Model selection for Gaussian mixtures

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MSc Data Science

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Gaussian mixture models

We have some data $\mathbf{x}_1, ..., \mathbf{x}_N \in \mathbb{R}^D$. 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 $\theta = (\pi_1, ..., \pi_K, \boldsymbol{\mu}_1, ..., \boldsymbol{\mu}_K, \boldsymbol{\Sigma}_1, ..., \boldsymbol{\Sigma}_K)$.

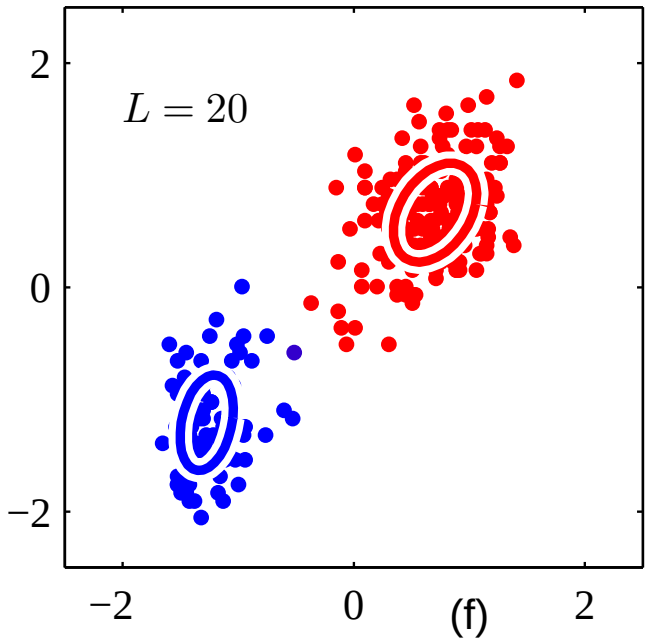

Figure: **Figure 9.8 from Bishop's book.**

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

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

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

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

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

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

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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

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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

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The means $\boldsymbol{\mu}_1, ..., \boldsymbol{\mu}_K$ are simply vectors in $\mathbb{R}^D$. This will lead to KD free parameters.

The covariances $\boldsymbol{\Sigma}_1, ..., \boldsymbol{\Sigma}_K$ 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.

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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 $y_1, ..., y_{n_1}$ 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.