

Model selection for Gaussian mixtures



Pierre-Alexandre Mattei

<http://pamattei.github.io> – @pamattei
pierre-alexandre.mattei@inria.fr

MSc Data Science

Recap on GMMs

Model selection for GMMs

GMMs beyond clustering

Recap on GMMs

Model selection for GMMs

GMMs beyond clustering

Gaussian mixture models

We have some data $\mathbf{x}_1, \dots, \mathbf{x}_N \in \mathbb{R}^D$. A **Gaussian mixture model with K clusters** is a statistical model $(p_\theta, \theta \in \Theta_K)$ with the following density

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

with $\theta = (\pi_1, \dots, \pi_K, \boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_K, \boldsymbol{\Sigma}_1, \dots, \boldsymbol{\Sigma}_K)$.

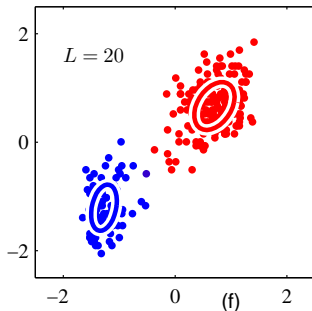


Figure: Figure 9.8 from Bishop's book.

The parameters of a Gaussian mixture model

Consider the model

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

with $\theta = (\pi_1, \dots, \pi_K, \boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_K, \boldsymbol{\Sigma}_1, \dots, \boldsymbol{\Sigma}_K)$.

What are the constraints on the parameters? In other words, in which space the proportions, means, and covariances live?

The proportions and means

The proportions must sum to one! So

$$(\pi_1, \dots, \pi_K) \in \Delta_K,$$

with $\Delta_K = \{\mathbf{t} \in \mathbb{R}^K, t_1 + \dots + t_K = 1\}$. This set is usually called the **simplex**.

The means $\boldsymbol{\mu}_1, \dots, \boldsymbol{\mu}_K$ are simply vectors in \mathbb{R}^D .

The covariances $\boldsymbol{\Sigma}_1, \dots, \boldsymbol{\Sigma}_K$ must be symmetric positive definite matrices. This means that they are symmetric and all their eigenvalues are strictly positive.

Recap on GMMs

Model selection for GMMs

GMMs beyond clustering

Choosing the number of clusters as model selection

The goal is to choose the number of clusters K . This is a **model selection** problem. Each number of clusters corresponds indeed to a model (i.e. a parametric family of densities)

$$\mathcal{M}_k = (p_\theta, \theta \in \Theta_K).$$

What model selection techniques do you know?

Model selection

The goal is to choose the number of clusters K . This is a **model selection** problem. Each number of clusters corresponds indeed to a model (i.e. a parametric family of densities)

$$\mathcal{M}_k = (p_\theta, \theta \in \Theta_K).$$

What model selection techniques do you know?

Penalised model selection

A first important school of techniques for model selection is to maximise a **penalised likelihood criterion**:

$$\mathcal{L}(\mathcal{M}_k) = \sum_{i=1}^n \log p_{\hat{\theta}_k}(x_i) - \text{penalty}(\mathcal{M}_k),$$

where $\hat{\theta}_k$ is the maximum likelihood estimate for model \mathcal{M}_k .

At the end, we choose the model with the largest $\mathcal{L}(\mathcal{M}_k)$.

The role of the penalty is to **discourage overly complex models**, and avoid overfitting. What does "overly complex" mean in a clustering context?

Penalised model selection

$$\mathcal{L}(\mathcal{M}_k) = \sum_{i=1}^n \log p_{\hat{\theta}_k}(x_i) - \text{penalty}(\mathcal{M}_k),$$

Overly complex can (for example) mean "with too many clusters". One way to formalise this is by **counting the number of free parameters** $q_k = \dim(\Theta_k)$. This leads to the following (famous?) penalties:

- $\text{penalty}_{\text{AIC}} = q_k$
- $\text{penalty}_{\text{BIC}} = q_k \log(n)/2$.

The BIC also has a Bayesian interpretation, but we won't talk about it today.

Validation using the likelihood

Another way of doing model selection is to compute the likelihood on a validation set, and choose the model with the largest validation likelihood.

A more advanced approach would be to use **cross-validation**.

Counting GMM parameters

The proportions must sum to one! So

$$(\pi_1, \dots, \pi_K) \in \Delta_K,$$

with $\Delta_K = \{\mathbf{t} \in \mathbb{R}^K, t_1 + \dots + t_K = 1\}$. This set is usually called the **simplex**. This will lead to **$K - 1$ free parameters**.

Counting GMM parameters

The proportions must sum to one! So

$$(\pi_1, \dots, \pi_K) \in \Delta_K,$$

with $\Delta_K = \{\mathbf{t} \in \mathbb{R}^K, t_1 + \dots + t_K = 1\}$. This set is usually called the **simplex**. This will lead to $K - 1$ free parameters.

The means μ_1, \dots, μ_K are simply vectors in \mathbb{R}^D . This will lead to KD free parameters.

The covariances $\Sigma_1, \dots, \Sigma_K$ must be symmetric positive definite matrices. This means that they are symmetric and all their eigenvalues are strictly positive. Because of the symmetry, this leads to $KD(D + 1)/2$ free parameters.

Recap on GMMs

Model selection for GMMs

GMMs beyond clustering

Classification with mixture discriminant analysis

Another interesting application of GMMs is **mixture discriminant analysis**. It is a generative model for classification that assumes that, for each class c ,

$$p(\mathbf{x}|c) = \sum_{k=1}^K \pi_{kc} \mathcal{N}(\mathbf{x} | \boldsymbol{\mu}_{kc}, \boldsymbol{\Sigma}_{kc}).$$

One can train this with EM, and then do classification by computing

$$p(c|\mathbf{x}) = \frac{p(\mathbf{x}|c)p(c)}{p(\mathbf{x})}.$$

Question. What would the EM look like?

Semi supervised learning

When some labels y_1, \dots, y_{n_1} are observed, it is a **semi supervised learning** setting. A GMM can still be learned by maximising the **observed likelihood**

$$\sum_{i=1}^{n_1} \log p(x_i, y_i) + \sum_{i=n_1+1}^n \log p(x_i).$$

We'll talk more about this when we talk about **missing data**. An EM can be used again to maximise the likelihood.

