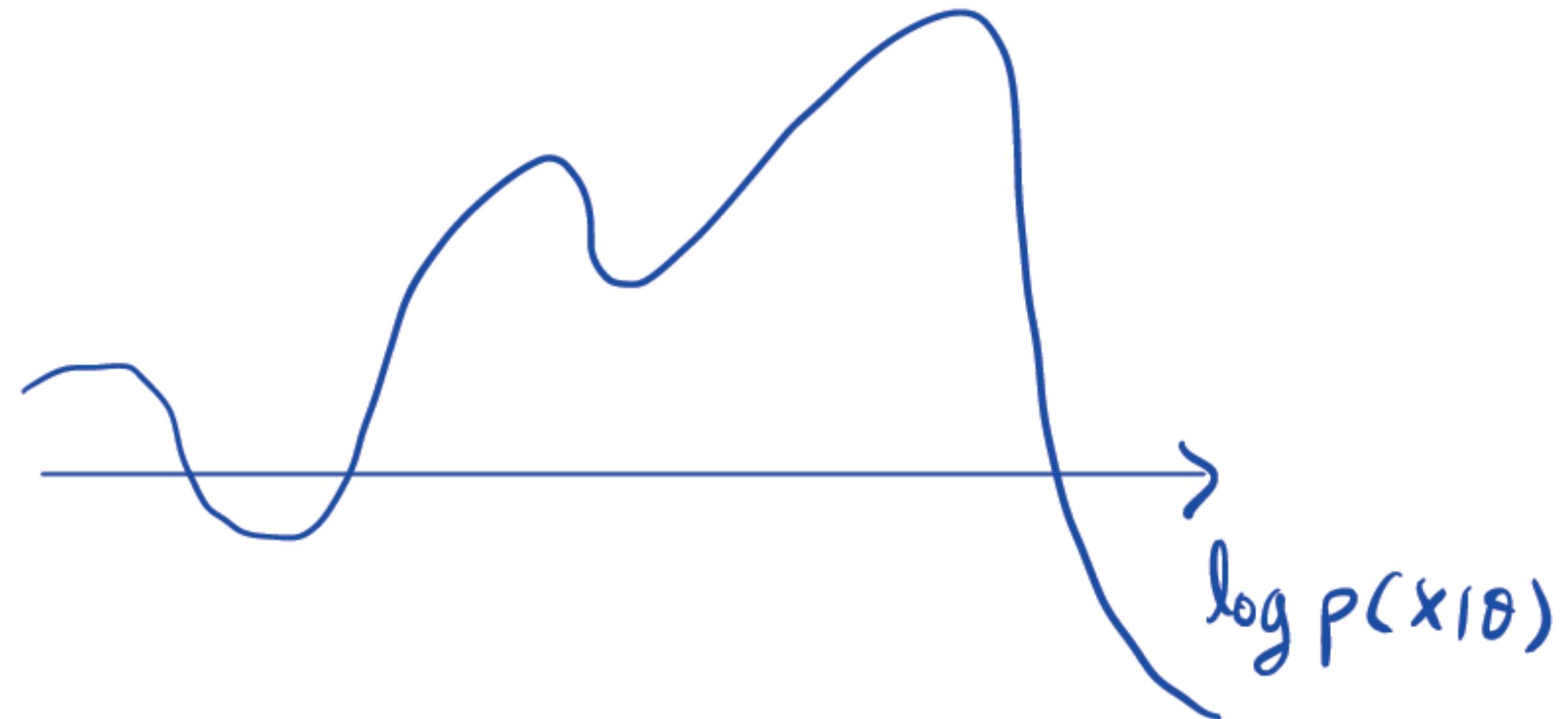


$$p(x_i | \theta) = \sum_{k=1}^4 p(x_i, t_i=k | \theta)$$

$$\log P(x | \theta) \underset{\text{Jensen}}{\geq} \mathcal{L}(\theta, q)$$



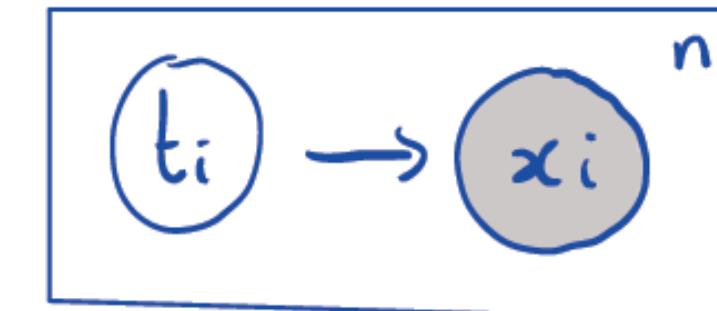
$$\hat{\theta} = \arg \max_{\theta} \left\{ \log P(x | \theta) \right\}$$



## 2.b. Expectation-Maximization algorithm

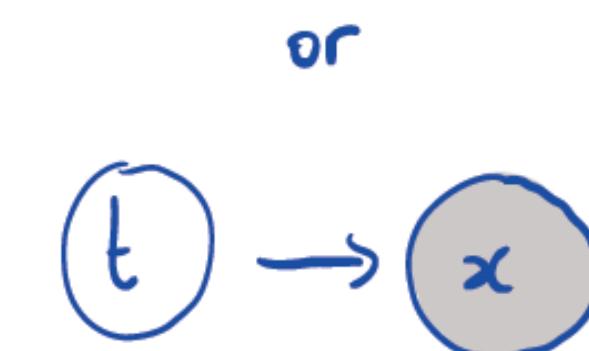
### EM algorithm : E-step

Our aim is to find :  $\hat{\theta}^{MLE} = \arg \max_{\theta} p(\mathbf{x} | \theta) = \arg \max_{\theta} \log p(\mathbf{x} | \theta)$

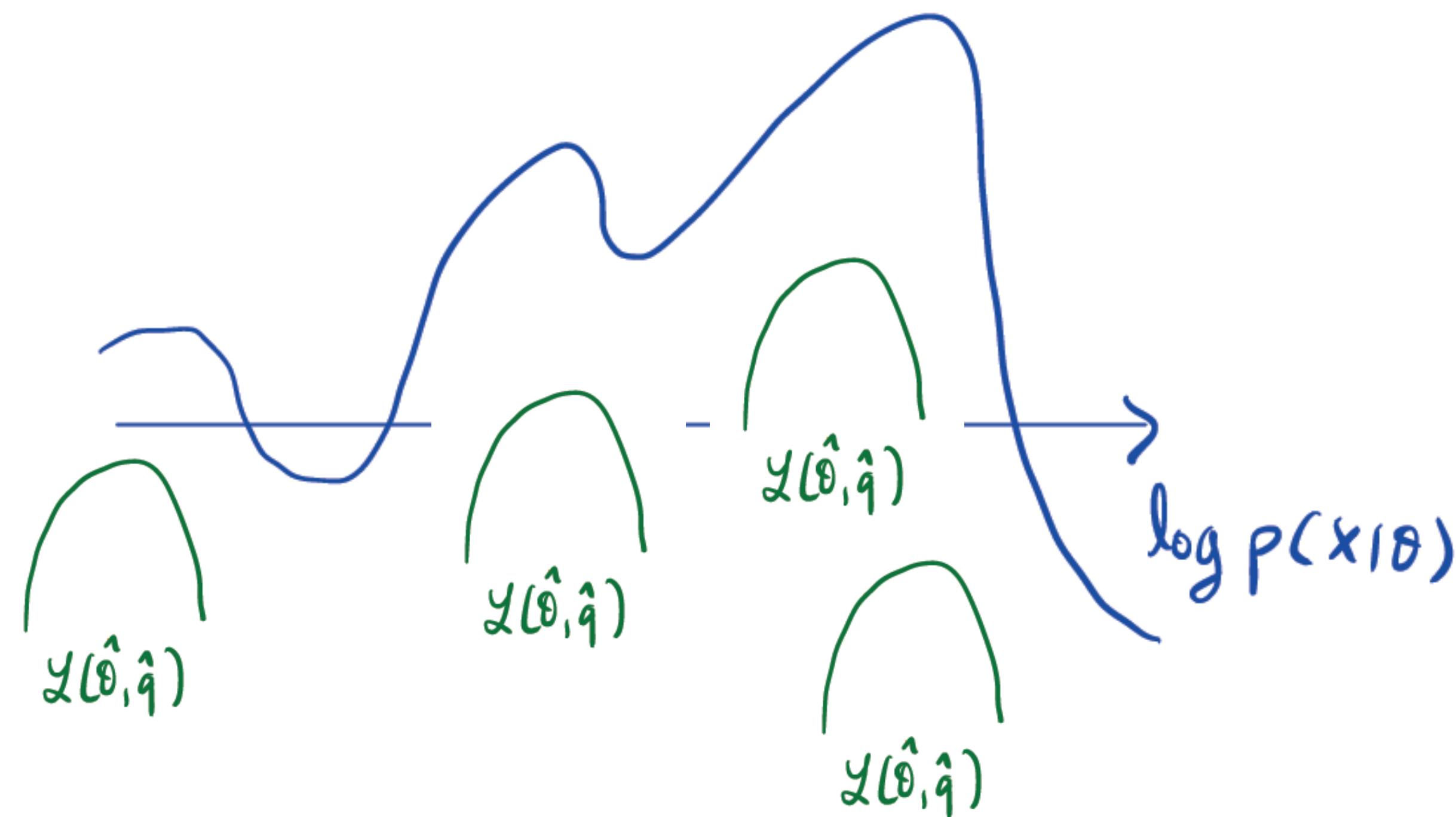


$$p(x_i | \theta) = \sum_{k=1}^4 p(x_i, t_i=k | \theta)$$

$$\log P(x | \theta) \underset{\text{Jensen}}{\geq} \mathcal{L}(\theta, q)$$



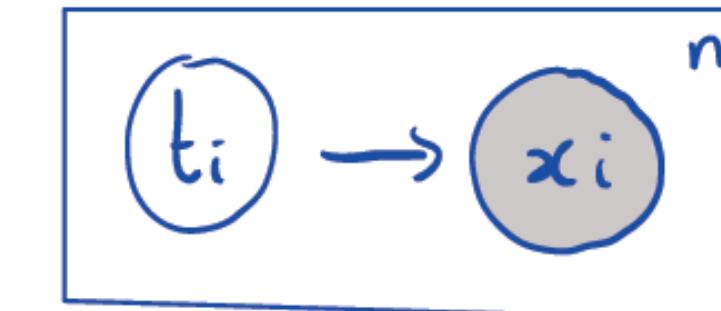
$$\hat{\theta} = \arg \max_{\theta} \left\{ \log P(x | \theta) \right\}$$



## 2.b. Expectation-Maximization algorithm

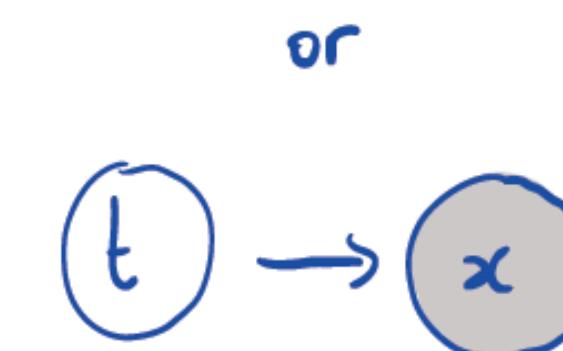
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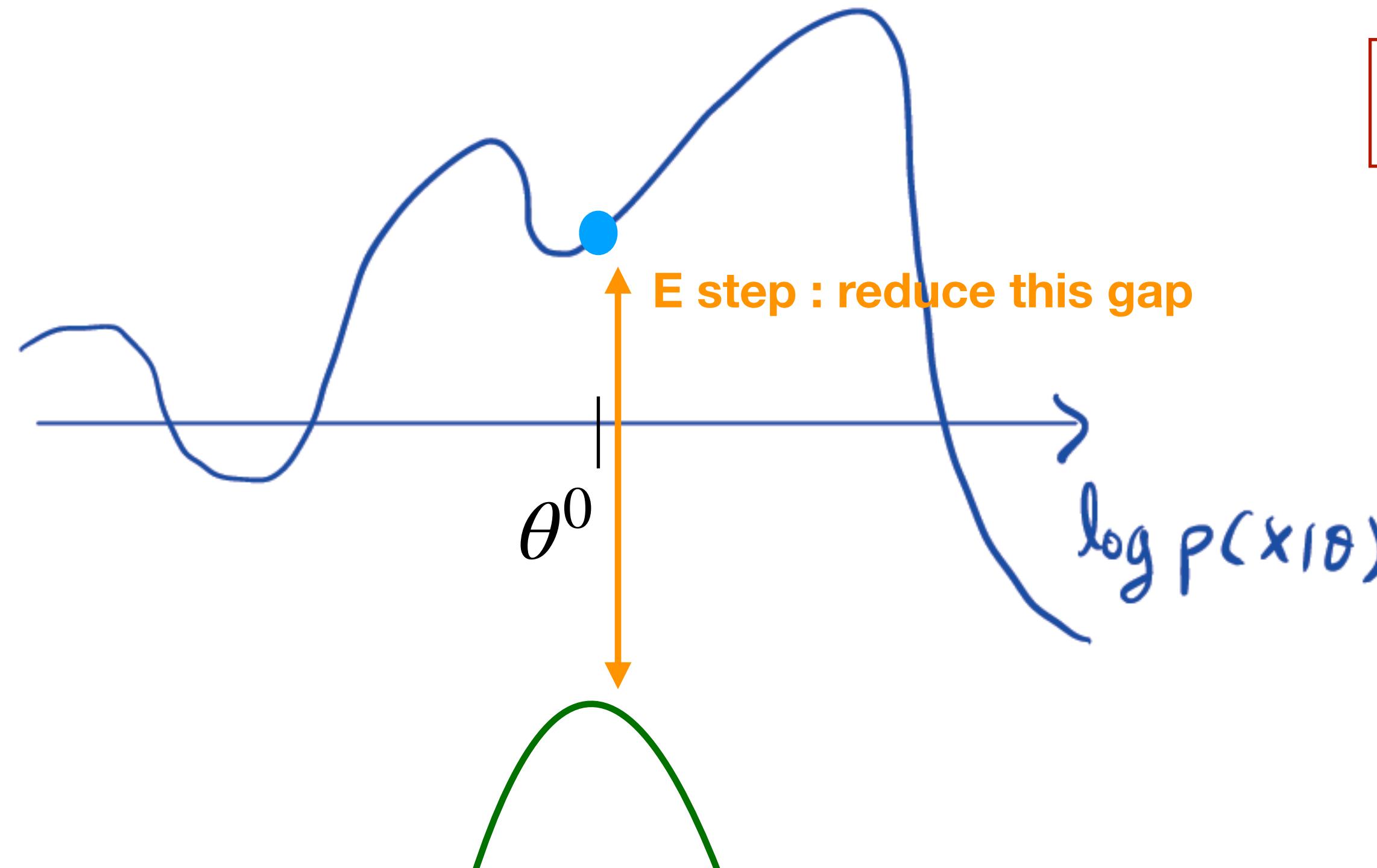


$$p(\mathbf{x} | \theta) = \sum_{k=1}^4 p(x_i, t_i=k | \theta)$$

$$\log P(\mathbf{x} | \theta) \underset{\text{Jensen}}{\geq} \mathcal{L}(\theta, q)$$



$$\hat{\theta} = \arg \max_{\theta} \left\{ \log P(\mathbf{x} | \theta) \right\}$$

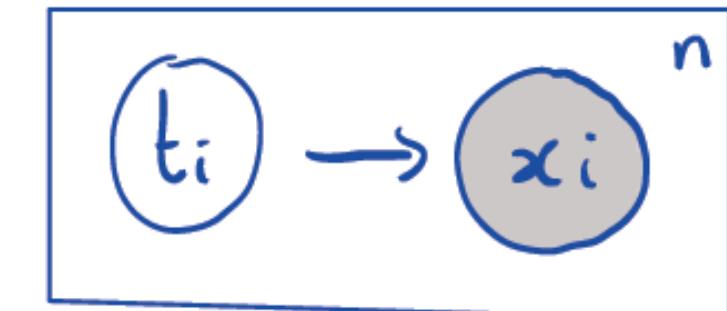


**Expectation step :**  $q^{k+1} = \arg \max_{q \in \text{Family}} \mathcal{L}(\theta^k, q)$

## 2.b. Expectation-Maximization algorithm

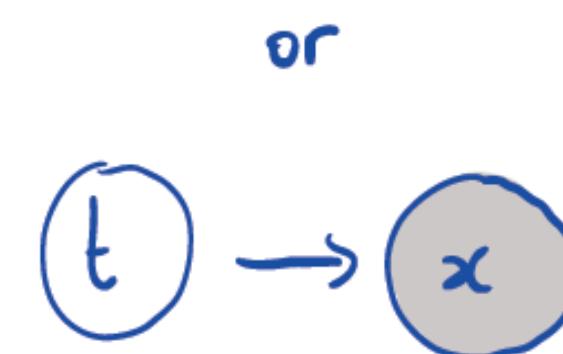
### EM algorithm : E-step

Our aim is to find :  $\hat{\theta}^{MLE} = \arg \max_{\theta} p(\mathbf{x} | \theta) = \arg \max_{\theta} \log p(\mathbf{x} | \theta)$

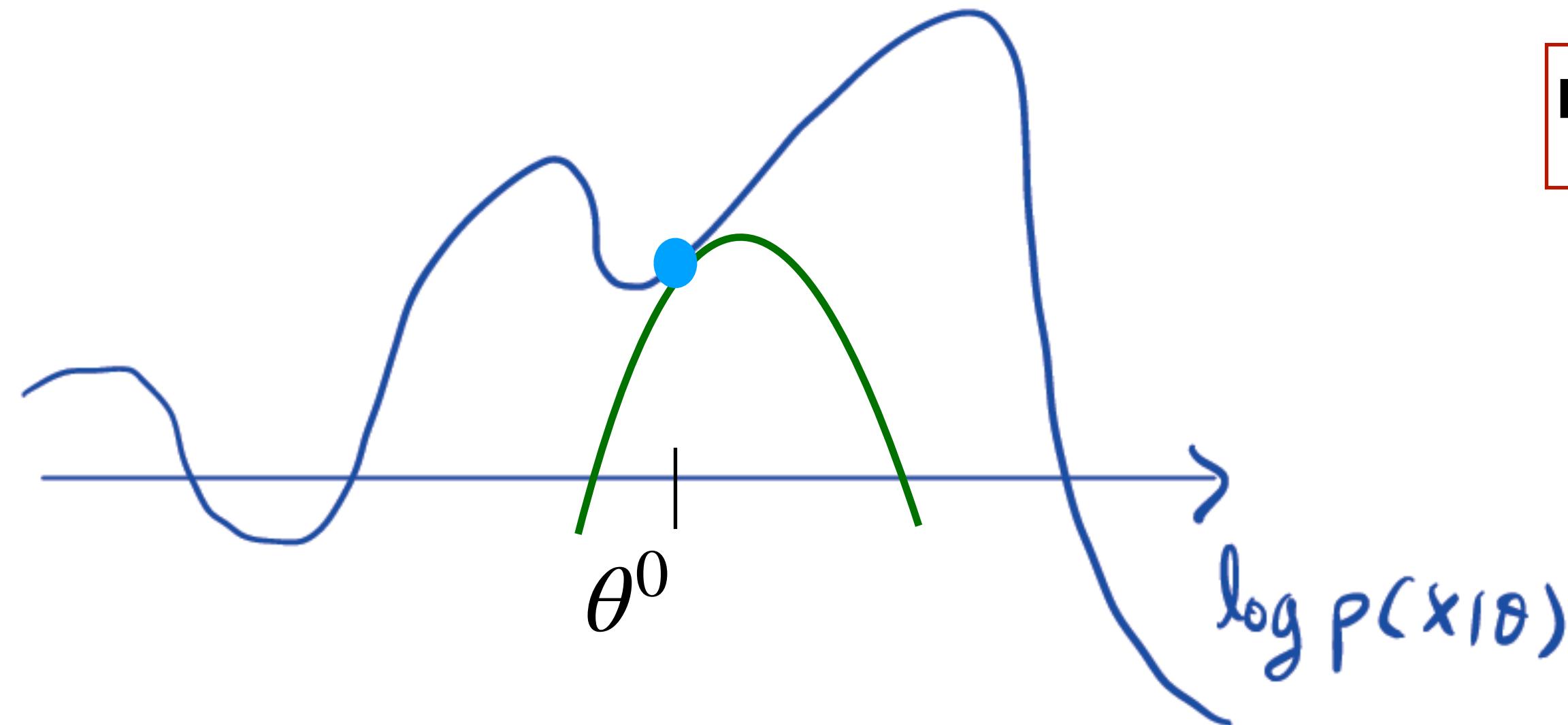


$$p(\mathbf{x} | \theta) = \sum_{k=1}^4 p(x_i, t_i=k | \theta)$$

$$\log P(\mathbf{x} | \theta) \underset{\text{Jensen}}{\geq} \mathcal{L}(\theta, q)$$



$$\hat{\theta} = \arg \max_{\theta} \left\{ \log P(\mathbf{x} | \theta) \right\}$$

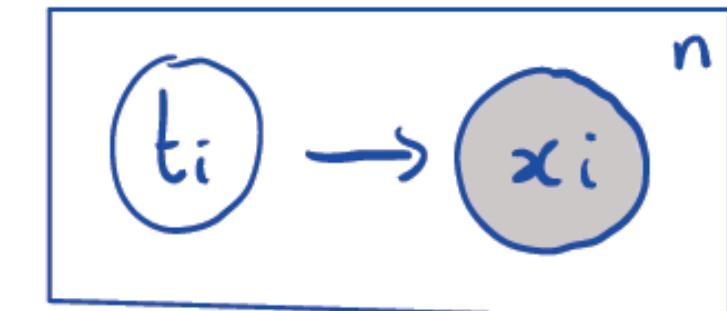


**Expectation step :**  $q^{k+1} = \arg \max_{q \in \text{Family}} \mathcal{L}(\theta^k, q)$

## 2.b. Expectation-Maximization algorithm

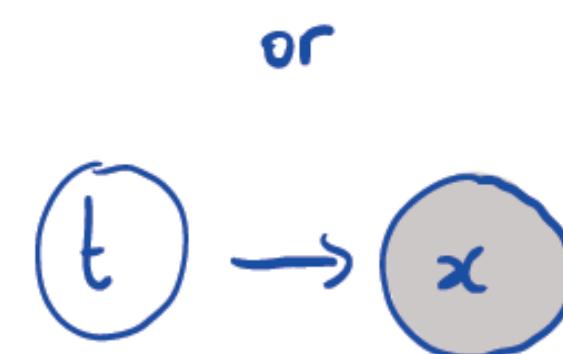
### EM algorithm : M-step

Our aim is to find :  $\hat{\theta}^{MLE} = \arg \max_{\theta} p(\mathbf{x} | \theta) = \arg \max_{\theta} \log p(\mathbf{x} | \theta)$

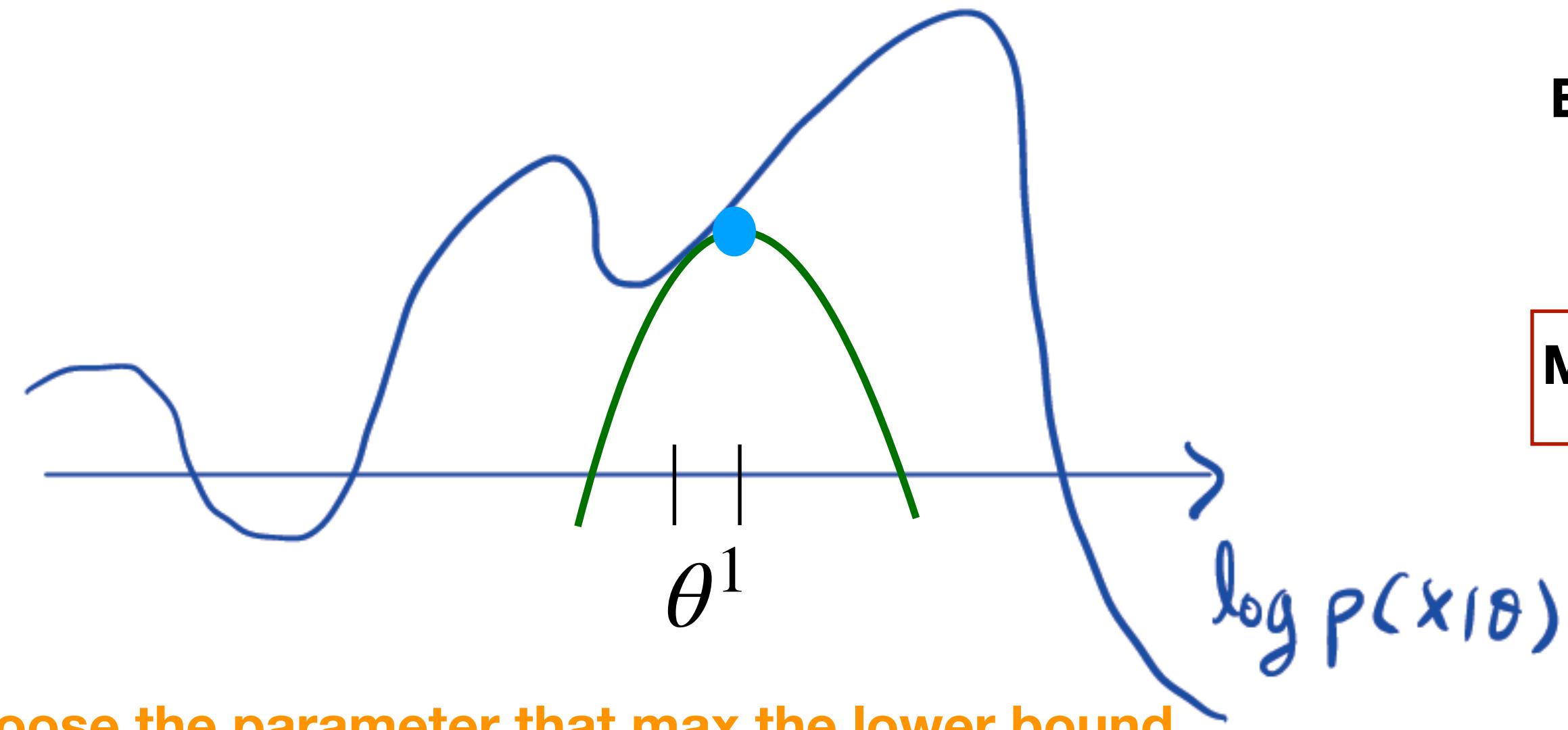


$$p(x_i | \theta) = \sum_{k=1}^4 p(x_i, t_i=k | \theta)$$

$$\log P(x | \theta) \underset{\text{Jensen}}{\geq} \mathcal{L}(\theta, q)$$



$$\hat{\theta} = \arg \max_{\theta} \left\{ \log P(x | \theta) \right\}$$



**Expectation step :**  $q^{k+1} = \arg \max_{q \in \text{Family}} \mathcal{L}(\theta^k, q)$

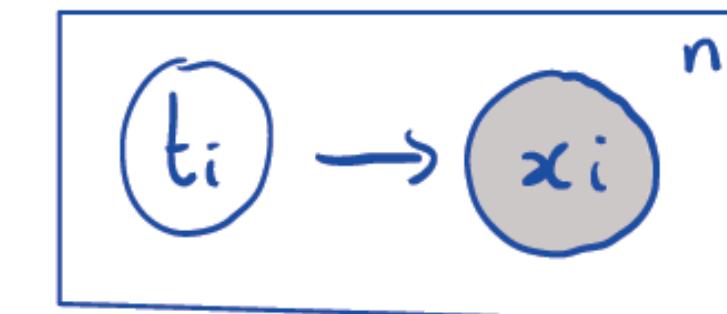
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M step : choose the parameter that max the lower bound

## 2.b. Expectation-Maximization algorithm

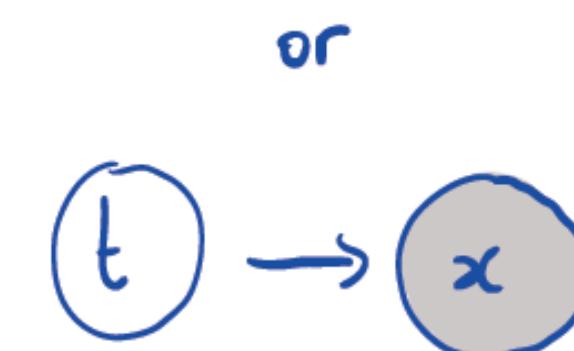
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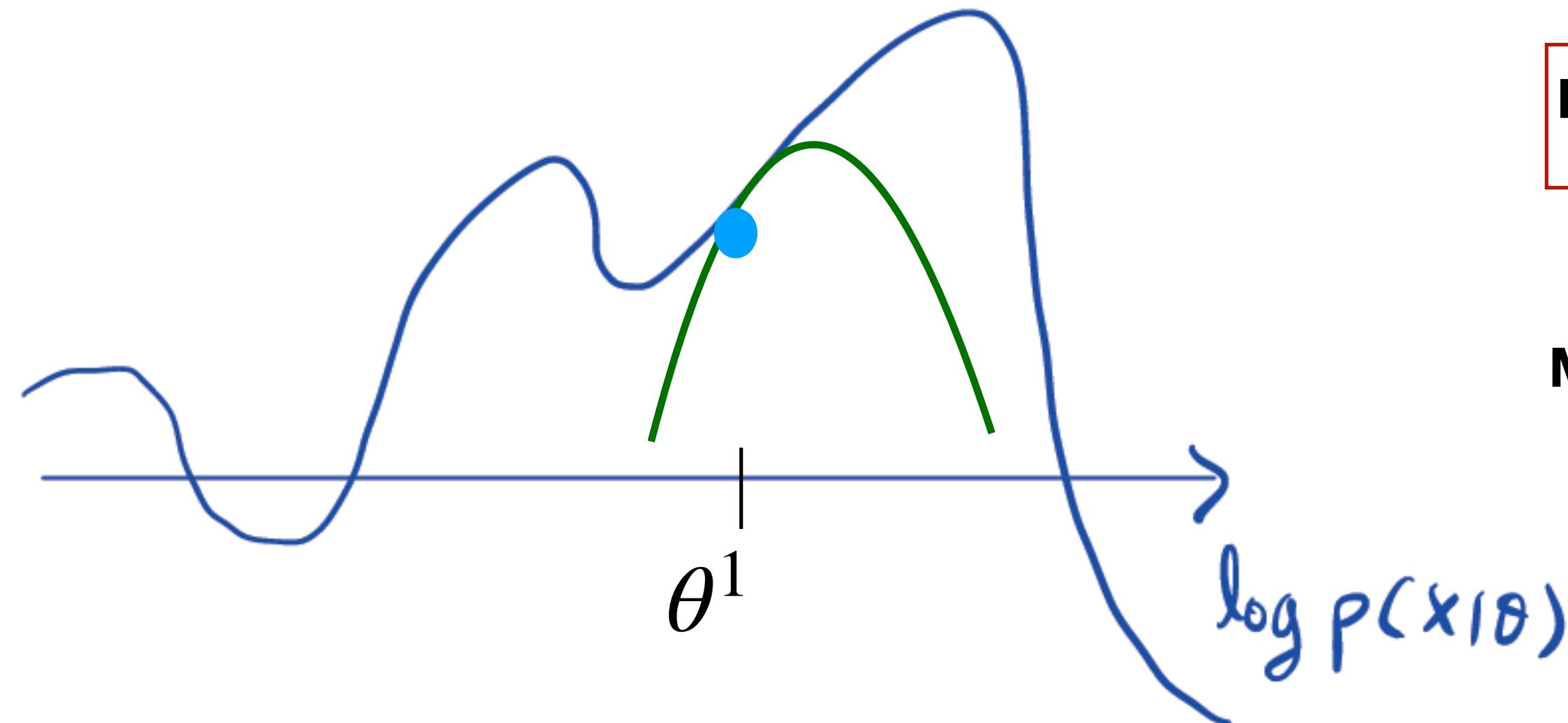


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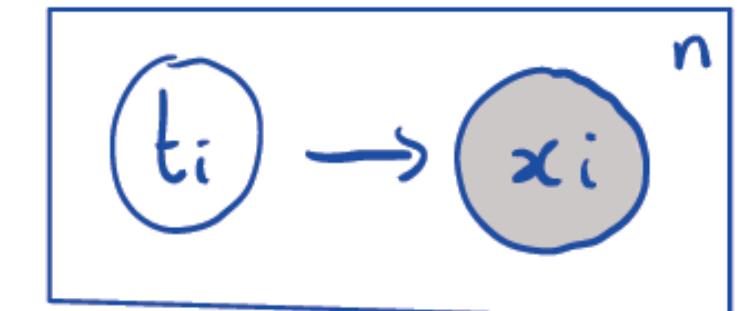
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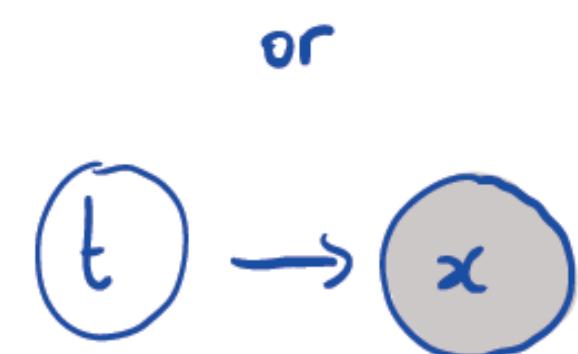
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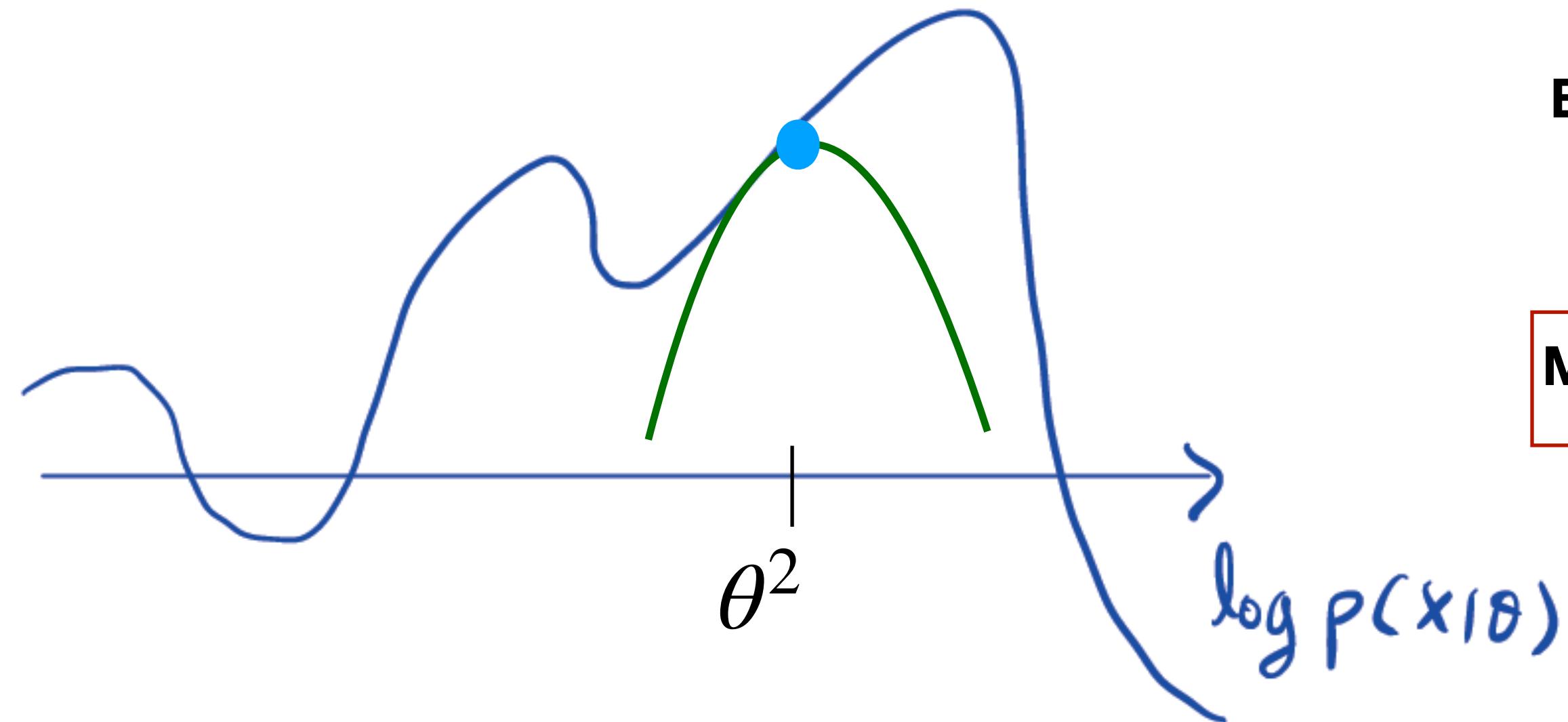


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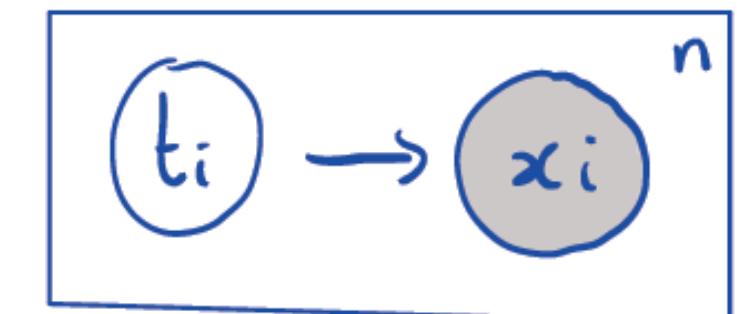
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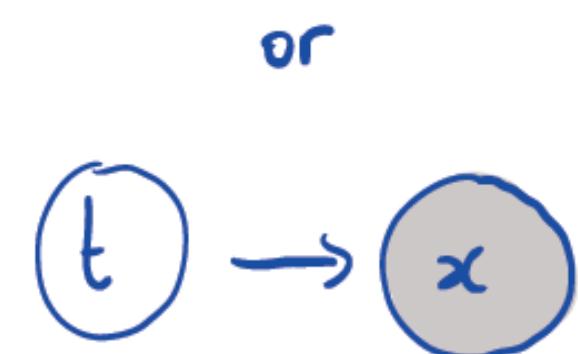
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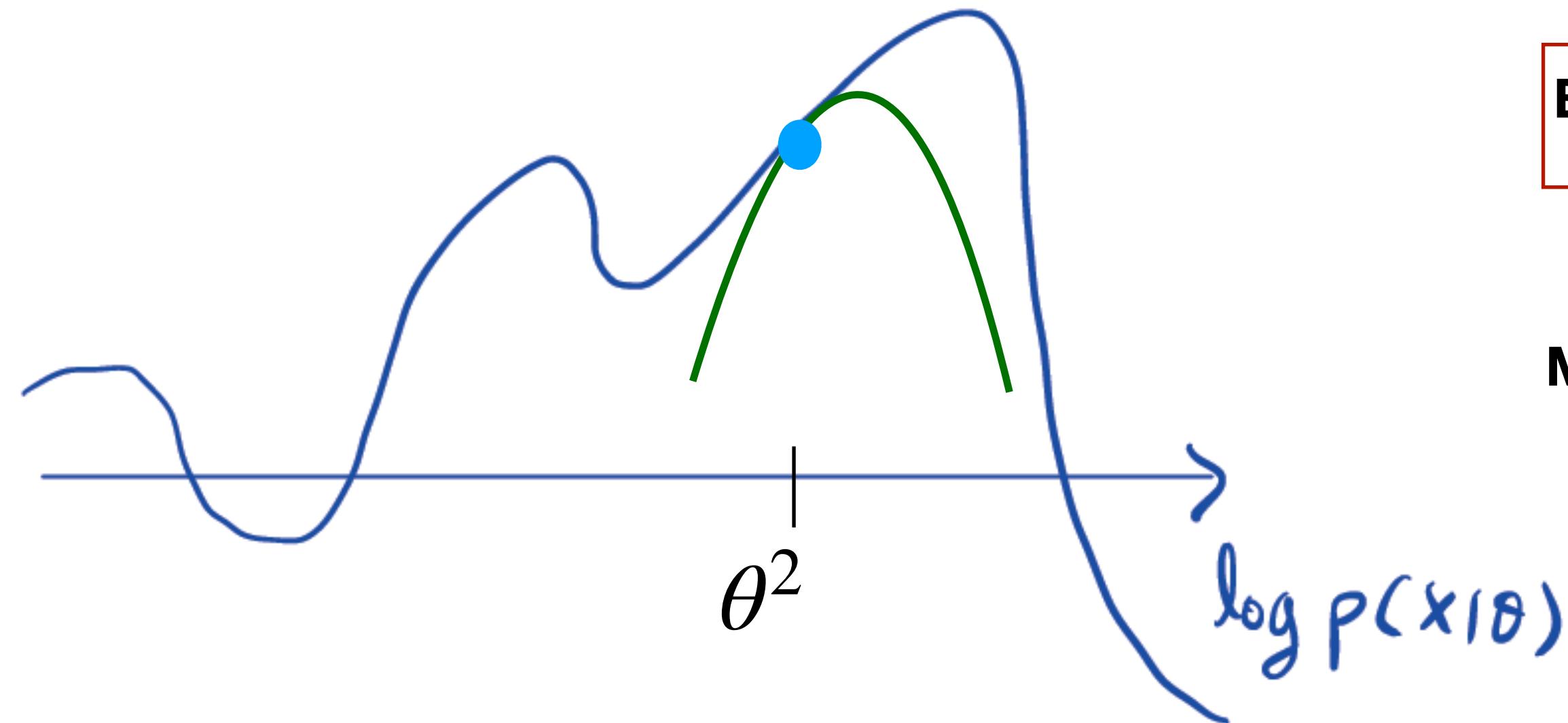


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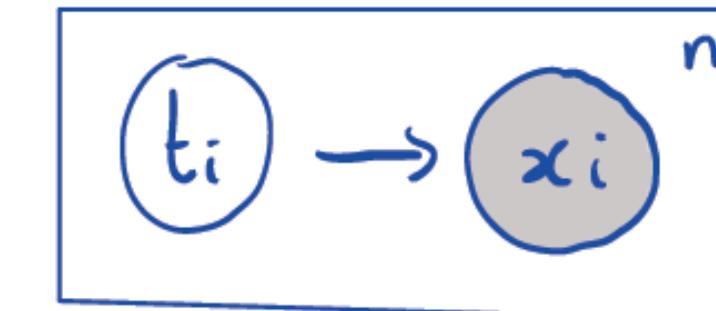
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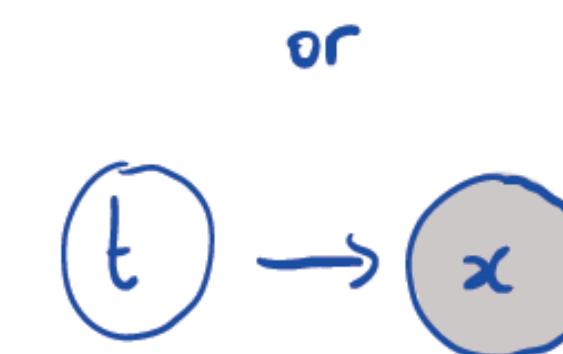
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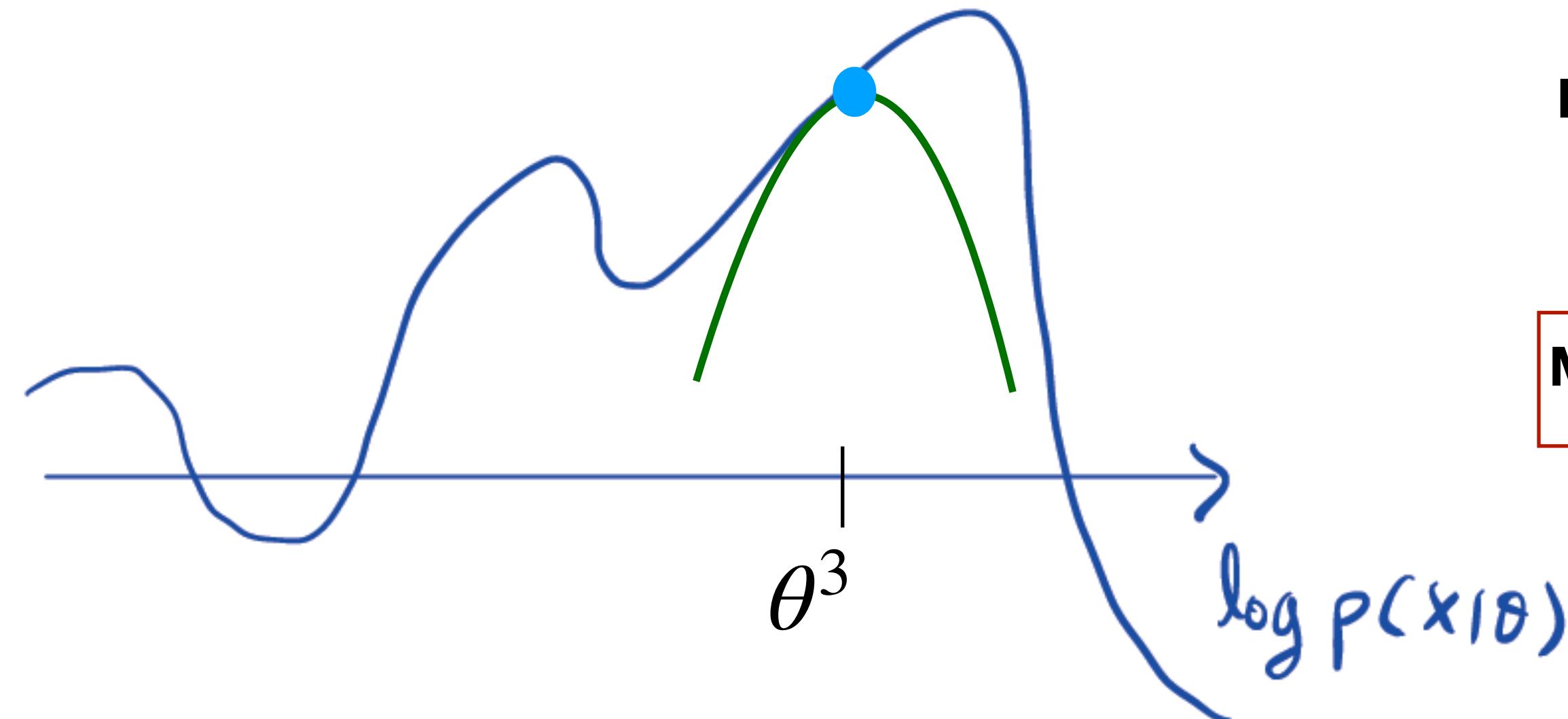


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And so on ... until we reach a local maximum

## 2.b. Expectation-Maximization algorithm

### EM algorithm : more details

**E-step :**

$$q^{k+1} = \arg \max_{q \in \text{Family}} \mathcal{L}(\theta^k, q) \iff q(t_i) = p(t_i | x_i, \theta)$$

**M-step :**

$$\theta^{k+1} = \arg \max_{\theta} \mathcal{L}(\theta, q^{k+1}) \iff \theta^{k+1} = \arg \max_{\theta} \mathbb{E}_{q^{k+1}}[\log p(X, T | \theta)]$$

## 2.b. Expectation-Maximization algorithm

### EM algorithm : back to GMM

**E-step :**

$$q^{k+1} = \arg \max_{q \in \text{Family}} \mathcal{L}(\theta^k, q) \iff q(t_i) = p(t_i | x_i, \theta)$$

**GMM** : for each point we indeed computed  $q(t_i) = p(t_i | x_i, \theta)$

**M-step :**

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**GMM** : we updated the gaussian parameters with

$$\mu_{soft}^{MLE} = \frac{\sum_i p(\textcolor{orange}{t=2} | x, \theta) x_i}{\sum_i p(\textcolor{orange}{t=2} | x, \theta)}$$

which indeed is the M-step of the EM algorithm

## 2.b. Expectation-Maximization algorithm

### EM algorithm : back to GMM

**E-step :**

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which indeed is the M-step of the EM algorithm

$$\sum_{i=1}^n E_{q(t_i)} \log p(x_i, t_i | \theta) = \sum_{i=1}^n \sum_{k=1}^4 q(t_i=k) \log \left( \frac{1}{\text{const}} e^{-\frac{(x_i - \mu_k)^2}{2\sigma_k^2}} \times \pi_k \right)$$

$$= \sum_{i=1}^n \sum_{k=1}^4 q(t_i=k) \left( \log \left( \frac{\pi_k}{\text{const}} \right) - \frac{(x_i - \mu_k)^2}{2\sigma_k^2} \right)$$

$$\frac{\partial}{\partial \mu_2} \left( \sum_{i=1}^n \sum_{k=1}^4 q(t_i=k) \left( \log \left( \frac{\pi_k}{\text{const}} \right) - \frac{(x_i - \mu_k)^2}{2\sigma_k^2} \right) \right)$$

$$= \sum_{i=1}^n q(t_i=2) \left( 0 + \frac{(x_i - \mu_2)^2}{\sigma_2^2} \right) = 0$$

$$\Rightarrow \sum_{i=1}^n q(t_i=2) \times x_i - \mu_2 \sum_{i=1}^n q(t_i=2) = 0$$

$$\Leftrightarrow \boxed{\mu_2 = \frac{\sum_{i=1}^n q(t_i=2) \times x_i}{\sum_{i=1}^n q(t_i=2)}}$$



3

## Probabilistic dimensionality reduction and EM-algorithm

### 3. Probabilistic dimensionality reduction

#### Dimensionality reduction : reminder

**Dimensionality reduction** : transformation of data from a **high-dimensional** space **into a low-dimensional** space

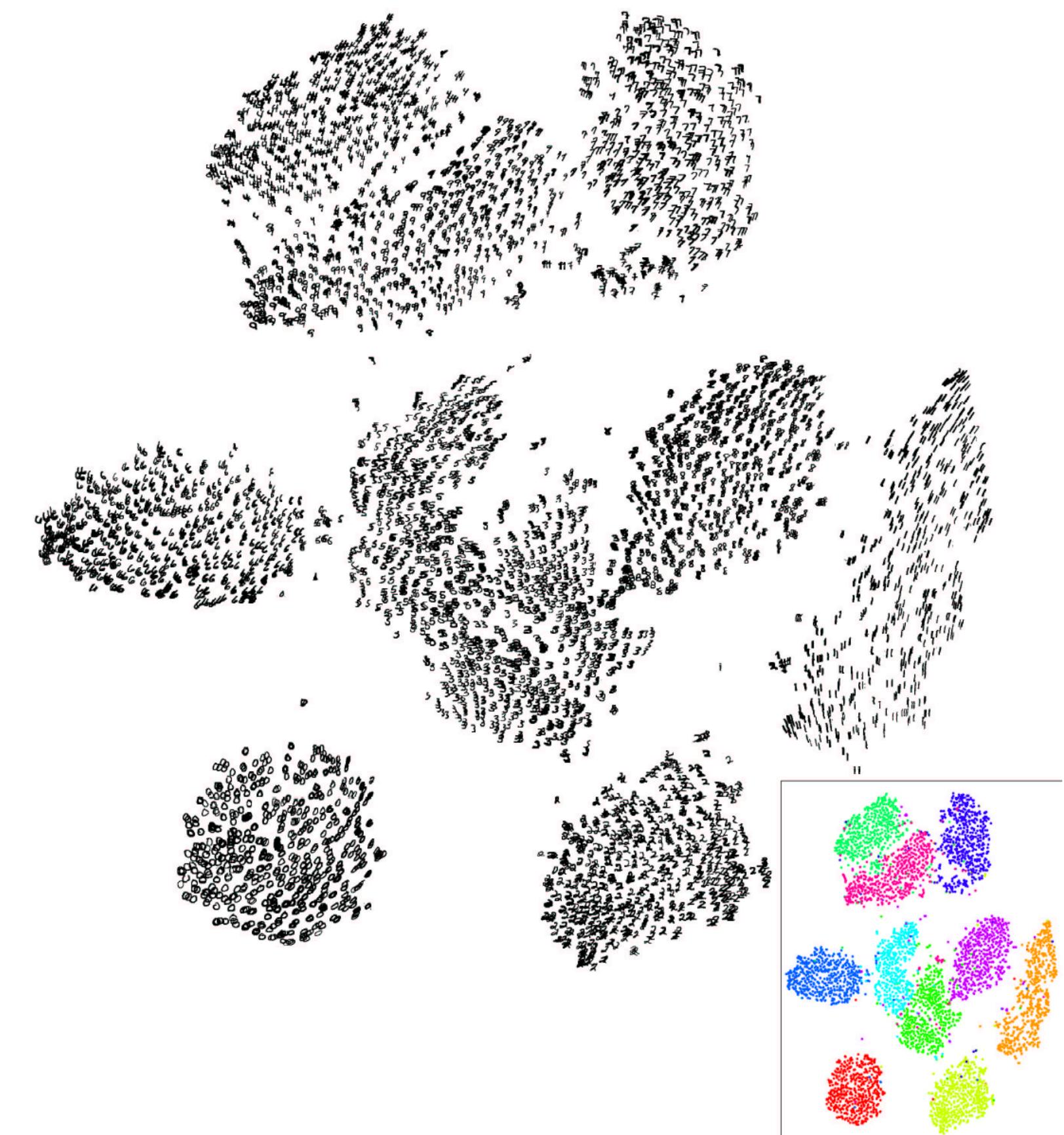
# 3. Probabilistic dimensionality reduction

## Dimensionality reduction : reminder

**Dimensionality reduction** : transformation of data from a **high-dimensional** space **into a low-dimensional** space

### Why do we care ?

- **Avoid curse of dimensionality :**  
a high-dimensional data can be dangerous if the data is too sparse
- **Noise reduction :**  
In a High-dimensional dataset there might be too much noise.
- **Data visualisation (2D or 3D visualisation) :**  
We cannot visualise a high-dimensional data (dimension > 3)

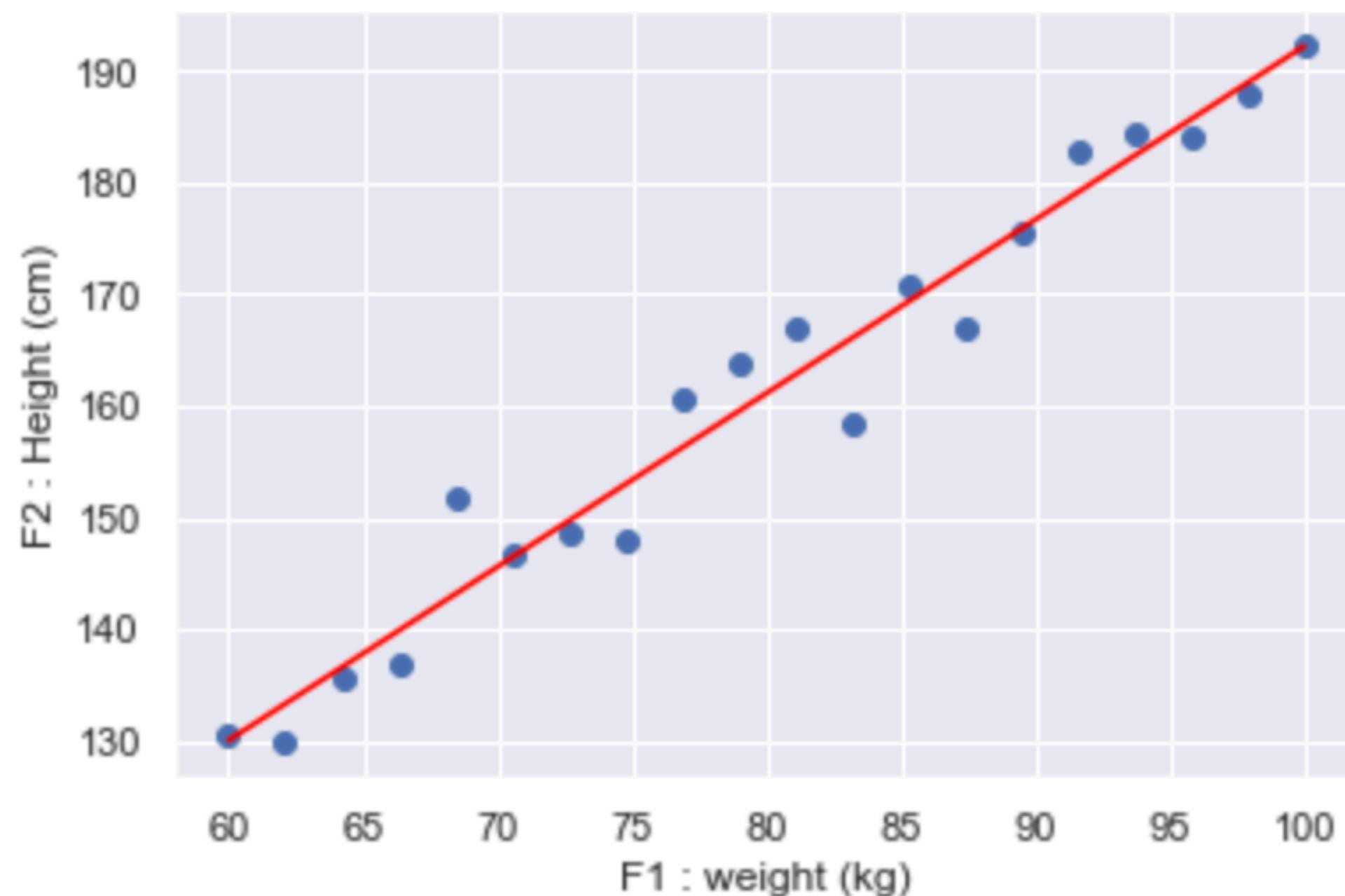


### 3. Probabilistic dimensionality reduction

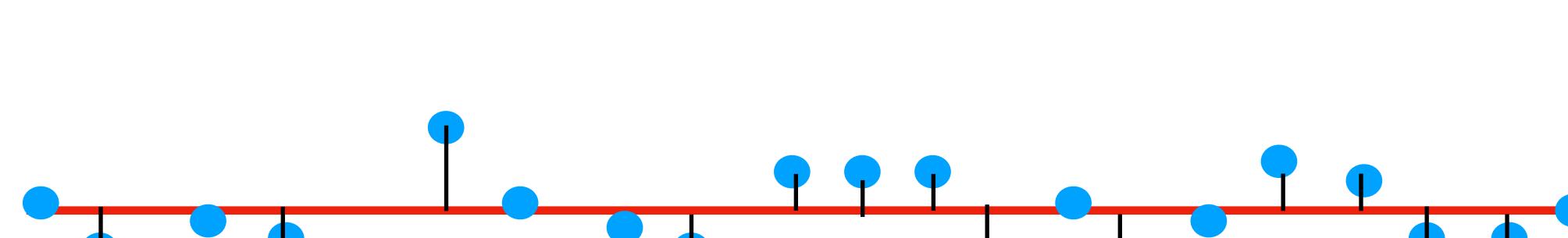
#### Dimensionality reduction : PCA

**Dimensionality reduction** : transformation of data from a **high-dimensional space** into a **low-dimensional space**

**Principal Component Analysis (PCA)** : **Linear approach** to dimensionality reduction : the idea is to linearly project the high-dimensional data into a low-dimensional data



The two features F1 and F2 have a positive correlation

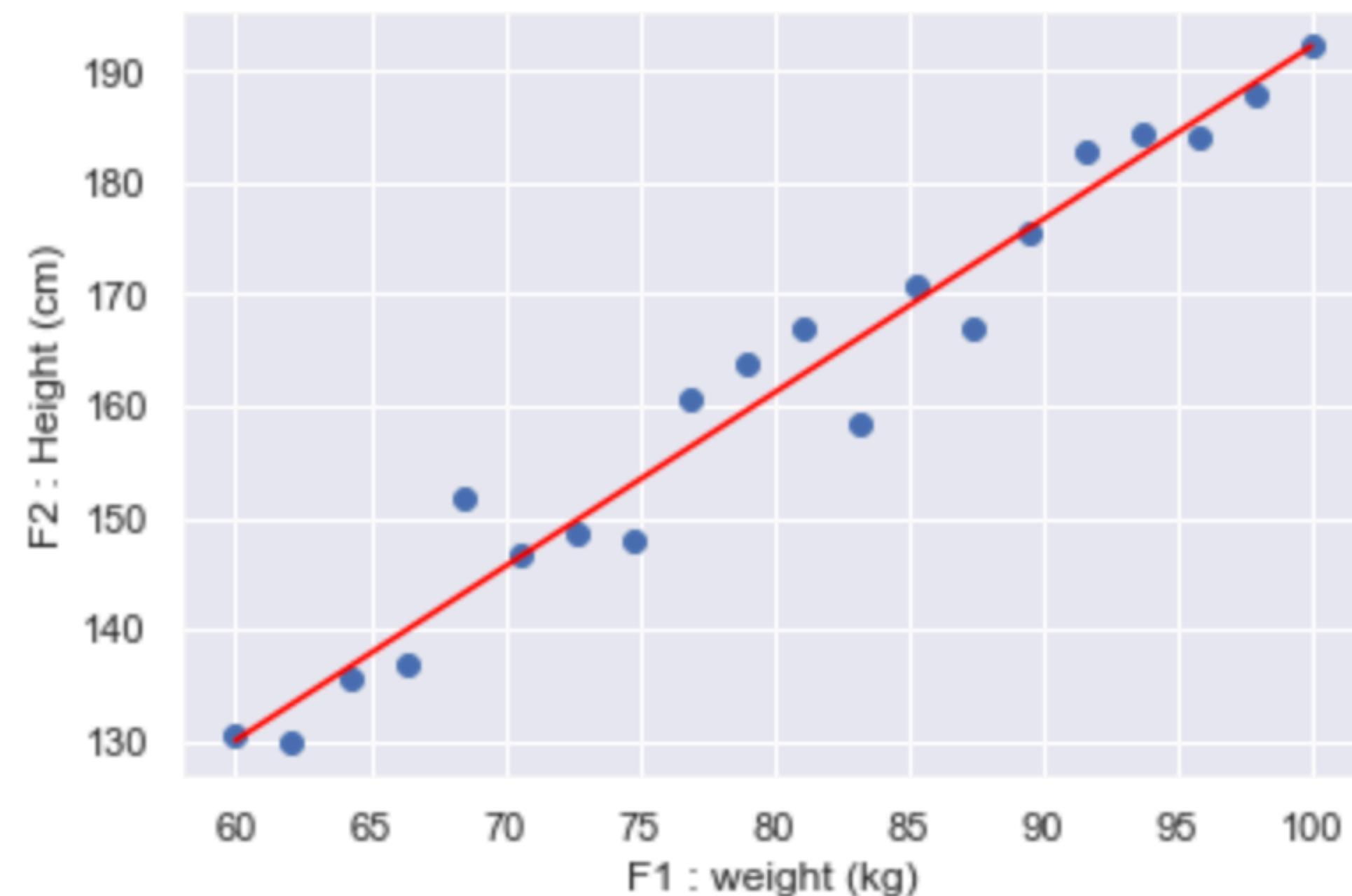


# 3. Probabilistic dimensionality reduction

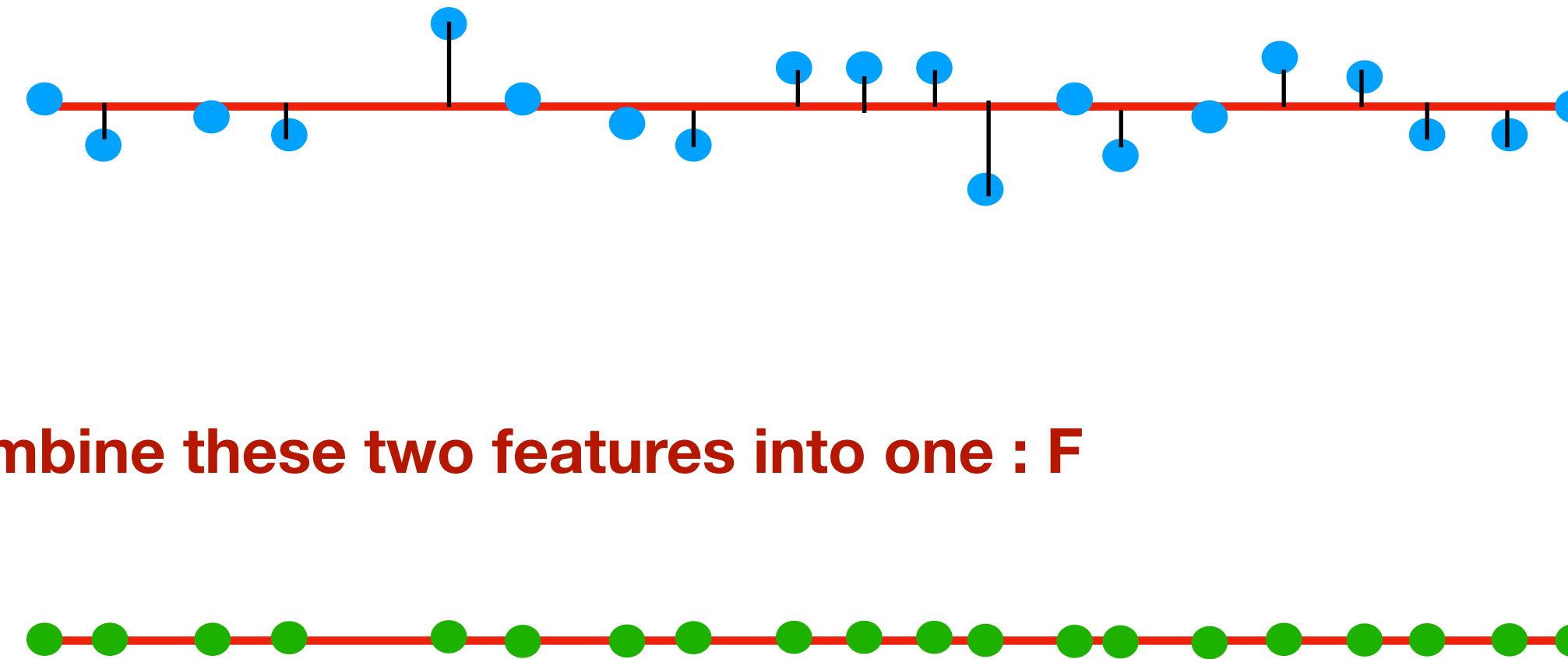
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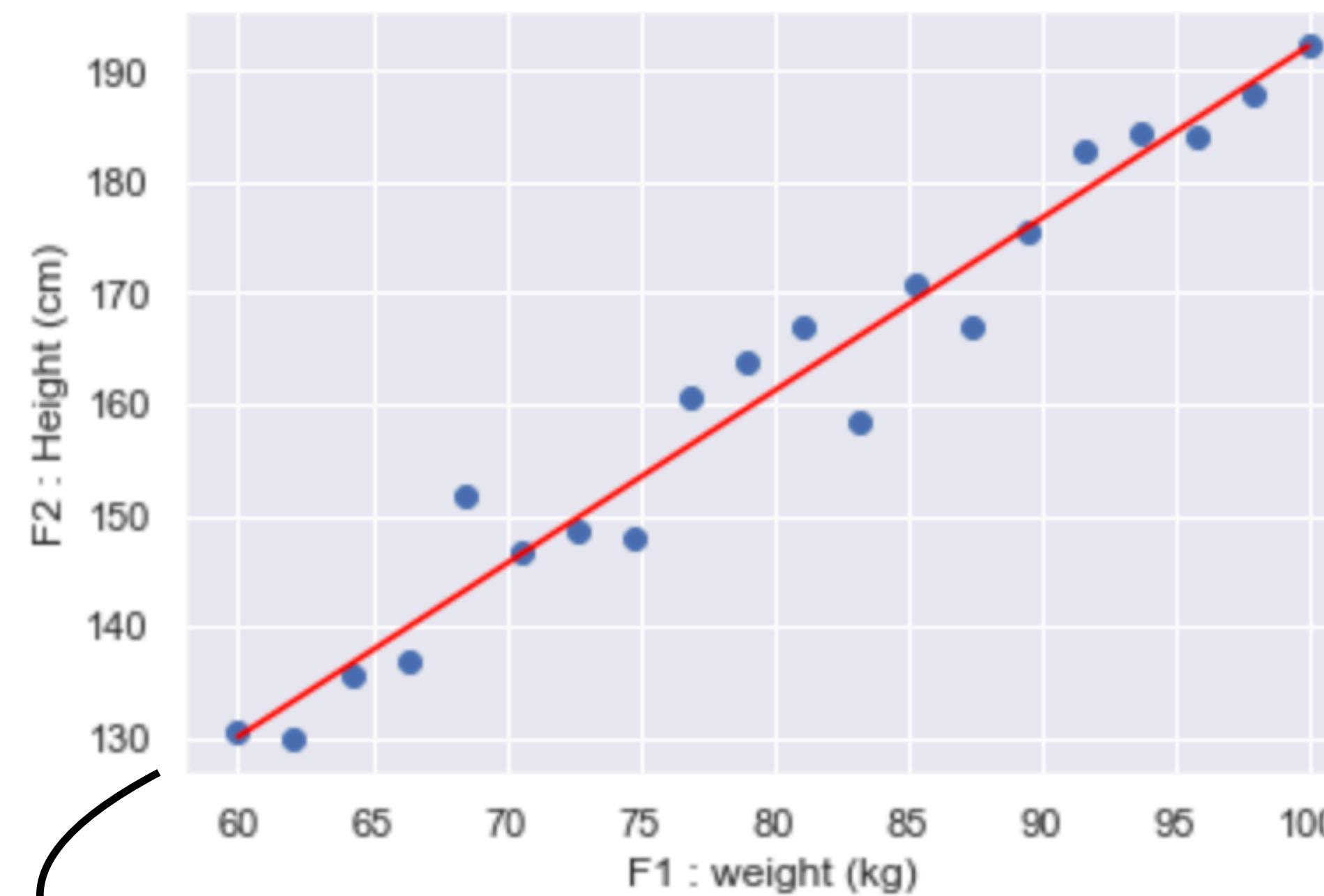


# 3. Probabilistic dimensionality reduction

## Dimensionality reduction : PCA

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The two features F1 and F2 have a positive correlation

Combine these two features into one : F



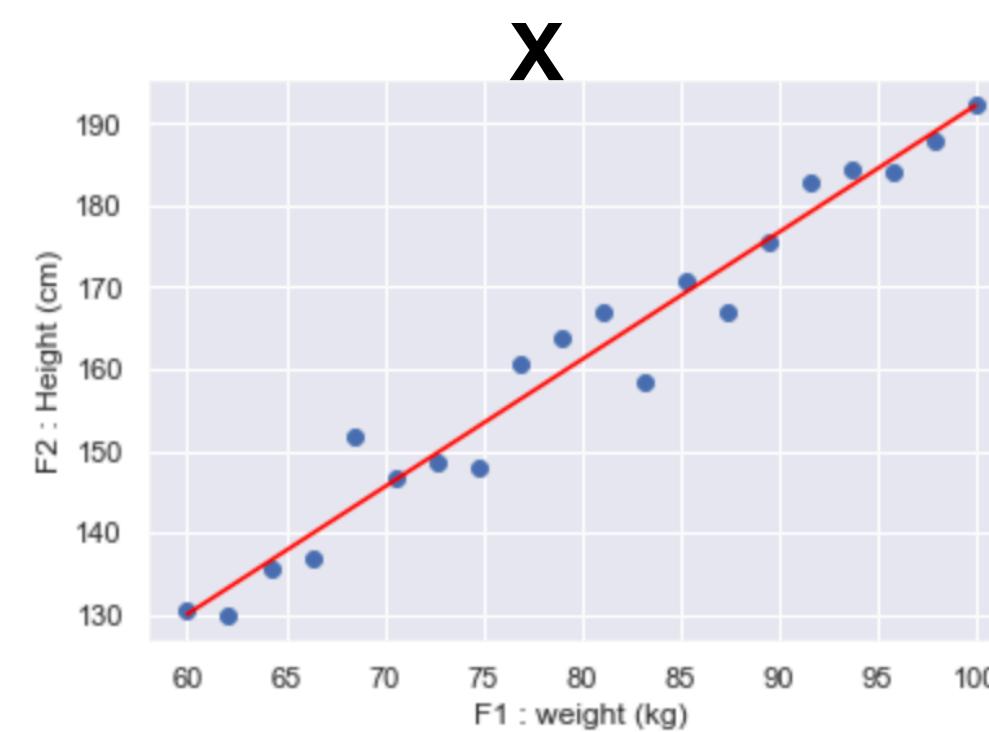
This line corresponds to the eigenvector associated to the greatest eigenvalue of the covariance matrix

### 3. Probabilistic dimensionality reduction

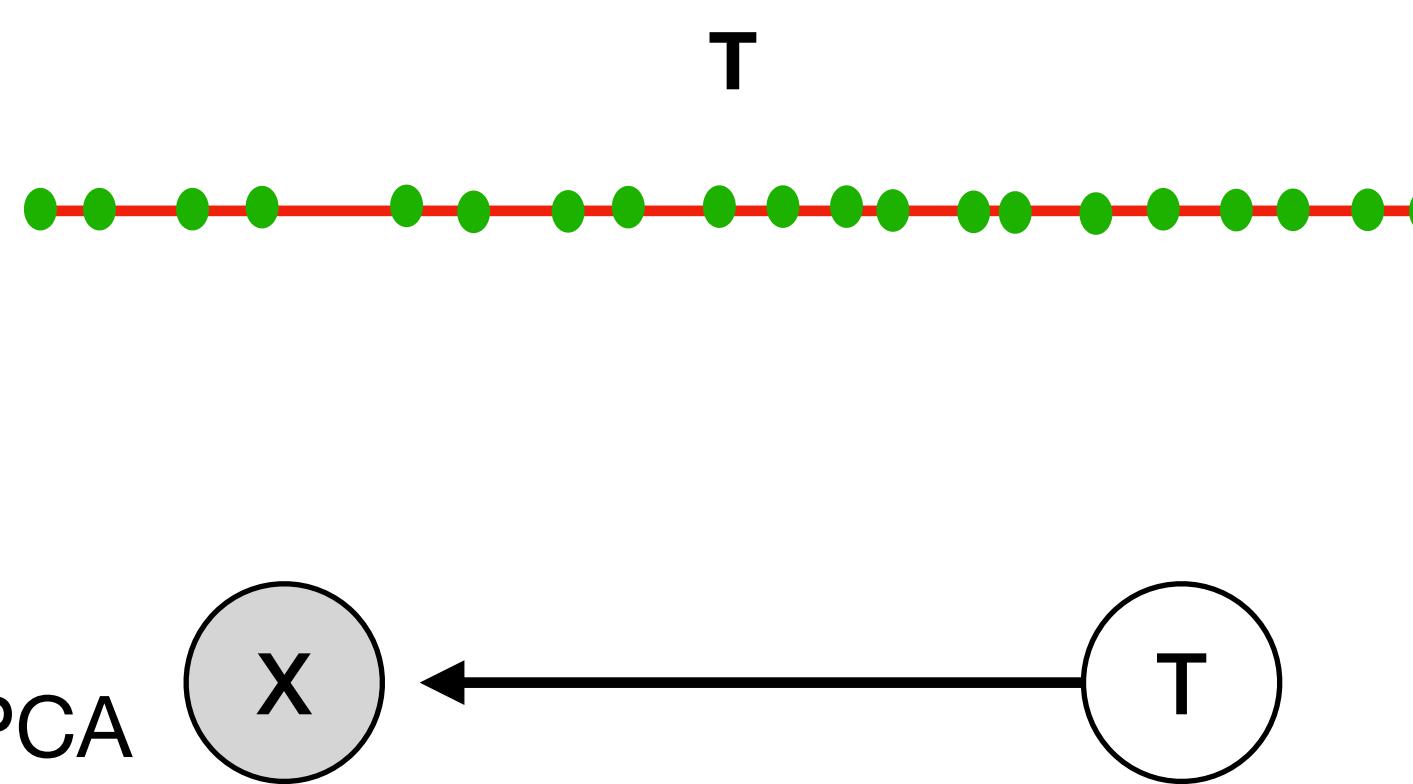
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How do we **reduce** ?



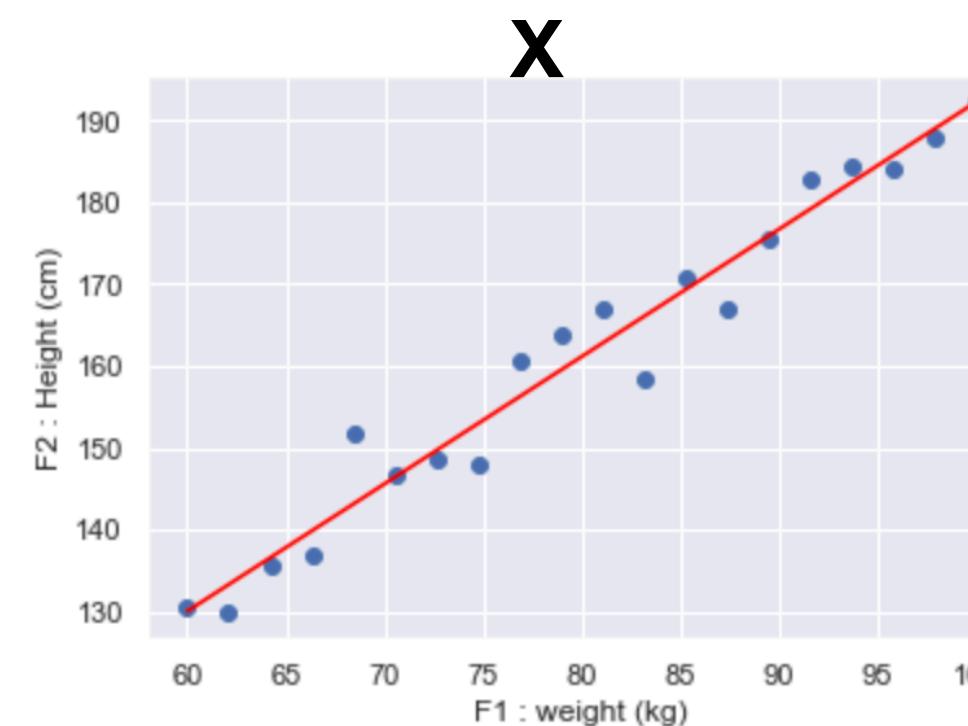
**Probabilistic PCA** : a probabilistic point of view of PCA

# 3. Probabilistic dimensionality reduction

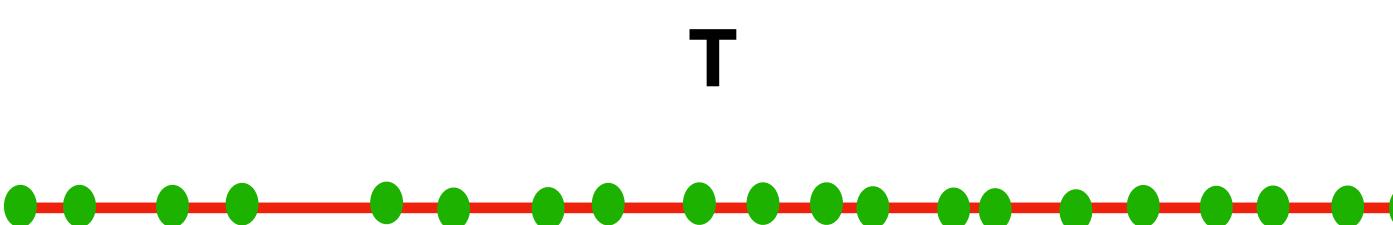
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**Probabilistic PCA** : a probabilistic point of view of PCA



$$p(t_i) = \mathcal{N}(t_i | 0, I_2)$$

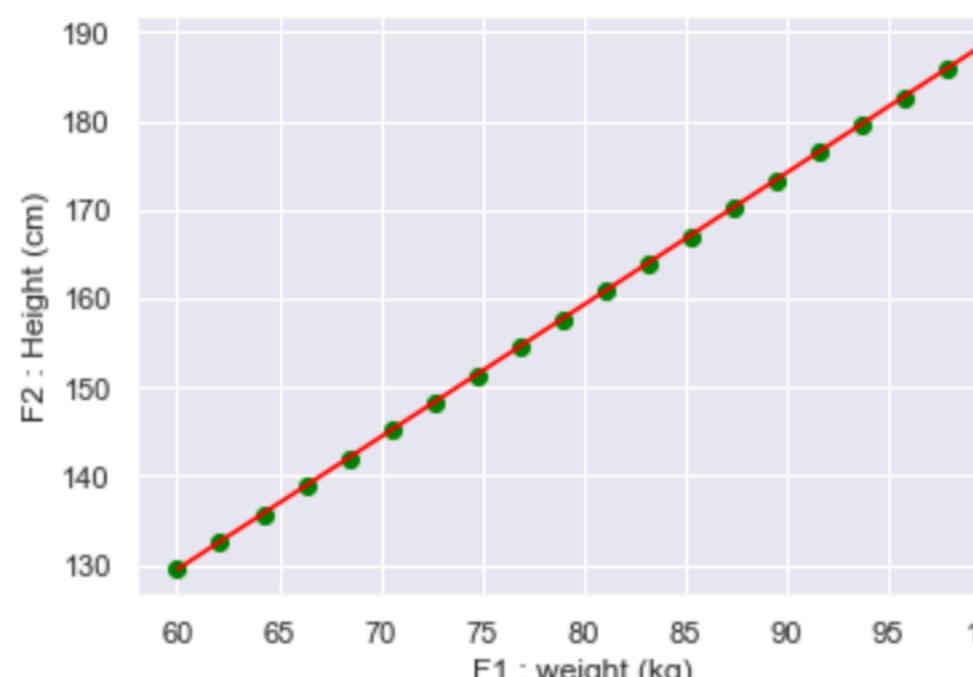
$$x_i = W t_i + b$$

$$x_i = W t_i + b + \epsilon_i \text{ with } \epsilon_i \sim \mathcal{N}(0, \Sigma)$$

$$p(x_i | t_i, \theta) = \dots$$



How do we **generate** ?

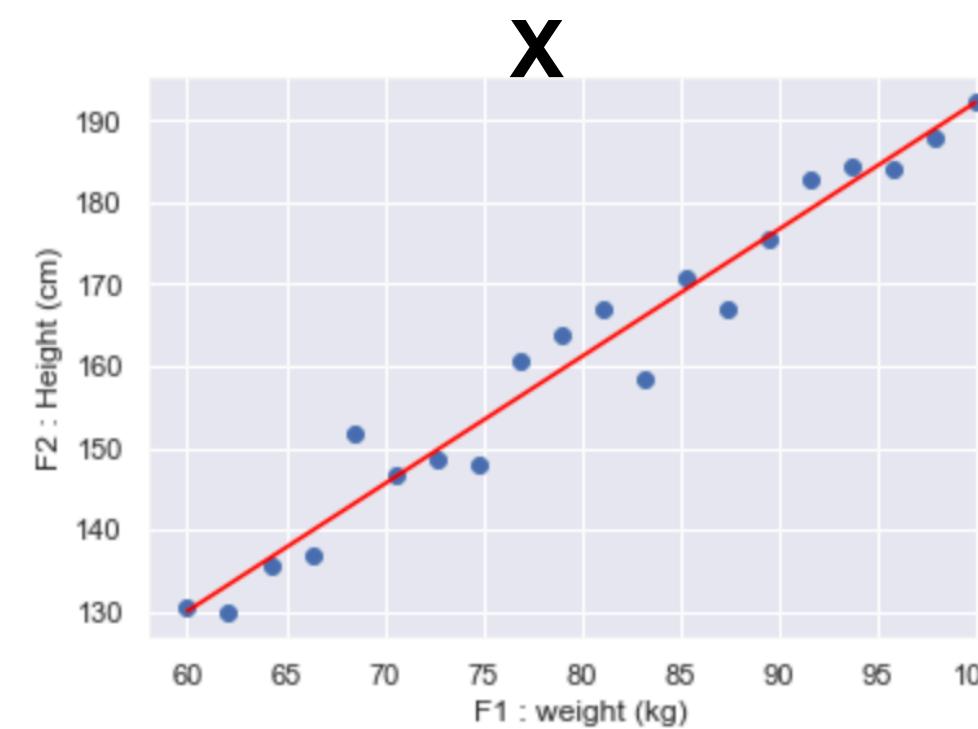


# 3. Probabilistic dimensionality reduction

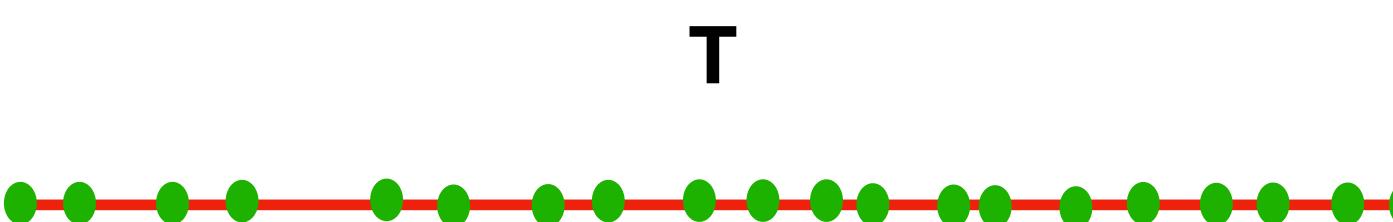
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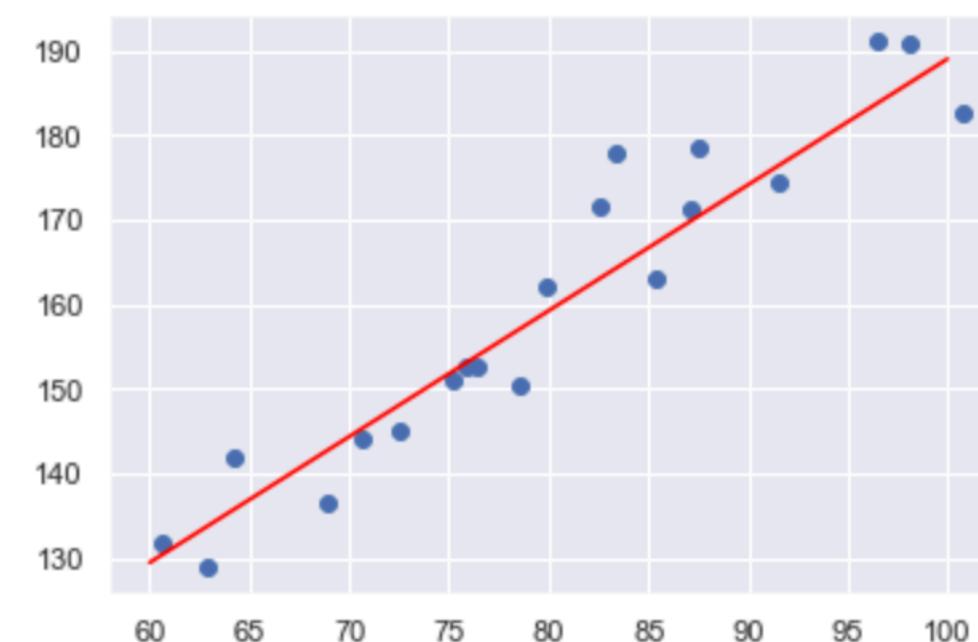
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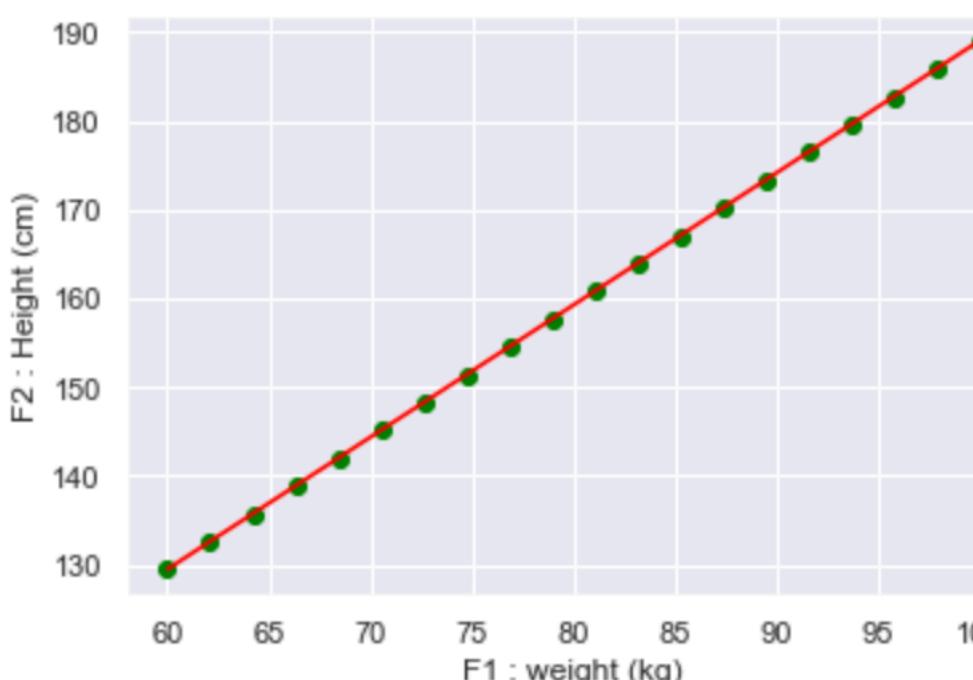
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$$\begin{aligned} p(x | \theta) &= \prod_{i=1, \dots, n} p(x_i | \theta) \\ &= \prod_{i=1, \dots, n} \int p(x_i | t_i, \theta) p(t_i) dt_i \end{aligned}$$



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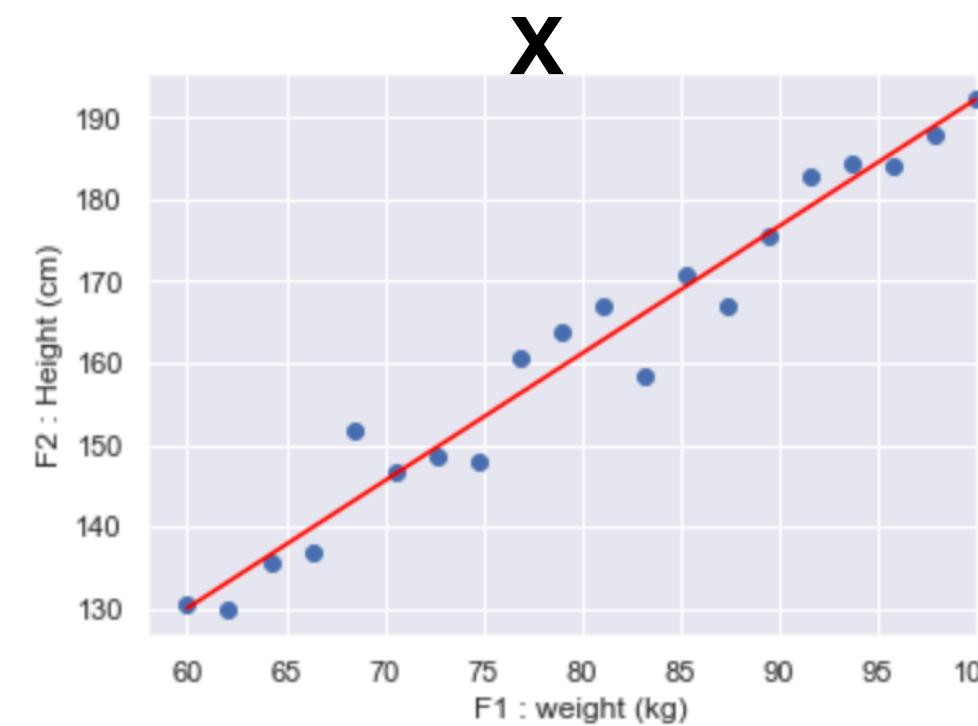


# 3. Probabilistic dimensionality reduction

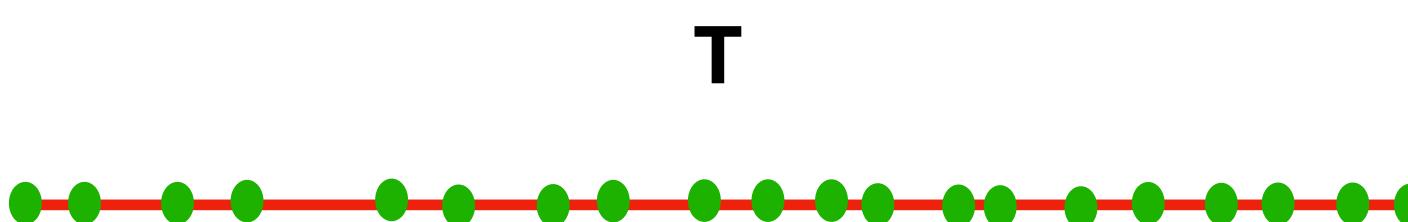
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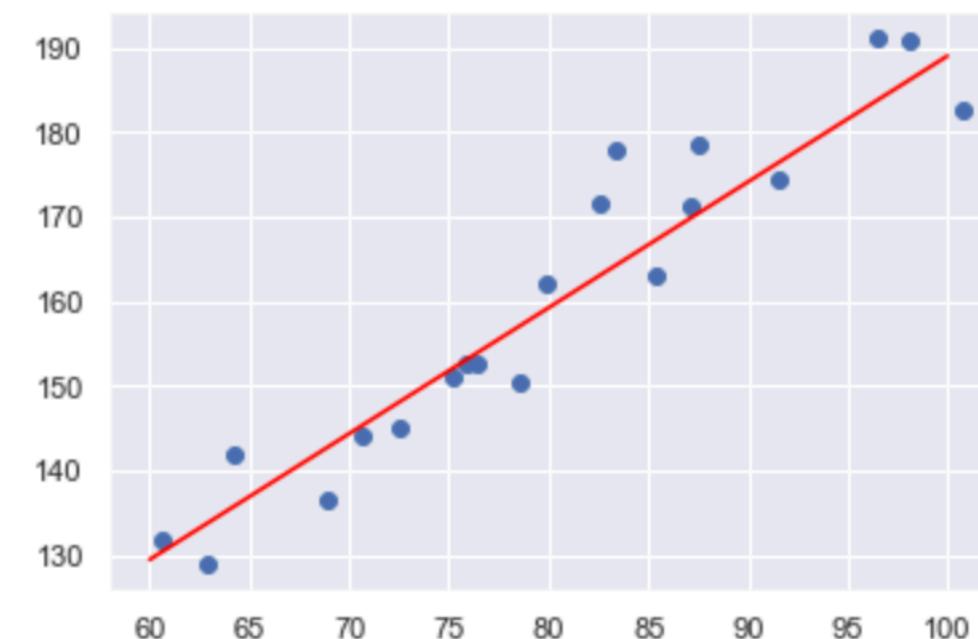
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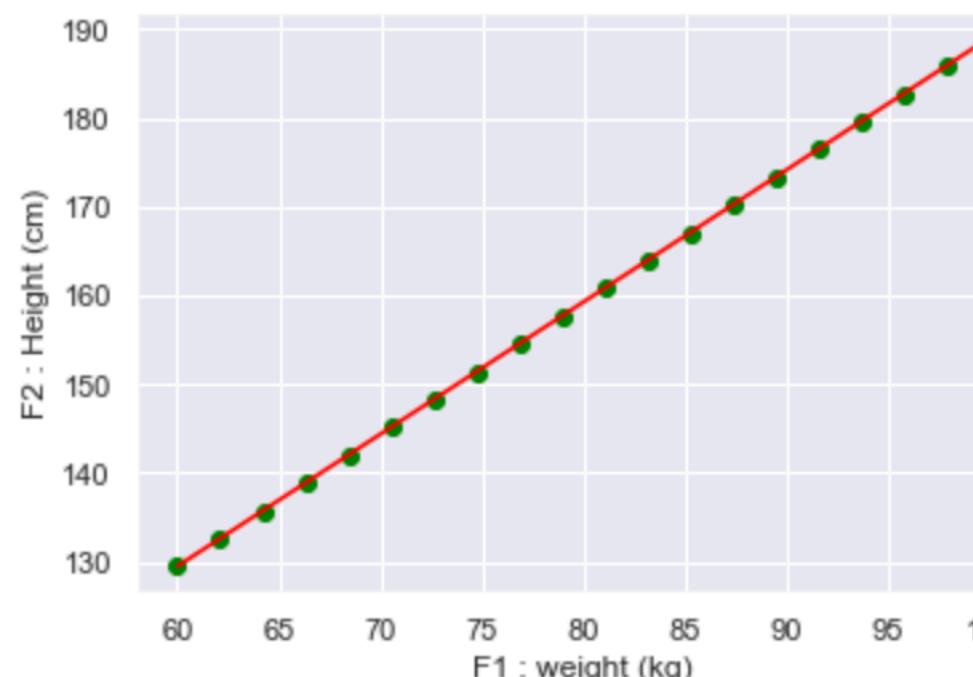
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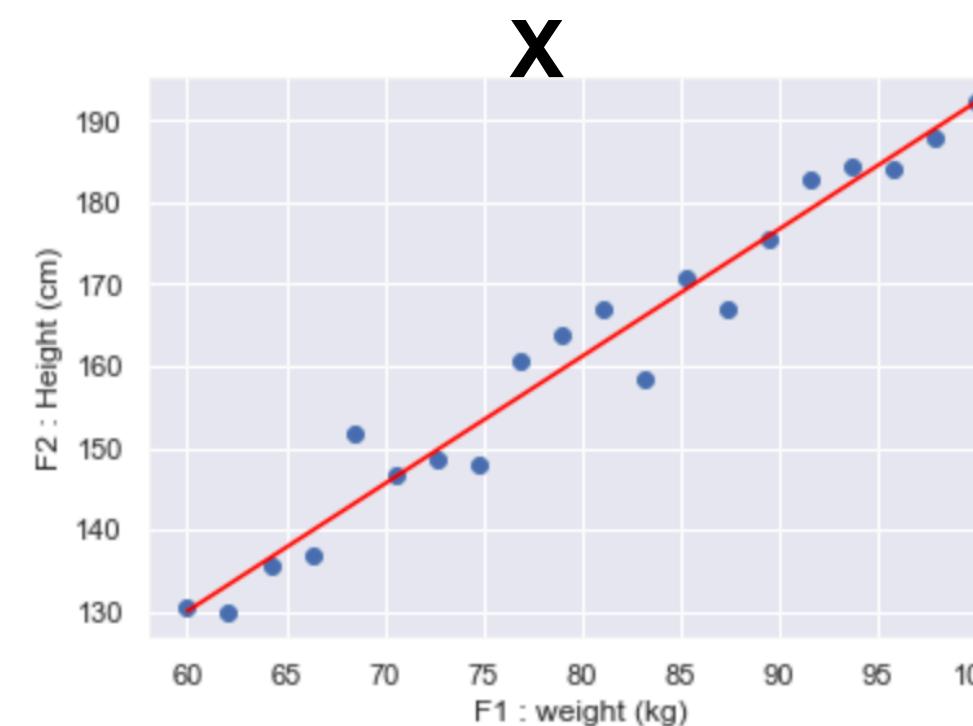
Normal conjugacy !

# 3. Probabilistic dimensionality reduction

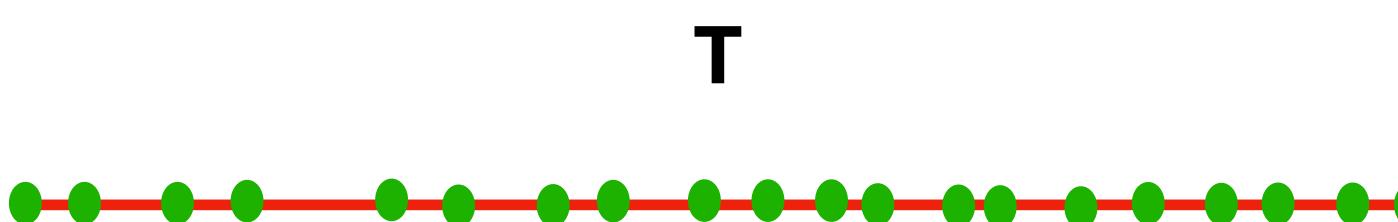
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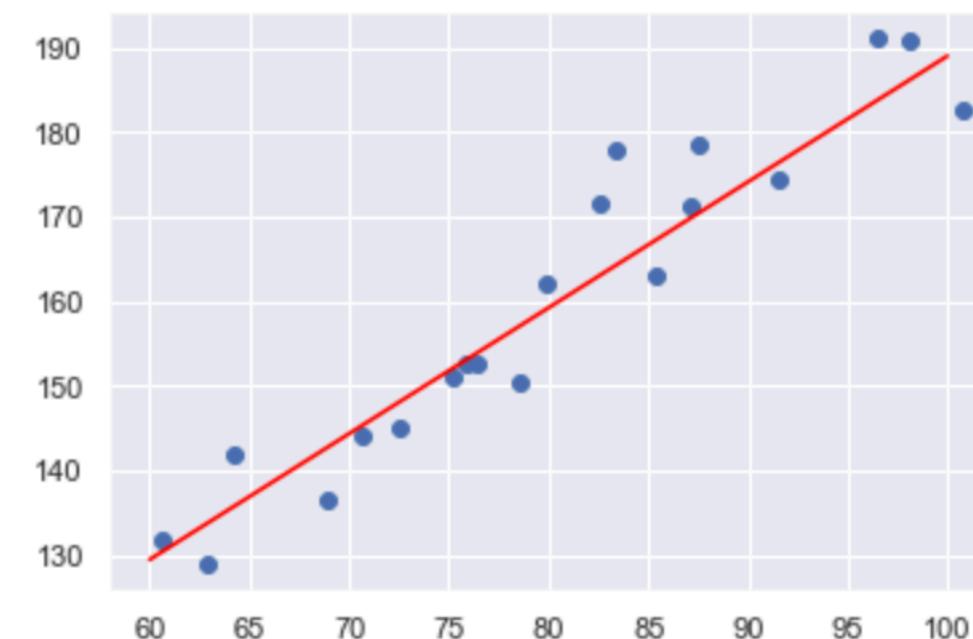
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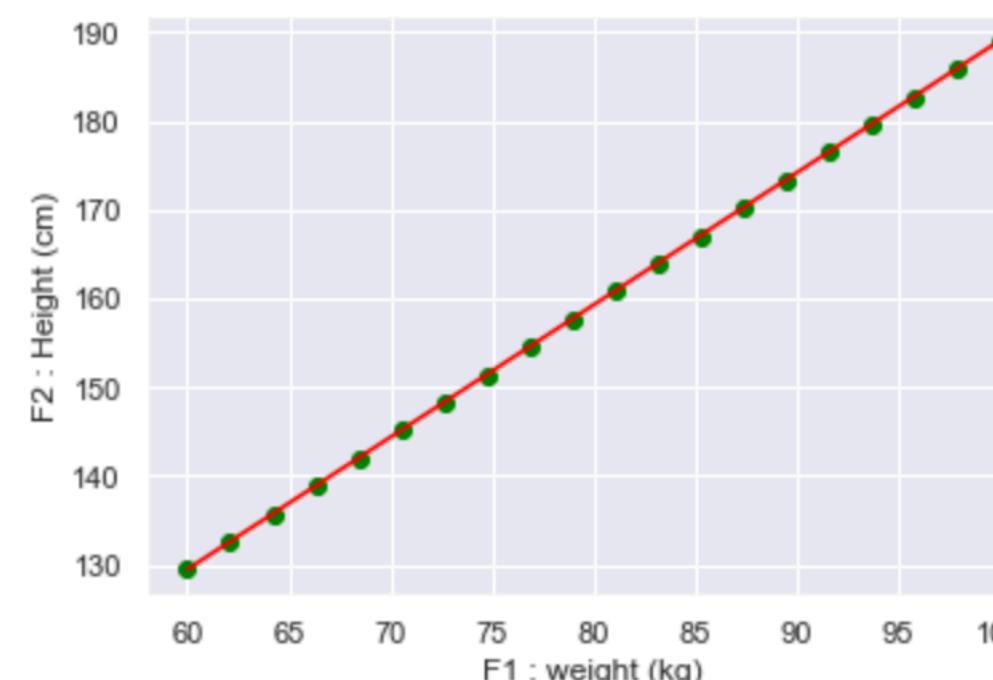
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Normal conjugacy !

*Easy to do EM here !*

# 3. Probabilistic dimensionality reduction

## Dimensionality reduction : probabilistic PCA (PPCA)

Probabilistic PCA : a probabilistic point of view of PCA



EM for PPCA :

E-step :  $q(t_i) = p(t_i | x_i, \theta) = \frac{p(x_i | t_i, \theta) p(t_i)}{\text{constant}}$  prior conjugacy

M-step :  $\max_{\theta} \leftarrow E_{q(t)} \sum_i \log p(x_i | t_i, \theta) p(t_i)$   
 $= \sum_i E_{q(t_i)} \log \left( \frac{1}{\text{const}} e^{-\frac{(x_i - w t_i + b)^2}{2\sigma^2}} e^{-\frac{t_i^2}{2}} \right)$   
 $= \sum_i \log \left( \frac{1}{\text{const}} \right) + \underbrace{\sum_i E_{q(t_i)} \log \left( e^{-\frac{(x_i - w t_i + b)^2}{2\sigma^2}} e^{-\frac{t_i^2}{2}} \right)}$

Some cool things with PPCA :

- We can fill **missing values**
- **Hyperparameters** tuning
- We can do **mixture of PPCA**

quadratic function on  $t$ ,  
so we can do it analytically



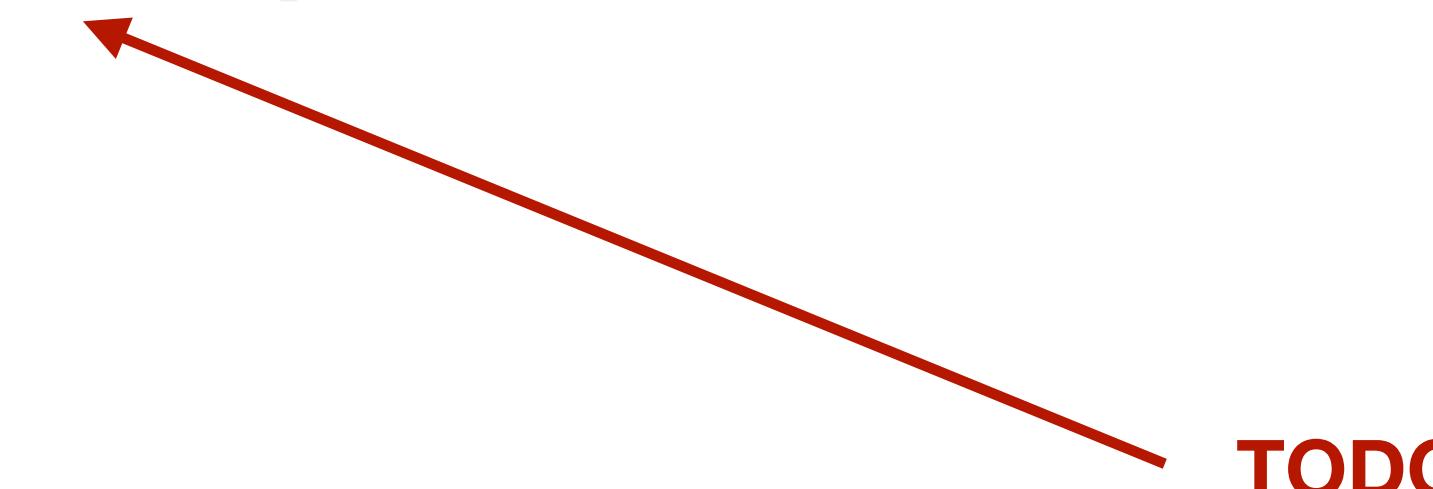
4

## **Applications and examples : notebook**

# Application and examples

website : <https://curiousml.github.io/>

- Master of Science in Artificial Intelligence Systems : **Bayesian Machine Learning** by [François HU](#)
  - **Lecture 1** : Bayesian statistics [[Lecture](#)]
  - **Lecture 2** : Latent Variable Models and EM-algorithm [Soon available]
  - **Lecture 3** : Variational Inference and intro to NLP [Soon available]
  - **Lecture 4** : Markov Chain Monte Carlo [Soon available]
  - **Lecture 5** : [Oral presentations]
  - **Training session / prerequisite** : Statistics with python [[Notebook](#)], [[Data](#)]
  - **Practical work 1** : Conjugate distributions [[Notebook](#)] [[Correction](#)]
  - **Practical work 2** : Probabilistic K-means and probabilistic PCA [[Notebook](#)]
  - **Practical work 3** : Topic Modeling with LDA [Soon available]
  - **Practical work 4** : MCMC samples [Soon available]



TODO

!

## Road map

## Bayesian statistics



1

**Bayesian perspective :**

$$P(\theta | X) = \frac{P(X, \theta)}{P(X)} = \frac{P(X | \theta) \cdot P(\theta)}{P(X)}$$

Likelihood      Prior distribution  
Posterior distribution

 $\theta$  parameters $X$  observations**Exemple :**  
Naive Bayes classifier,  
Linear regression, ....MAP :  $\arg \max_{\theta} P(X | \theta) \cdot P(\theta)$ 

Conjugate distribution

**Pros :**  
- exact posterior**Cons :**  
- conjugate prior  
maybe inadequate

## Latent variable models

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**Bayesian perspective :****Hidden variable models :**

$$P(X | \theta) = \sum_{t \in T_{\text{indexes}}} P(X, T = t | \theta)$$

$$P(X, T | \theta) = P(X | T, \theta)P(T | \theta)$$

**Exemple :**  
GMM, K-means, PCA/PPCA**Pros :**

- fewer parameters / simpler models
- hidden variable sometimes meaningful
- clustering / dimensionality reduction

**Cons :**

- harder to work with
- requires math
- only local maximum or saddle point
- EM : the posterior of T could be intractable

## Variational Inference

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## Causal Inference

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## Oral presentation & Extensions

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