Why is Mixture Modelling so popular?

Tony Robinson

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Outline

1. Heterogeneity - one model won't do!
2. Basic mixture formulation.
3. Ways to fit.
4. Inferential difficulties.
5. Cautionary example.
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Introduction - Model Heterogeneity.

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Why is Mixture Modelling so popular?
Finite Mixture Models

Idea is to model complex data as a finite mixture of component models, often of same type. Loosely, model $M$ is a weighted mixture of component models $\{M_i\}$, if

$$M = \sum_{i=1}^{g} w_i M_i$$

where $w_i$ represents the proportion of the data "explained" by $M_i$.

Example: Density estimation

$$f(x_j) = \sum_{i=1}^{g} w_i f_i(x_j),$$

where $f_i(x_j)$ are "standard" densities and $0 \leq w_i \leq 1$, and $\sum w_i = 1$.

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But this raises an immediate question? Do we know how many component models there are in the mixture? Or, do we need to find out?
Four?

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<table>
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| 0 | 20 | 40 | 60 | 80 |

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**Six?**

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Model-Based Clustering

The stamp data paper is likely to come from several different origins. Mixture modelling provides a natural framework for this situation. At its simplest, each component in the mixture represents a cluster within the total population. Assumes clusters are individually well fitted by the models $\{M_i\}$.
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Old Faithful Data

Why is Mixture Modelling so popular?
More Applications

Mixtures of regressions, linear Models, GLMs, survival,...
EG. Hurn et al. (2000)

Fig. 2. (left) Equivalence ratio against exhaust nitric oxide concentration (Source: Hurvich et al., 1998); (right) representation of the GNP and CO2 emission levels in 1996 for various countries (Source: OECD).
More Applications

Mixtures of Phylogenetic Models (Evolutionary tree of species)

Characters (ACGT) evolve according to a Markov process \( \Theta \) involving parameters such as mutation rates. BUT many sources of heterogeneity can mix any or all of:

- different \( \Theta \)s
- branch lengths
- topologies

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Social Networks Handcock et al (2006)

Figure 3: Estimates of clusters and latent positions for the relationship between monks within a monastery from the Bayesian estimation of the LPCM. The probability of assignment to each latent clusters is shown by a colored pie chart.
Fitting Mixture Models

Two popular methods of fitting.

1. EM Algorithm

The EM algorithm involves assessing to which component $j$ of the mixture each datum is expected to belong. Once this is established for all the data, fitting by usual MLE proceeds for the parameters of model $j$. McMC may also utilise this device for completing the “missing” part of the data.
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Resulting allocation vector $Z = (Z_1, ..., Z_n)$
Any Problems?

Model selection, inference and interpretation can be complicated by several factors.
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Model selection, inference and interpretation can be complicated by several factors.

- What is $g$?
- $g$ large $\Rightarrow$ many parameters.
- Identifiability?
Label Switching

In a mixture model, if all the components belong to the same parametric family, then the mixture density is invariant under the permutations of the component labels.

The likelihood \( \text{Lik} = \prod_{i=1}^{n} \left\{ w_1 f(x_i; \theta_1) + \ldots + w_g f(x_i; \theta_g) \right\} \) is the same for all permutations of the labels \((1, 2, 3, \ldots, g)\).

The term label switching is used to describe the invariance of the likelihood under the relabelling of the components.

Often handled by imposing constraints, e.g. label components in increasing order of weight \(w_j\). Not always satisfactory.
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Identifiability v Nonidentifiability

For example, consider the allocation vectors

\[(4, 4, 3, 3, 4, 2, 2, 3, 1, 3)\]

and

\[(2, 2, 1, 1, 2, 3, 3, 1, 4, 1)\]

these are different models if each component can be identified from some information.

However these two vectors define the same partition of the data and so are identical models from the clustering viewpoint. Therefore we would like some unique representation of them that identifies their common partition, i.e.

\[\{\{1, 2, 5\}\}, \{\{3, 4, 8, 10\}\}, \{\{6, 7\}\}, \{\{9\}\}\].

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One simple solution is to relabel the allocations in increasing order as new components make an appearance, starting with label 0 or 1 for the first observation.

The restricted growth function representation of the two allocation vectors above is \{1, 1, 2, 2, 1, 3, 3, 2, 4, 2\}.

Given allocation vectors from a sampler possibly suffering from label switching, we convert them to an unambiguous sample from space of possible partitions.
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So estimating $g$ as well as Gaussian parameters and weights.

Standard approach to clustering is typically:

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2. Given $g$, estimate likely clustering.
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Old Faithful “Standard” Clustering

The figure below shows the posterior distribution of the number of components $k$ which has a prominent mode at 3. Alongside is the classification into 3 clusters obtained by standard hierarchical clustering using the number of times each pair of observations appear in the same sample cluster as a distance measure. (O'Hagan)

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Old Faithful, Common Partitions

The figure below depicts the 3 most commonly occurring configurations—all contain just 2 components.

1. Modal Configuration, Posterior Probability = 0.3
2. Second Configuration, Posterior Probability = 0.095
3. Third Configuration, Posterior Probability = 0.0165

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Can we do more?

- Simple to explore the commonly occurring partitions.
- But what about variation in the sampled partition values?
- These live in a very complex and high dimensional discrete space.
- Could we get some insight into nature of this sample distribution?
- Dissimilarity between each pair of partitions - number of pairs of observations that agree in the two partitions, ie. either both in same group or both in different groups.
Why is Mixture Modelling so popular?

MDS plot of Old Faithful partitions

Here is a 2D configuration obtained from a nonmetric multidimensional scaling based on the computed dissimilarities between the 1172 sampled cluster configurations.
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Here is a 2D configuration obtained from a nonmetric multidimensional scaling based on the computed dissimilarities between the 1172 sampled cluster configurations.

isoMDS of unique sampled allocations

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- THANK YOU.