Gaussian Mixture Model
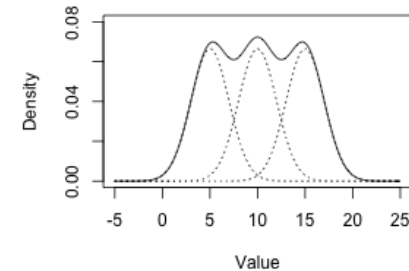
Gaussian mixture models are a probabilistic model for representing normally distributed subpopulations within an overall population. Mixture models in general don't require knowing which subpopulation a data point belongs to, allowing the model to learn the subpopulations automatically. Since subpopulation assignment is not known, this constitutes a form of unsupervised learning.

A Gaussian mixture of three normal distributions.[1]

For example, in modeling human height data, height is typically modeled as a normal distribution for each gender with a mean of approximately 5'10" for males and 5'5" for females. Given only the height data and not the gender assignments for each data point, the distribution of all heights would follow the sum of two scaled (different variance) and shifted (different mean) normal distributions. A model making this assumption is an example of a Gaussian mixture model (**GMM**), though in general a GMM may have more than two components. Estimating the parameters of the individual normal distribution components is a canonical problem in modeling data with GMMs.

GMMs have been used for feature extraction from speech data, and have also been used extensively in object tracking of multiple objects, where the number of mixture components and their means predict object locations at each frame in a video sequence.

Contents

Motivation

One hint that data might follow a mixture model is that the data looks multimodal, i.e. there is more than one "peak" in the distribution of data. Trying to fit a multimodal distribution with a unimodal (one "peak") model will generally give a poor fit, as shown in the example below. Since many simple distributions are unimodal, an obvious way to model a multimodal distribution would be to assume that it is generated by multiple unimodal distributions. For several theoretical reasons, the most commonly used distribution in modeling real-world unimodal data is the Gaussian distribution. Thus, modeling multimodal data as a mixture of many unimodal Gaussian distributions makes intuitive sense. Furthermore, GMMs maintain many of the theoretical and computational benefits of Gaussian models, making them practical for efficiently modeling very large datasets.
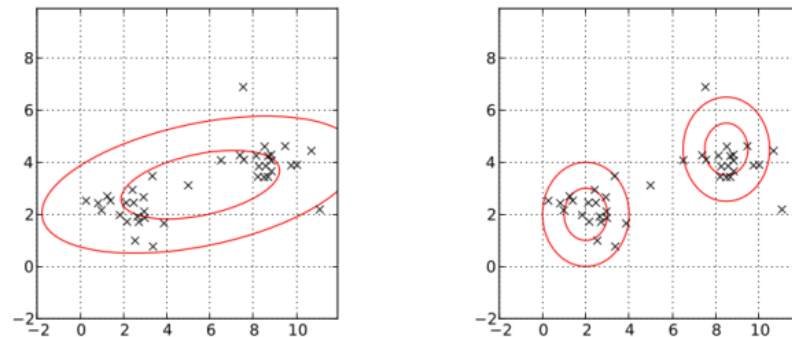
(Left) Fit with one Gaussian distribution (Right) Fit with Gaussian mixture model with two components

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TRY IT YOURSELF

Which of the following data sets is most likely to be well-modeled by a Gaussian mixture model?

○ Numbers of pregnancies across many humans

○ Speeds across cars just before reaching a specific traffic light

○ Student scores on a specific standardized test

The Model

A Gaussian mixture model is parameterized by two types of values, the mixture **component weights** and the component **means** and **variances/covariances**. For a Gaussian mixture model with K components, the kth component has a mean of μ_k and variance of σ_k for the univariate case and a mean of $\vec{\mu}_k$ and covariance matrix of Σ_k for the multivariate case. The mixture component weights are defined as ϕ_k for component C_k, with the constraint that $\sum_{i=1}^{K} \phi_i = 1$ so that the total probability distribution normalizes to 1. If the component weights aren't learned, they can be viewed as an a-priori distribution over components such that $p(x \text{ generated by component } C_k) = \phi_k$. If they are instead learned, they are the a-posteriori estimates of the component probabilities given the data.

One-dimensional Model

$$p(x) = \sum_{i=1}^{K} \phi_i \mathcal{N}(x \mid \mu_i, \sigma_i)$$

$$\mathcal{N}(x \mid \mu_i, \sigma_i) = \frac{1}{\sigma_i \sqrt{2\pi}} \exp\left(-\frac{(x - \mu_i)^2}{2\sigma_i^2}\right)$$

$$\sum_{i=1}^{K} \phi_i = 1$$

Multi-dimensional Model

$$p(\vec{x}) = \sum_{i=1}^{K} \phi_i \mathcal{N}(\vec{x} \mid \vec{\mu}_i, \Sigma_i)$$

$$\mathcal{N}(\vec{x} \mid \vec{\mu}_i, \Sigma_i) = \frac{1}{\sqrt{(2\pi)^K |\Sigma_i|}} \exp\left(-\frac{1}{2}(\vec{x} - \vec{\mu}_i)^{\mathrm{T}} \Sigma_i^{-1} (\vec{x} - \vec{\mu}_i)\right)$$

$$\sum_{i=1}^{K} \phi_i = 1$$

Learning the Model

If the number of components K is known, expectation maximization is the technique most commonly used to estimate the mixture model's parameters. In frequentist probability theory, models are typically learned by using maximum likelihood estimation techniques, which seek to maximize the probability, or likelihood, of the observed data given the model parameters. Unfortunately, finding the maximum likelihood solution for mixture models by differentiating the log likelihood and solving for 0 is usually analytically impossible.

Expectation maximization (**EM**) is a numerical technique for maximum likelihood estimation, and is usually used when closed form expressions for updating the model parameters can be calculated (which will be shown below). Expectation maximization is an iterative algorithm and has the convenient property that the maximum likelihood of the data strictly increases with each subsequent iteration, meaning it is guaranteed to approach a local maximum or saddle point.

EM for Gaussian Mixture Models

Expectation maximization for mixture models consists of two steps.

The first step, known as the **expectation** step or **E** step, consists of calculating the expectation of the component assignments C_k for each data point $x_i \in X$ given the model parameters ϕ_k, μ_k, and σ_k.

The second step is known as the **maximization** step or **M** step, which consists of maximizing the expectations calculated in the E step with respect to the model parameters. This step consists of updating the values ϕ_k, μ_k, and σ_k.

The entire iterative process repeats until the algorithm converges, giving a maximum likelihood estimate. Intuitively, the algorithm works because knowing the component assignment C_k for each x_i makes solving for ϕ_k, μ_k, and σ_k easy, while knowing ϕ_k, μ_k, and σ_k makes inferring $p(C_k|x_i)$ easy. The expectation step corresponds to the latter case while the maximization step corresponds to the former. Thus, by alternating between which values are assumed fixed, or known, maximum likelihood estimates of the non-fixed values can be calculated in an efficient manner.

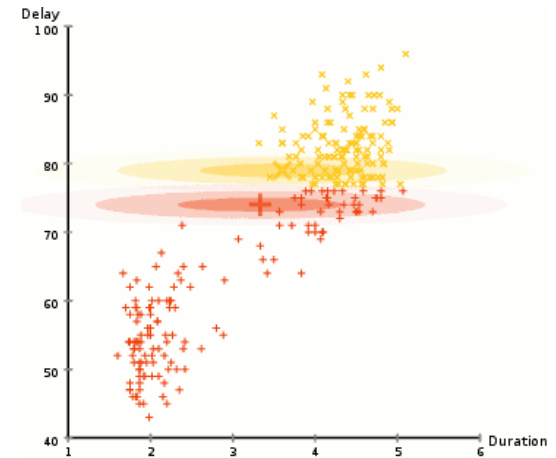**Algorithm for Univariate Gaussian Mixture Models**

The expectation maximization algorithm for Gaussian mixture models starts with an initialization step, which assigns model parameters to reasonable values based on the

data. Then, the model iterates over the expectation (E) and maximization (M) steps until the parameters' estimates converge, i.e. for all parameters θ_t at iteration t, $|\theta_t - \theta_{t-1}| \leq \epsilon$ for some user-defined tolerance ϵ. A graphic of the EM algorithm in action for a two-component, bivariate Gaussian mixture model is displayed on the right.

The EM algorithm for a univariate Gaussian mixture model with K components is described below. A variable denoted $\hat{\theta}$ denotes an estimate for the value θ. All equations can be derived algebraically by solving for each parameter as outlined in the section above titled *EM for Gaussian Mixture Models*.

The EM algorithm updating the parameters of a two-component bivariate Gaussian mixture model.[2]

Initialization Step:

- Randomly assign samples without replacement from the dataset $X = \{x_1, ..., x_N\}$ to the component mean estimates $\hat{\mu}_1, ..., \hat{\mu}_K$. E.g. for $K = 3$ and $N = 100$, set $\hat{\mu}_1 = x_{45}, \hat{\mu}_2 = x_{32}, \hat{\mu}_3 = x_{10}$.
- Set all component variance estimates to the sample variance $\hat{\sigma}_1^2, ..., \hat{\sigma}_K^2 = \frac{1}{N} \sum_{i=1}^{N} (x_i - \bar{x})^2$, where $\bar{x}$ is the sample mean $\bar{x} = \frac{1}{N} \sum_{i=1}^{N} x_i$.
- Set all component distribution prior estimates to the uniform distribution $\hat{\phi}_1, ..., \hat{\phi}_K = \frac{1}{K}$.

Expectation (E) Step:

Calculate $\forall i, k$

$$\hat{\gamma}_{ik} = \frac{\hat{\phi}_k \mathcal{N}(x_i \mid \hat{\mu}_k, \hat{\sigma}_k)}{\sum_{j=1}^{K} \hat{\phi}_j \mathcal{N}(x_i \mid \hat{\mu}_j, \hat{\sigma}_j)},$$

where $\hat{\gamma}_{ik}$ is the probability that x_i is generated by component C_k. Thus, $\hat{\gamma}_{ik} = p(C_k | x_i, \hat{\phi}, \hat{\mu}, \hat{\sigma})$.

Maximization (M) Step:

Using the $\hat{\gamma}_{ik}$ calculated in the expectation step, calculate the following in that order $\forall k$:

- $\hat{\phi}_k = \sum_{i=1}^{N} \dfrac{\hat{\gamma}_{ik}}{N}$

- $\hat{\mu}_k = \dfrac{\sum_{i=1}^{N} \hat{\gamma}_{ik} x_i}{\sum_{i=1}^{N} \hat{\gamma}_{ik}}$

- $\hat{\sigma}_k^2 = \dfrac{\sum_{i=1}^{N} \hat{\gamma}_{ik} (x_i - \hat{\mu}_k)^2}{\sum_{i=1}^{N} \hat{\gamma}_{ik}}.$

When the number of components K is not known a priori, it is typical to guess the number of components and fit that model to the data using the EM algorithm. This is done for many different values of K. Usually, the model with the best trade-off between fit and number of components (simpler models have fewer components) is kept.

The EM algorithm for the multivariate case is analogous, though it is more complicated and thus is not expounded here.
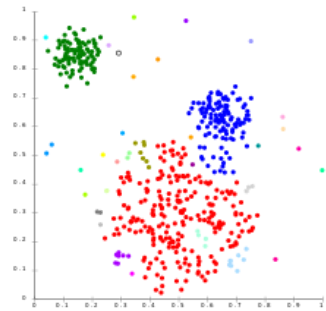
Unsupervised Learning

Once the EM algorithm has run to completion, the fitted model can be used to perform various forms of inference. The two most common forms of inference done on GMMs are density estimation and clustering.

Density Estimation

Since the GMM is completely determined by the parameters of its individual components, a fitted GMM can give an estimate of the probabilities of both in-sample and out-of-sample data points, known as density estimation. Furthermore, since numerically sampling from an individual Gaussian distribution is possible, one can easily sample from a GMM to create synthetic datasets.

Sampling from a GMM consists of the following steps:

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1. Sample the Gaussian component according to the distribution defined by $p(C_s) = \phi_s$.

2. Sample x from the distribution for component C_s, according to the distribution defined by $\mathcal{N}(x \mid \mu_s, \sigma_s)$.

Clustering using a Gaussian mixture model. Each color represents a different cluster according to the model.[3]

Clustering

Using Bayes' theorem and the estimated model parameters, one can also estimate the posteriori component assignment probability. Knowing that a data point is likely from one component distribution versus another provides a way to learn clusters, where cluster assignment is determined by the most likely component assignment. Clustering has many uses in machine learning, ranging from tissue differentiation in medical imaging to customer segmentation in market research.

Given a univariate model's parameters, the probability that a data point x belongs to component C_i is calculated using Bayes' theorem:

$$p(C_i \mid x) = \frac{p(x, C_i)}{p(x)} = \frac{p(C_i)p(x \mid C_i)}{\sum_{j=1}^{K} p(C_j)p(x \mid C_j)} = \frac{\phi_i \mathcal{N}(x \mid \mu_i, \sigma_i)}{\sum_{j=1}^{K} \phi_j \mathcal{N}(x \mid \mu_j, \sigma_j)}.$$

Recent Applications

GMMs have been used recently for feature extraction from speech data for use in speech recognition systems[4]. They have also been used extensively in object tracking of multiple objects, where the number of mixture components and their means predict object locations at each frame in a video sequence[5]. The EM algorithm is used to update the component means over time as the video frames update, allowing object tracking.

See Also

- Normal Distribution

- Multivariate Normal Distribution

References

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