Density Estimation

Data Science I

Cristóbal Donoso O.

September 26, 2018

We have been working...

- Methods for exploring and quantifying structure in a multivariate distribution of points (Exploratory Data Analysis)
- Statistical description of the structure observed to fit models
- The space in the sample can be real physical or space spanned by the measured quantities (attributes)

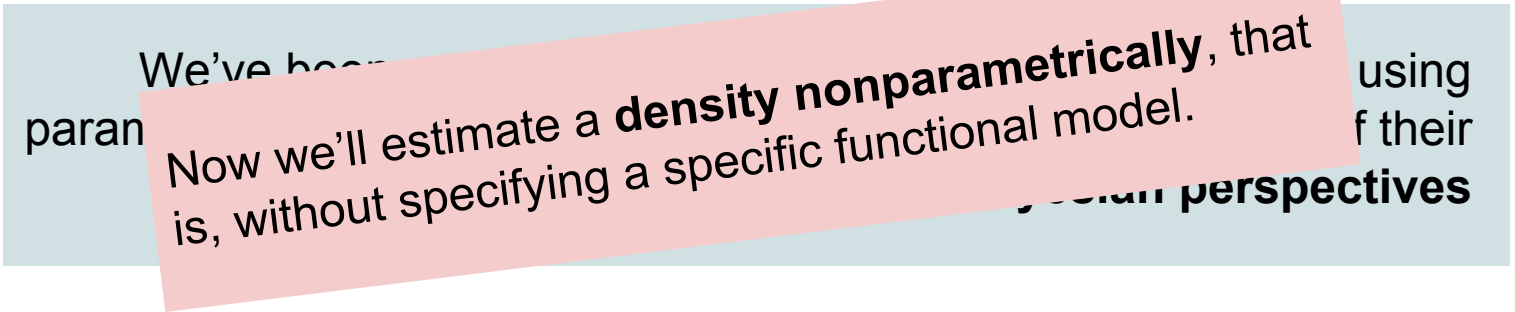
Density Estimation

- To infer the Probabilistic Density Function (PDF) from a sample of data
- Given a PDF estimated from a point data we can generated simulated distributions of a data and compare them against observations
- We can estimate the pdf for each subsample in a set of different labeled samples (Classification)

We've been estimating the underlying density of the data using parametrics models from **density functions** and estimations of their parameters from **Frequentist and Bayesian perspectives**

Density Estimation

- To infer the Probabilistic Density Function (PDF) from a sample of data
- Given a PDF estimated from a point data we can generated simulated distributions of a data and compare them against observations
- We can estimate the pdf for each subsample in a set of different labeled samples (Classification)



Histograms

- A straightforward way to estimate densities is to use Histograms.
- **Each point contributes one unit to the height** of the histogram at the position of it's bin
- The exact locations of the bins **can make a difference**

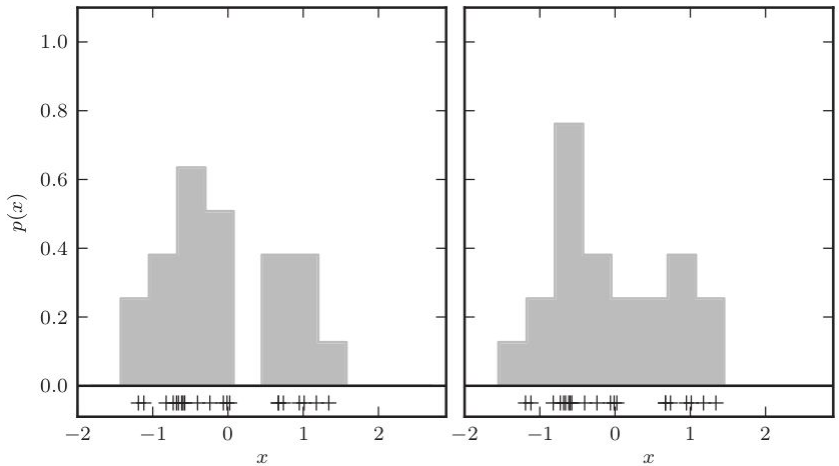


Image Source: Statistics, Data Mining and Machine Learning in Astronomy - Chapter 6 page 252

Improving the basic histogram

- Each point could have it’s own bin
- Allow the bins to overlap
- Each point is **replaced by a box** of unit **height** and some predefined **width**
- The box is usually named **kernel**

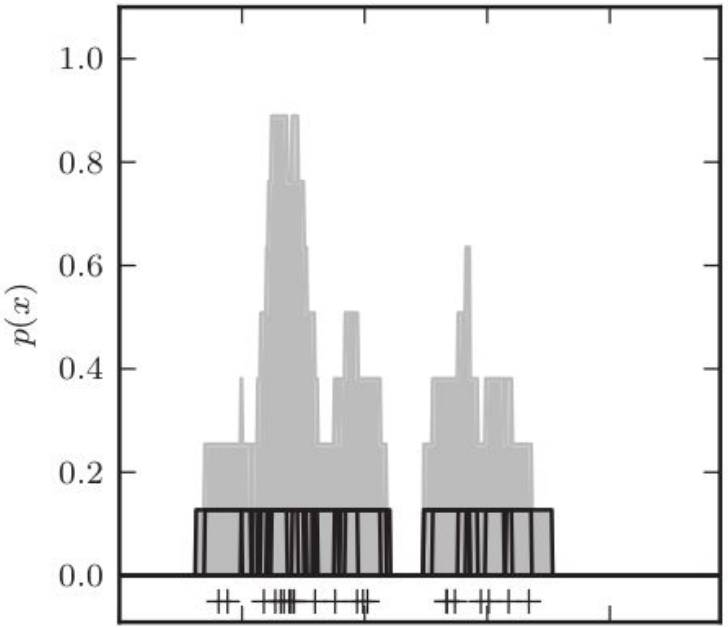


Image Source: Statistics, Data Mining and Machine Learning in Astronomy - Chapter 6 page 252

Kernel Density Estimation

- The **rectangular kernel** does not lead to a **smooth distribution** and can display **suspicious spikes**

- We can use a **Gaussian Kernel** among others

$$\widehat{f}_N(x) = \frac{1}{Nh^D} \sum_{i=1}^{N} K\left(\frac{d(x, x_i)}{h}\right)$$

- The function is estimated as a weighted mean of all points, where the weights are specified via K (u)

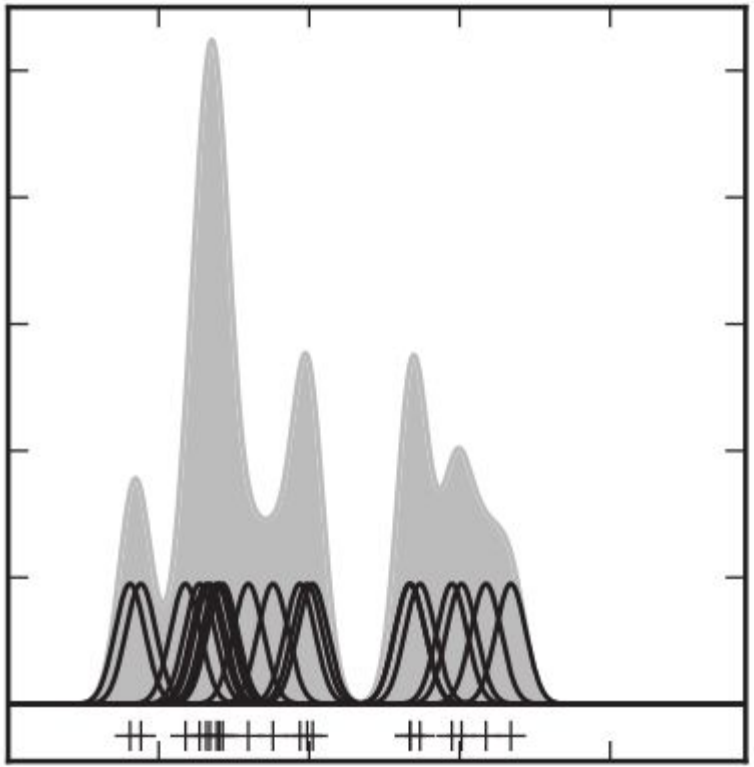


Image Source: Statistics, Data Mining and Machine Learning in Astronomy - Chapter 6 page 252

Kernel Density Estimation

- We can use a **Gaussian Kernel** among others

$$\widehat{f}_N(x) = \frac{1}{Nh^D} \sum_{i=1}^{N} K\left(\frac{d(x, x_i)}{h}\right)$$

- The function is estimated as a weighted mean of all points, where the weights are specified via K(u)
- K(u) is constrained by
  - $(K(u) \geq 0),$ (positives values)
  - $\int K(u)\, du = 1$ (normalized)
  - $\int uK(u)\, du = 0$ (mean)
  - $\sigma_K^2 = \int u^2 K(u)\, du \geq 0),$ (variance)

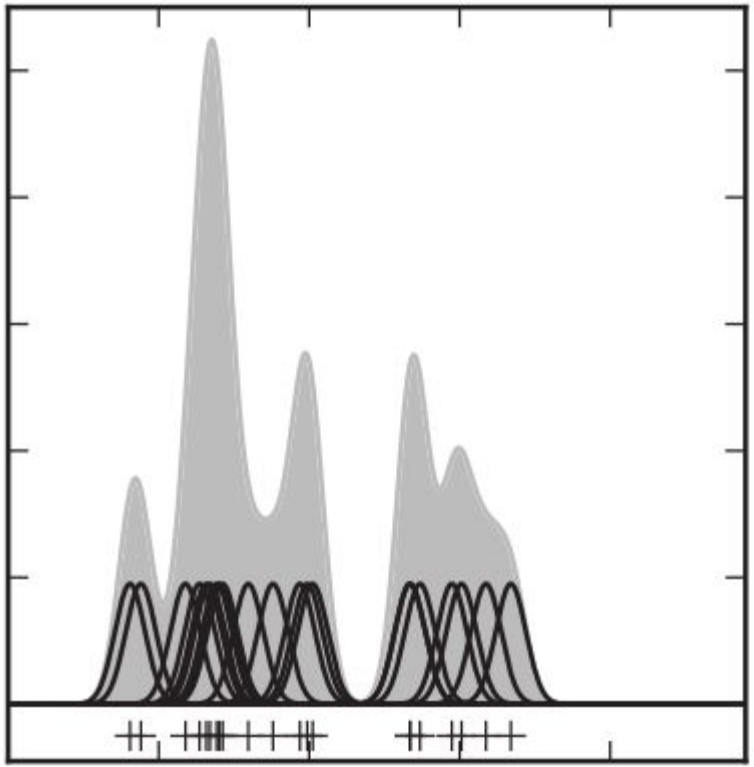


Image Source: Statistics, Data Mining and Machine Learning in Astronomy - Chapter 6 page 252

Types of Kernels

Gaussian Kernel

$$K(u) = \frac{1}{(2\pi)^{D/2}} e^{-u^2/2}$$

Top-hat Kernel

$$K(u) = \begin{cases} \frac{1}{V_D(1)} & \text{if } u \leq 1, \\ 0 & \text{if } u > 1, \end{cases}$$

Exponential Kernel

$$K(u) = \frac{1}{D!\, V_D(1)} e^{-|u|},$$

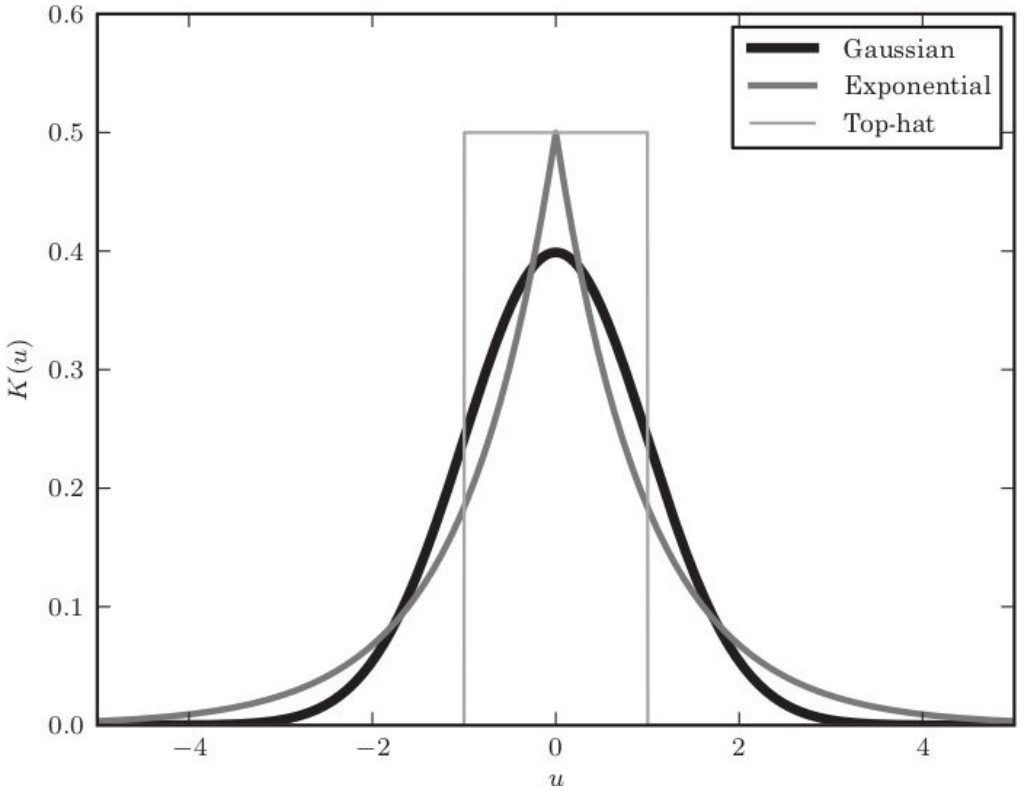
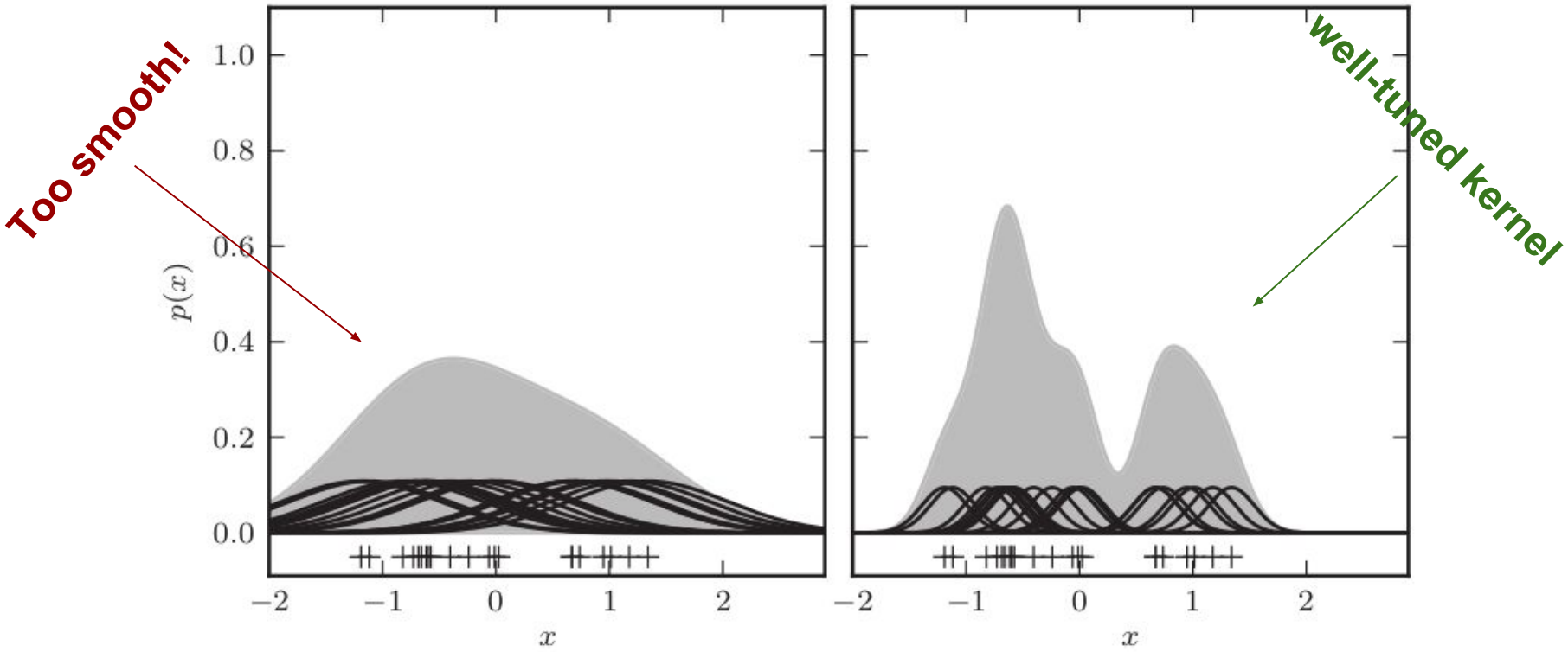


Image Source: Statistics, Data Mining and Machine Learning in Astronomy - Chapter 6 page 252

The amplitude (or bandwidth) of the kernel could generate densities that are too smooth and deleting important information from peaks



Selecting the bandwidth

1. Assuming an underlying Gaussian distribution: Scott's rule:

$$h = 3.5\sigma / N^{1/3}$$

2. Non-Gaussian distributions:

$$h = 2(q_{75} - q_{25}) / N^{1/3}$$

3. Cross-validation: Given **n** data points in the original sample then, **n-p samples are used to train the model** and **p points are used as the validation set**. This is repeated for all combinations in which original sample can be separated this way, and then the error is averaged for all trials, to give overall effectiveness (*).

(*) https://towardsdatascience.com/cross-validation-in-machine-learning-72924a69872f

Cross-validation to select the bandwidth

An alternative to likelihood cross-validation is to use the mean integrated square error

$$\int (\widehat{f}_h - f)^2 = \int \widehat{f}_h^2 - 2\int \widehat{f}_h f + \int f^2.$$

As before, the first term can be obtained analytically, and the last term does not depend on h. For the second term we have expectation value

$$\mathbb{E}\left[\int \widehat{f}_h(x) f(x)\, dx\right] = \mathbb{E}\left[\frac{1}{N}\sum_{i=1}^{N} \widehat{f}_{h,-1}(x)\right].$$

This motivates the L2 cross-validation score:

$$\mathrm{CV}_{L_2}(h) = \int \widehat{f}_h^2 - 2\frac{1}{N}\sum_{i=1}^{N} \widehat{f}_{h,-i}(x_i)$$

Cross-validation to select the bandwidth

An alternative to likelihood cross-validation is to use the mean integrated square error

$$\int (\widehat{f}_h - f)^2 = \int \widehat{f}_h^2 - 2\int \widehat{f}_h f + \int f^2.$$

As before, the first term can be obtained analytically, and the last term does not depend on h. For the second term we have expectation value

$$\mathbb{E}\left[\int \widehat{f}_h(x) f(x)\, dx\right] = \mathbb{E}\left[\frac{1}{N}\sum_{i=1}^{N} \widehat{f}_{h,-1}(x)\right].$$

This motivates the L2 cross-validation score:

$$\mathrm{CV}_{L_2}(h) = \int \widehat{f}_h^2 - 2\frac{1}{N}\sum_{i=1}^{N} \widehat{f}_{h,-i}(x_i) \quad \xrightarrow{\text{Optimal h}} \quad \mathrm{argmax}_h\, \mathrm{CV}_{L_2}(h)$$

Cross-validation to select the bandwidth

This motivates the L 2 cross-validation score:

$$\mathrm{CV}_{L_2}(h) = \int \widehat{f}_h^2 - 2\frac{1}{N}\sum_{i=1}^{N} \widehat{f}_{h,-i}(x_i)$$

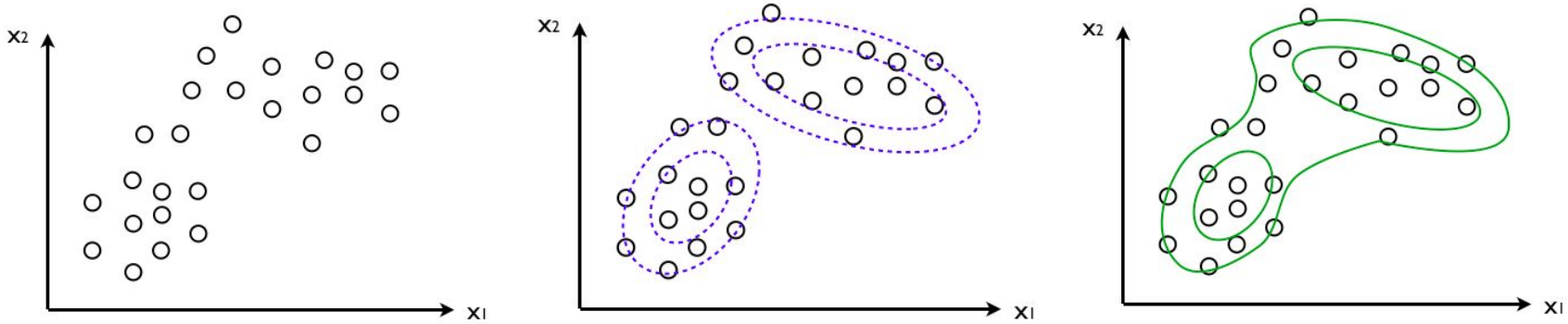
When doing density estimation we are actually estimating the pdf of our parameters. In that sense, we can use our test set (leave-one-out) to directly estimate the likelihood of that set of points.

$$\mathrm{CV}_l(h) = \frac{1}{N}\sum_{i=1}^{N} \log \widehat{f}_{h,-i}(x_i),$$

Optimal h → $\mathrm{argmax}_h CV_l(h)$

Parametric Density Estimation

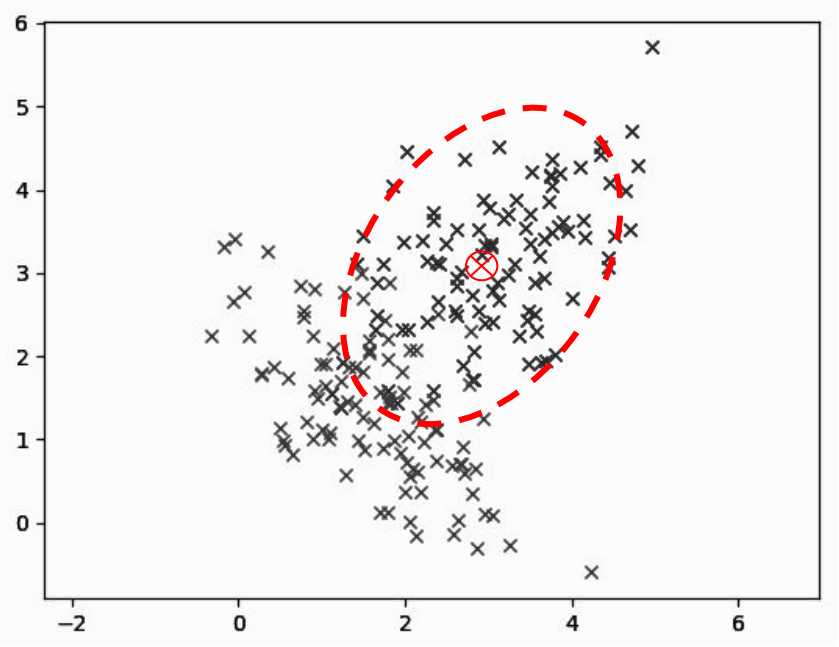
- We can use fewer kernels, and fit for the kernel locations as well as the widths



- The contribution of the full set of clusters at any given point
- The location and size of each component is assumed to reflect some underlying property of the data

Parametric Density Estimation: Gaussian Approach

- We can use Gaussians to model the behavior of the data



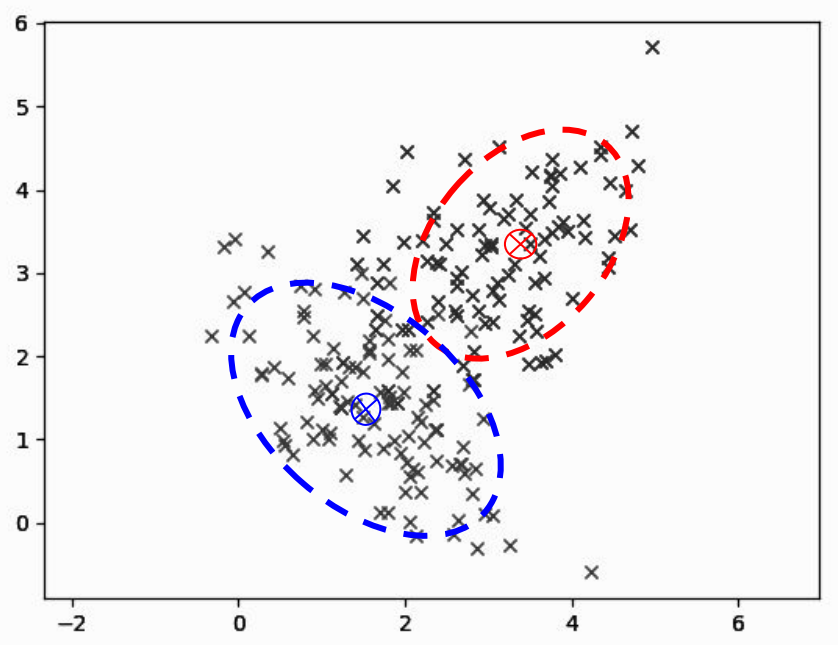
- We assume that exists some **latent variable** which generate the data
- This **latent variable** follows:

$$p(\boldsymbol{x}|z) = \mathcal{N}(\boldsymbol{x}|\mu\square, C\square)$$

- We could not capture distributions of minority data groups

Parametric Density Estimation: Gaussian Approach

- If one gaussian doesn't work, we could use several of them



- We assume that exists a group of latent variables $z \in \{e_1, \ldots, e_\square\}$, where e is a categorical vector which is used to select a particular variable z
- The density of each data point

$$p(\mathbf{x}|z = e_k) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

- The marginal distribution of **x** is then obtained by summing the joint distribution over all possible states of **z**

$$p(\mathbf{x}) = \sum_{\mathbf{z}} p(\mathbf{z})p(\mathbf{x}|\mathbf{z}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$$

Gaussian Mixture Model

GMM models the underlying density (pdf) of points as a sum of Gaussians.

The density of the points is given by

$$\rho(\mathbf{x}) = Np(\mathbf{x}) = N\sum_{k=1}^{K}\pi_k\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k) \xrightarrow{\text{log-likelihood}} \sum_{n=1}^{N}\ln\left\{\sum_{k=1}^{K}\pi_k\mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k,\boldsymbol{\Sigma}_k)\right\}.$$

where

- K is the number of Gaussian
- μ□ means or locations of the Gaussians
- Σ□ covariances of the Gaussians
- $\boldsymbol{\pi}$□ mixing coefficient for each Gaussian, restricte $\sum_{k=1}^{K}\pi_k = 1.$

Gaussian Mixture Model: Optimizing parameters

- **MLE** is more complicated for optimization in multiple dimensions
- Alternatively, we can use the **expectation maximization** method, where the model depends on unobserved latent variables:
- The goal of this technique is to assume some initial mean μ, standard deviation **Σ** and normalization factors **α** and **iteratively improve the estimate**
    - **E-step:** calculate the expected joint (data + latent variable) log-likelihood at iteration t.
    - **M-step:** maximize such likelihood in terms of the model parameters. $\theta=(\alpha,\{\mu\square\},\{C\square\})$

EM for Gaussian Mixture Model: Expectation step

Making the derivatives of $\ln p(\mathbf{X}|\boldsymbol{\pi}, \boldsymbol{\mu}, \boldsymbol{\Sigma})$ w.r.t each means μ to zero

$$0 = -\sum_{n=1}^{N} \underbrace{\frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)}{\sum_j \pi_j \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_j, \boldsymbol{\Sigma}_j)}}_{\gamma(z_{nk})} \boldsymbol{\Sigma}_k(\mathbf{x}_n - \boldsymbol{\mu}_k)$$

where $\gamma(z_{nk})$ is the **responsibility**. It can be viewed as the posterior probability once we have observed x.

In this step **we evaluate the responsibilities using the current parameter values**

EM for Gaussian Mixture Model: Maximization Step

Re-estimate the parameters using the **current responsibilities**

$$\boldsymbol{\mu}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \mathbf{x}_n$$

$$\boldsymbol{\Sigma}_k^{\text{new}} = \frac{1}{N_k} \sum_{n=1}^{N} \gamma(z_{nk}) \left(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}}\right) \left(\mathbf{x}_n - \boldsymbol{\mu}_k^{\text{new}}\right)^{\mathrm{T}}$$

$$\pi_k^{\text{new}} = \frac{N_k}{N}$$

where

$$N_k = \sum_{n=1}^{N} \gamma(z_{nk}).$$

EM for Gaussian Mixture Model: Evaluating convergence

In order to stop the iterative process we shall define a convergence criterion. We have to:

1. evaluate the log-likelihood, using the maximized parameters and check the convergence.

$$\ln p(\mathbf{X}|\boldsymbol{\mu}, \boldsymbol{\Sigma}, \boldsymbol{\pi}) = \sum_{n=1}^{N} \ln \left\{ \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) \right\}$$

2. if the statement is not satisfied, go back and repeat the EM steps

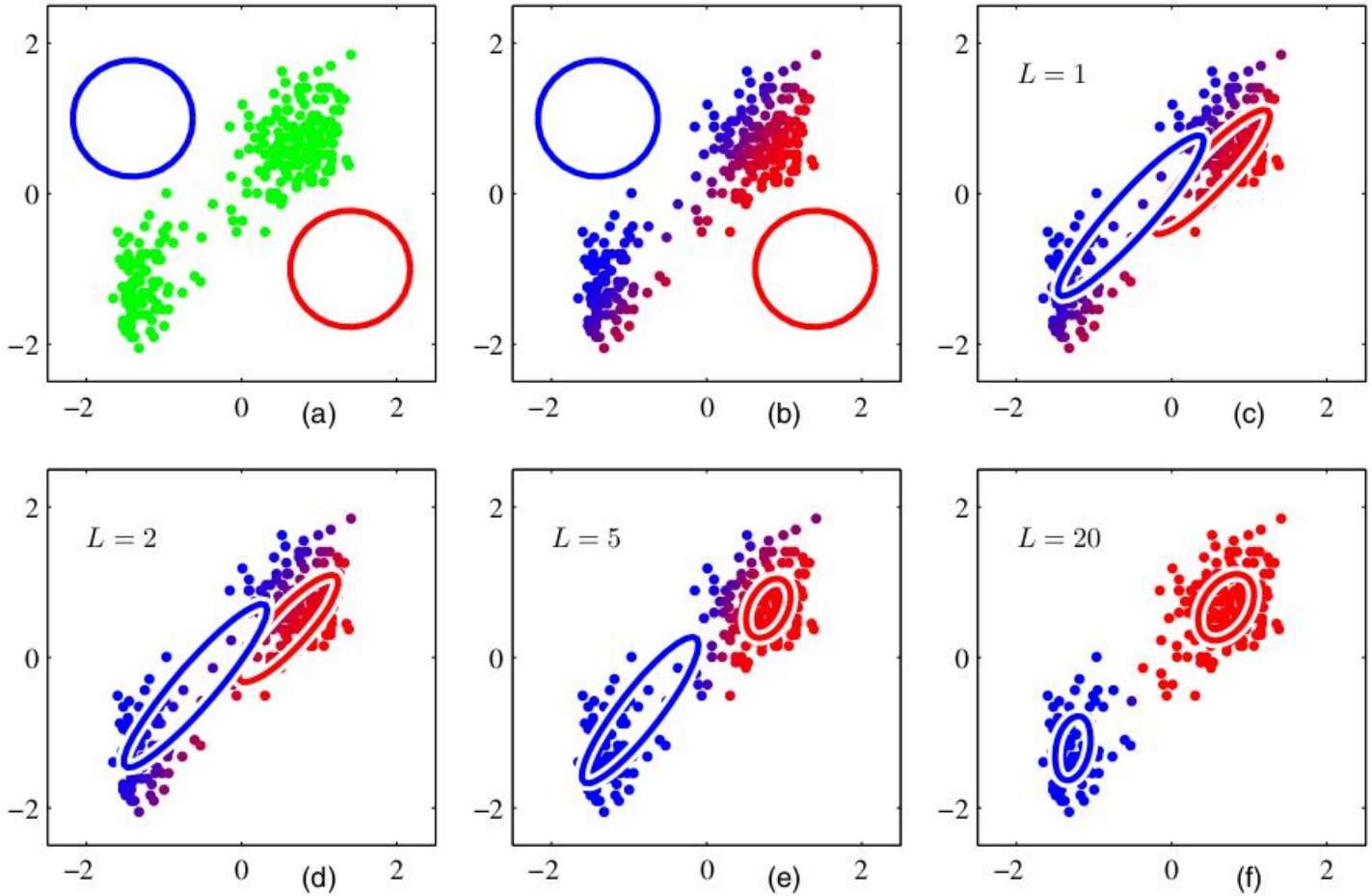


Figure source: Bishop - Pattern Recognition and Machine Learning - pag 437

Ok, we've obtain a fitted beautiful Gaussian from data, but

How many Gaussians should we use?

Model Selection

As we have seen before, in order to compare different models, the prefered technique is cross-validation. Nevertheless, there are classical methods that are easy to use and often effective for simple models. Two of those are

1. the Akaike Information Criterion (AIC)

2. the Bayesian Information Criterion (BIC).

Model Selection: Akaike Information Criterion (AIC)

Akaike Information Criterion penalizes the model based on its complexity. It is defined a

$$AIC(\theta) = -2\log p(X|\theta) + 2k$$

where,

- θ is the model
- X is the input data
- $\log p(X|\theta)$ is the log likelihood
- k is the number of parameters

Source: https://pdfs.semanticscholar.org/9063/d849a9cf4c9f7abf39d5416721ef90ff9e57.pdf

Model Selection: Bayesian Information Criterion (BIC).

BIC gives us a way to choose between different models with different numbers of parameters by **selecting the one which gives us the lowest BIC score**.

$$BIC(\theta) = -2logp(X|\theta) + k\log(n)$$

It is only valid for sample size n much larger than the number k of parameters in the model.

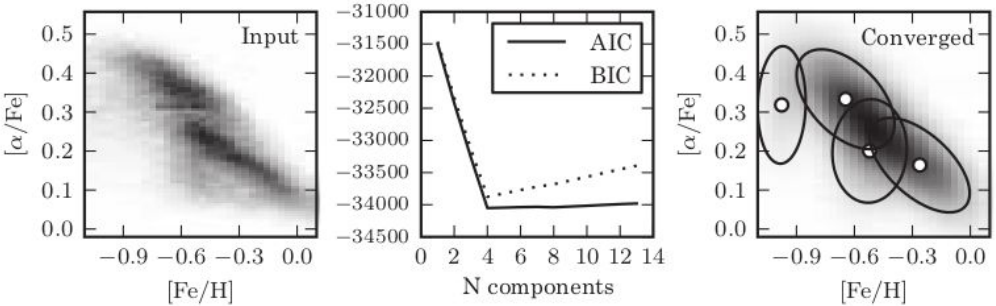
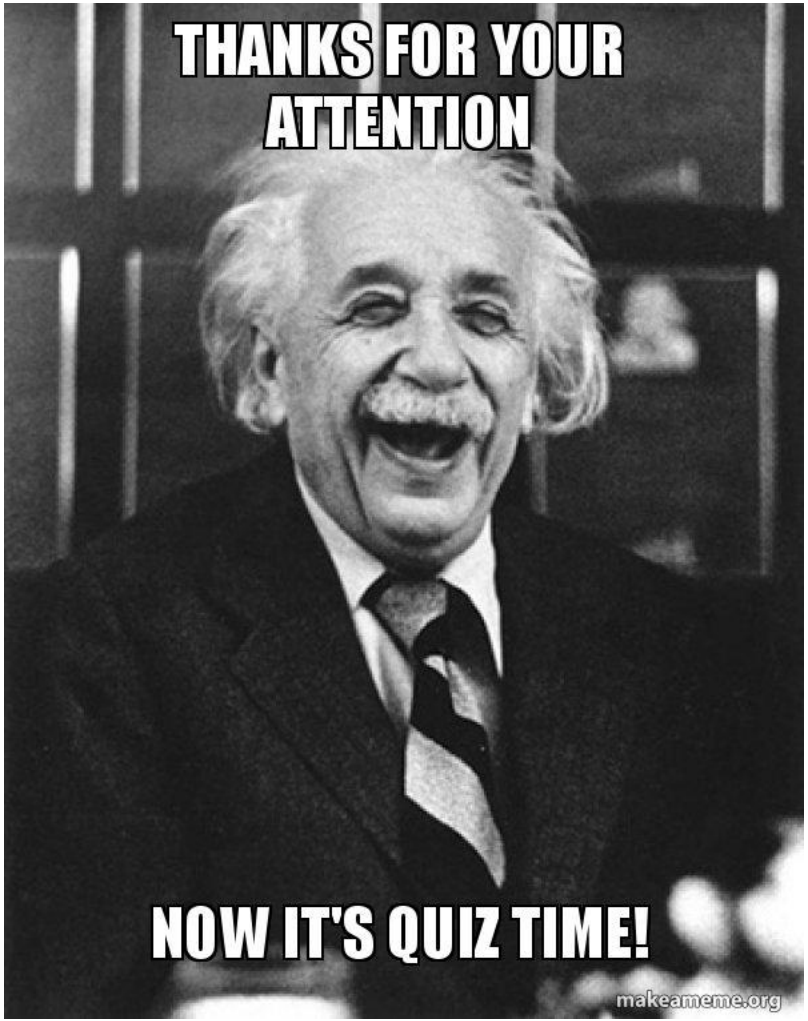


Image Source: Statistics, Data Mining and Machine Learning in Astronomy - Chapter 6 page 252


THANKS FOR YOUR ATTENTION
NOW IT'S QUIZ TIME!
makeameme.org