Fractionally-Supervised Classification

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Abstract

Traditionally, there are three species of classification: unsupervised, supervised, and semi-supervised. Supervised and semi-supervised classification differ by whether or not weight is given to unlabelled observations in the classification procedure. In unsupervised classification, or clustering, either there are no labelled observations or the labels are ignored altogether. A priori it can very difficult to choose the optimal level of supervision, and the consequences of a sub-optimal choice can be rather severe. A flexible fractionally-supervised approach to classification is introduced, where any level of supervision — ranging from unsupervised to supervised — can be attained. Our approach uses a weighted likelihood, wherein weights control the level of supervision. Gaussian mixture models are used as a vehicle to illustrate our fractionally-supervised classification approach; however, it is broadly applicable and variations on the postulated model can easily be made by adjusting the weights. A comparison between our approach and the traditional species is presented using benchmark model-based clustering data.

Keywords. Discriminant analysis, classification, clustering, weighted likelihood, mixture models, semi-supervised, supervised.

1 Introduction

Broadly, classification is concerned with assigning labels to observations so that they are partitioned into classes. Classification can be supervised, semi-supervised, or unsupervised, and we refer to these as the three species of classification. In supervised classification, or discriminant analysis, only observations that are already labelled are used to find labels for the unlabelled observations. In semi-supervised classification, all observations are used to
label the unlabelled observations. In unsupervised classification, or clustering, all observations are unlabelled or as treated as such; accordingly all observations are used to find labels. The choice over which species of classification, i.e., supervised, semi-supervised, or unsupervised, should be used in a particular analysis is not straightforward unless none of the labels are known. In all other cases, the three species are available and the choice can be highly consequential. The purpose of this paper is to remove the burden of this choice by introducing a fractionally-supervised classification (FSC) paradigm.

FSC includes all three species as special cases but allows for any level of supervision between unsupervised and supervised. Derived from the maximum-entropy principle, our FSC paradigm is based on weighted likelihoods and provides a middle ground for classification. Herein, we use Gaussian mixture model-based approaches to classification to illustrate our FSC approach; however, it is broadly applicable. The remainder of this paper is organized as follows. In Section 2 mixture model-based approaches to discriminant analysis, classification, and clustering are reviewed using notation that will facilitate the later work herein. Then, the general theory used in the construction of the FSC algorithm is described (Section 3) and the model is laid out along with mathematical details (Section 4). In Section 5 the FSC approach is illustrated and compared to the three species of classification. The paper concludes with a discussion and suggestions for future work (Section 6).

2 Mixture Models and Classification

2.1 Finite Mixture Models

Finite mixture models have been established as an effective means of classification since they were first used for clustering by Wolfe [1963]. The model assumes that population is comprised of a finite number of subgroups, or components, each following some parametric distribution. The density of a finite mixture model is a convex combination of these component densities, given by

$$M(x \mid \Theta) = \sum_{g=1}^{G} \pi_g \phi(x \mid \theta_g),$$

where $$\pi_g > 0$$, with $$\sum_{g=1}^{G} \pi_g = 1$$, are the mixing proportions, $$\phi(\cdot \mid \theta_g)$$ is the $$g$$th component density, parameterized by $$\theta_g$$, and $$\Theta = (\pi_1, \ldots, \pi_G, \theta_1, \ldots, \theta_G)$$ is the vector of parameters. Note that in general, we could have different densities for each component, so that $$\phi(x \mid \theta_g)$$ would be replaced by $$\phi_g(x \mid \theta_g)$$ in (1); however, we use Gaussian mixture models herein and so we have the density in (1), where $$\phi(x \mid \theta_g)$$ is the density of a $$p$$-dimensional Gaussian random variable with $$\theta_g = (\mu_g, \Sigma_g)$$. 

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2.2 Model-Based Classification

Consider a sample of \( n \) \( p \)-dimensional observations, independently drawn from \([1]\). Suppose that we know the labels, i.e., the components of origin, for a subset of the observations so that \( \mathbf{x} = (\mathbf{x}_1^\top, \mathbf{x}_2^\top)^\top \) comprises the labelled data \( \mathbf{x}_1 = (x_{11}^\top, x_{12}^\top, \ldots, x_{1n_1}^\top)^\top \) and the unlabelled data \( \mathbf{x}_2 = (x_{21}^\top, x_{22}^\top, \ldots, x_{2n_2}^\top)^\top \), where \( n_1 + n_2 = n \). Suppose that \( \mathbf{x}_k \) has component indicator matrix \( \mathbf{z}_k = (z_{k1}^\top, z_{k2}^\top, \ldots, z_{kn_k}^\top)^\top \), where \( z_{kj} \) is the element in the \( j \)-th row and \( k \)-th column of \( \mathbf{z}_k \) with elements

\[
\begin{align*}
z_{jk}^{(k)} &= \begin{cases} 
1, & \text{if } x_{kj} \text{ arises from group } g \\
0, & \text{otherwise,}
\end{cases}
\end{align*}
\]  

for \( k \in \{1, 2\} \) and \( j = 1, \ldots, n_k \). The problem of classification can be reformulated as estimating \( \mathbf{z}_2 \), the component indicator matrix for the unlabelled data, on the basis of the some or all of the observed values \( \mathbf{x}_1, \mathbf{x}_2 \), and \( \mathbf{z}_1 \).

The observed likelihood function of \( \Theta \), given the observed data \( (\mathbf{x}, \mathbf{z}_1) \), has the form

\[
\mathcal{L}_o(\Theta \mid \mathbf{x}, \mathbf{z}_1) = \prod_{j=1}^{n_1} \prod_{g=1}^{G} [\pi_g \phi(x_{1j} \mid \theta_g)]^{z_{1j}^{(1)}} \times \prod_{k=1}^{n_2} \prod_{h=1}^{H} [\pi_h \phi(x_{2k} \mid \theta_h)]^{z_{2k}^{(2)}}.
\]  

To maximize \([3]\) with respect to \( \Theta \), we make use of the expectation maximization (EM) algorithm \([\text{Dempster et al. 1977}]\). The EM algorithm is based on the complete-data \( (\mathbf{x}, \mathbf{z}) \), where \( \mathbf{z} = (\mathbf{z}_1, \mathbf{z}_2) \), which is the observed data \( (\mathbf{x}, \mathbf{z}_1) \) plus the missing data \( \mathbf{z}_2 \). The likelihood of \( \Theta \) given the complete-data, more commonly referred to as the complete-data likelihood, is given by

\[
\mathcal{L}_c(\Theta \mid \mathbf{x}, \mathbf{z}) = \prod_{j=1}^{n_1} \prod_{g=1}^{G} [\pi_g \phi(x_{1j} \mid \theta_g)]^{z_{1j}^{(1)}} \times \prod_{h=1}^{H} \prod_{k=1}^{n_2} [\pi_h \phi(x_{2k} \mid \theta_h)]^{z_{2k}^{(2)}},
\]  

where \( H \geq G \). As is common practice in classification problems, we subsequently restrict ourselves to \( H = G \).

The EM algorithm cycles through an expectation step (E-step) and a maximization step (M-step) until convergence. We start with an initial estimate \( \Theta^{(0)} \) for \( \Theta \), and the EM algorithm proceeds as follows.

**E-step** Calculate

\[
\hat{z}_{jk}^{(2)} = \frac{\pi_g^{(t)} \phi(x_{2n_2} \mid \theta_g^{(t)})}{\sum_{g=1}^{G} \pi_g^{(t)} \phi(x_{2n_2} \mid \theta_g^{(t)})}
\]

**M-step** Find

\[
\Theta^{(t+1)} = \arg\max_{\Theta} \sum_{i=1}^{m} \sum_{j=1}^{n_i} \sum_{g=1}^{G} \hat{z}_{jk}^{(1)} \log [\pi_g^{(t)} \phi(x_{in_i} \mid \theta_g^{(t)})]
\]

If converged, stop. Otherwise, set \( t \leftarrow t + 1 \) and repeat.
Define
\[ Q(\Theta \mid \Theta^{(t)}) = E_{p(z|x)} \left[ \ell_c(\Theta \mid x, z) \mid x, \Theta^{(t)} \right], \tag{6} \]
where \( \ell_c(\Theta \mid x, z) := \log \mathcal{L}_c(\Theta \mid x, z) \). Now, (5a) is equivalent to calculating (6) based on the current fit of parameters \( \Theta^{(t)} \) (E-step) and (5b) is equivalent to maximizing (6) with respect to \( \Theta \) using the known component matrix \( z_1 \) and the current estimate \( \hat{z}_2 = \{ \hat{z}_{2jg} : j = 1, \ldots, n_2, g = 1, \ldots, G \} \) (M-step).

2.3 Model-Based Discriminant Analysis

Model-based discriminant analysis is a supervised approach to classification that uses labelled data \( x_1 \), and their labels \( z_1 \), to infer the parameters and thereby the unknown labels \( z_2 \). We consider the quadratic discriminant analysis (QDA) rule that determines the class of subject \( j \) by
\[
\hat{\tau}^{(2)}_{jg} = \frac{\hat{\pi}_g \phi(x_{1j} \mid \hat{\theta}_g)}{\sum_{g=1}^G \hat{\pi}_g \phi(x_{1j} \mid \hat{\theta}_g)},
\]
where \( x_{1j} \) is classified to component, or class, \( g \) if \( \hat{\tau}^{(2)}_{jg} > \hat{\tau}^{(2)}_{jk} \) for all \( k \neq g \), and \( \hat{\Theta} = \{ \hat{\pi}_g, \hat{\theta}_g \}_{g=1,\ldots,G} \) are the estimates found by maximizing
\[
\mathcal{L}(\Theta \mid x_1, z_1) = \prod_{j=1}^{n_1} \prod_{g=1}^G [\pi_g \phi(x_{1j} \mid \theta_g)]^{z_{1jg}}. \tag{7}
\]
Unlike model-based classification, \( \hat{\Theta} \) can be found using traditional likelihood maximization techniques. More specifically, given \( (x_1, z_1) \), maximizing (7) with respect to \( \Theta \) leads to the plug-in estimates,
\[
\hat{\pi}_g = \frac{\sum_{j=1}^{n_1} z_{1jg}^{(1)}}{n_1}, \tag{8a}
\]
\[
\hat{\mu}_g = \frac{\sum_{j=1}^{n_1} x_{1j} z_{1jg}^{(1)}}{\sum_{j=1}^{n_1} z_{1jg}^{(1)}}, \tag{8b}
\]
\[
\hat{\Sigma}_g = \frac{\sum_{j=1}^{n_1} z_{1jg}^{(1)} (x_{1j} - \mu_g)(x_{1j} - \mu_g)^\top}{\sum_{j=1}^{n_1} z_{1jg}^{(1)}}, \tag{8c}
\]
for \( g = 1, \ldots, G \). Although we use a QDA rule herein, we note that a linear discriminant analysis (LDA) rule, wherein the component covariance matrices are assumed to be equal, could also be used. More specifically, the LDA rule uses the pooled covariance matrix given by
\[
\tilde{\Sigma}_g = \tilde{\Sigma} = \frac{\sum_{i=1}^2 S_{ig}}{n}, \tag{9}
\]
in place of (8c), where \( S_{ig} = \sum_{j=1}^{n_i} z_{1jg}^{(i)} (x_{ij} - \mu_g)(x_{ij} - \mu_g)^\top \) and \( n = \sum_{i=1}^2 \sum_{j=1}^{n_i} z_{1jg}^{(i)} \).
2.4 Model-based Clustering

Model-based clustering is an unsupervised approach and so assumes no prior knowledge of class labels. Using the notation introduced in the previous sections, this method aims at finding \( z_2 \) based solely on the observed data \( x_2 \). Note that \( x_1 \) and \( z_1 \) are empty here. The observed likelihood in this case is given by

\[
L_o(\Theta | x_2) = \prod_{j=1}^{n_2} \sum_{g=1}^{G} \pi_g \phi(x_{2j} | \theta_g),
\]

and the complete-data log-likelihood by

\[
L_c(\Theta | x_2, z_2) = \prod_{j=1}^{n_2} \prod_{g=1}^{G} \left[ \pi_g \phi(x_{2j} | \theta_g) \right]^{\hat{z}_{2jg}^{(2)}}.
\]

The EM algorithm is carried out as in (5) with the M-step replaced by

\[
\Theta^{(t+1)} = \arg\max_{\Theta} \sum_{j=1}^{n_2} \sum_{g=1}^{G} \hat{z}_{2jg}^{(2)} \log \left[ \pi_g^{(t)} \phi(x_{2n_2} | \theta_g^{(t)}) \right].
\]

2.5 Classification and Classification Error

Maximum a posteriori (MAP) classification assigns \( x_{2j} \) to component \( g \) if \( \hat{z}_{2jg}^{(2)} > \hat{z}_{2jk}^{(2)} \) for all \( k \neq g \). In practice, the goal of model-based classification methods can be reduced to finding \( \hat{z}_{2jg}^{(2)} \) that corresponds to the smallest misclassification rate. In other words, if unlabelled observation \( x_{2j} \) originates from component \( g \), we would like to pick a classifier such that probability of classification error given by \( P(\text{MAP} \{ x_{2j} \} \neq g) \) is close to the minimal possible error rate. As discussed in the next section, the magnitude of this error can be affected by our choice of classification species.

2.6 Motivation

In classification problems, it can happen that the proportion of labelled data is small, and in some cases, it can be better to ignore known labels altogether (see Section 5 for two concrete examples of this phenomenon). Discriminant analysis can be unreliable in the event of small class sizes. In such cases, gains in classification accuracy can sometimes be achieved by using semi-supervised classification. Semi-supervised approaches have been employed with success in many applications including but not limited to Ratsaby and Venkatesh (1995), Baluja (1998), McCallum and Nigam (1998), Nigam et al. (2000), McNicholas (2010), and Andrews et al. (2011); see Seeger (2001) for a general review.

Although the inclusion of unlabelled data has proven to be beneficial in many classification applications, there has been some hesitation in concluding that unlabelled data should
always be used in defining a classifier (cf. Shahshahani and Landgrebe, 1994; Cozman et al., 2003). There are reasonable grounds for scepticism when we consider, for example, the argument made by Cozman et al. (2003), who show that unlabelled samples may lead to a larger classification error when the postulated model is incorrect. However, if the model is not misspecified, the inclusion of unlabelled data reduces the second-order Taylor series approximation of the expected error rates, provided the estimator used to construct the classification rule has negligible bias (Shahshahani and Landgrebe, 1994).

Despite conflicting arguments, we advocate the inclusion of all available information with the proviso that labelled and unlabelled data be treated separately. To substantiate this argument, we refer to the results of Castelli and Cover (1996), who considered a two-component Gaussian mixture with unknown mixing proportions and showed that labelled samples are exponentially more valuable than unlabelled samples in reducing classification error.

The proposed FSC approach is equipped for the tradeoff between using labelled and unlabelled data. It can be used to borrow more from unlabelled observations when there are few observations in a class, to emphasize the contribution of labelled or unlabelled observations to enhance our estimator, and to adjust for the complicated interplay between unlabelled data and classification error rates. We implement our FSC approach by adopting a weighted likelihood approach (Section 3).

3 Weighted Likelihood

The purpose of this paper is to provide a flexible classification approach, FSC, that allows the labeled and unlabelled data to exert different influence on parameter estimation. This can be accomplished by adopting a maximum weighted likelihood approach. The weighted likelihood assigns weights to the classic likelihood function, strengthening or diminishing the role of samples based on their relevance to the inference about the population of interest.

The notion of borrowing information from samples drawn from populations other than the population of direct interest, was explored in the seminal paper by Stein (1956). The author changed conventional estimation approaches when he showed that the maximum likelihood estimators (MLEs) for the means of independent Gaussian populations with known variance are inadmissible when the number of populations exceeds two. This phenomenon led to a number of alternative estimators that dominated the MLE, including but not limited to the celebrated James-Stein estimator (James and Stein, 1961), the modified James-Stein estimator (Berry, 1994), and the minimax estimators presented by Baranchik (1970) and Strawderman (1973). These Stein-type estimators are closely connected with weighted likelihood. In fact, when the weights are appropriately defined, the James-Stein estimator is a special case of the weighted likelihood estimator (Wang, 2006).

The evolution of the weighted likelihood moves to its closely connected forerunner, the relevance weighted likelihood (REWL; Hu, 1994, 1997; Hu and Zidek, 2001). The REWL
borrows information from distributions thought to be similar to the distribution of inferential interest, to produce better estimates — in terms of mean squared error — of the target distribution. The asymptotic properties of this class of estimators generalizes the work of [Wald (1949)] on the traditional MLE and are presented for the parametric case in [Hu (1997)]. Not long after, the weighted likelihood was formulated. Subsequently, it has been theoretically solidified and expounded upon by several authors (e.g., [Wang, 2001]; [Hu and Zidek, 2002]; [Wang, 2006]; [Wang et al., 2004]; [Wang and Zidek, 2005]; [Plante, 2008; 2009]). The weighted likelihood adopts a different paradigm than the REWL, which assumes information about Θ increases as the number of populations grows (cf. [Hu, 1997]). In contrast, the asymptotic theory employed in weighted likelihood assumes that the number of populations is fixed as sample size tends to infinity (cf. [Wang et al., 2004]). [Hu and Zidek (2002)] detail the derivation of both the non-parametric and parametric versions of their weighted likelihood.

The postulated model assumes that data come from m populations having similar, but not necessarily identical, distributions. To be more specific, let $X_i$ ($i = 1, \ldots, m$) be independent random vectors with probability density functions (PDFs) $f_i(\cdot | \Theta_i)$ and cumulative distribution functions $F_i$. We let $X = (X_1^\top, X_2^\top, \ldots, X_m^\top)^\top$, where $X_i = (X_{i1}, X_{i2}, \ldots, X_{in_i})$ and $X_{ij}$ are assumed to be iid random variables. If we assume that $f_2(\cdot | \Theta_2), \ldots, f_m(\cdot | \Theta_m)$ are similar to $f_1$, our primary PDF of interest, then the weighted likelihood takes on the form

$$L_w(\Theta | x) = \prod_{i=1}^{m} f_1(x_i | \Theta)^{\alpha_i} = \prod_{i=1}^{m} \prod_{j=1}^{n_i} f_1(x_{ij} | \Theta)^{\alpha_i},$$

where $\alpha_1, \alpha_2, \ldots, \alpha_m$ are positive-valued relevance weights that incorporate the importance of each population to the inference of $\Theta$, and we fix $\alpha_1 + \cdots + \alpha_m = 1$. Note that the restriction imposed on the weights could be relaxed to allow for negative weights (cf. [Hu and Zidek, 2002]). Furthermore, we obtain a traditional likelihood when $m = 1$. Naturally, the maximum weighted likelihood estimator (MWLE) is found by maximizing the weighted likelihood presented in (12). Asymptotic properties for the class of MWLE estimators are given by [Wang et al., 2004].

## 4 Fractionally-Supervised Classification

### 4.1 The Model

To describe our FSC approach, we first adopt the weighted likelihood in (12) with two populations (i.e., $m = 2$); the first population, specifically $f_1$, being of inferential interest. We view the samples $x_1$ and $x_2$ as being drawn from similar populations; however, the information provided by $x_1$ can be seen as ‘more exact’ than that provided by $x_2$ because we know from which component each observation $x_{1j}$ has arisen. Under the Gaussian mixture assumption, it might seem reasonable to estimate $f_1$ by plugging $x_1$ and $z_1$ into the class
sample-based MLEs given in (8). However, additional information from \( x_2 \) can be used to improve the inference of \( f_1 \).

The postulated FSC model assumes \( f_1 \) follows from a Gaussian mixture as defined in (1), and that the MWLE is derived from

\[
\arg\max_{\Theta} L_w(\Theta \mid x),
\]

where

\[
L_w(\Theta \mid x) = \prod_{i=1}^{2} f_1(x_i \mid \Theta)^{\alpha_i} = \prod_{i=1}^{2} \prod_{j=1}^{n_i} \sum_{g=1}^{G} \pi_g \phi(x_{ij} \mid \theta_g)^{\alpha_i}
\]

and \( \alpha_1 + \alpha_2 = 1 \). To illustrate the generality of this approach, notice the maximization of (13) with \( \alpha_1 = \alpha_2 = 1/2 \) reduces to maximization of the complete-data log-likelihood in (11) and so FSC amounts to preforming model-based classification. Similarly, \( (\alpha_1 = 1, \alpha_2 = 0) \) corresponds to model-based discriminant analysis (i.e., QDA). In the special case when \( x_1 \) and \( z_1 \) are empty, or are treated as empty, \( (\alpha_1 = 0, \alpha_2 = 1) \) corresponds to model-based clustering.

An EM algorithm is used for parameter estimation of our weighted model defined in (12).

We reformulate the maximization of \( L_w(\Theta \mid x) \) to maximizing \( \ell_w(\Theta \mid x) := \log\{L_w(\Theta \mid x)\} \), with

\[
f_1(x_{ij} \mid \Theta) = \frac{f_1(x_{ij}, z_{ij} \mid \Theta)}{f_1(z_{ij} \mid x_{ij}, \Theta)}.
\]

This recasts the problem in (13) as maximizing

\[
\ell_w(\Theta \mid x) = \sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i \log f_1(x_{ij} \mid \Theta)
\]

\[
= \sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i \left[ \log f_1(x_{ij}, z_{ij} \mid \Theta) - \log f_1(z_{ij} \mid x_{ij}, \Theta) \right]
\]

\[
= \sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i \left[ \log f_1(x_{ij}, z_{ij} \mid \Theta) - \log f_1(z_{ij} \mid x_{ij}, \Theta) + \log p(z_{ij} \mid x_{ij}) - \log p(z_{ij} \mid x_{ij}) \right]
\]

\[
= \sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i \left[ \log \frac{f_1(x_{ij}, z_{ij} \mid \Theta)}{p(z_{ij} \mid x_{ij})} - \log \frac{f_1(z_{ij} \mid x_{ij}, \Theta)}{p(z_{ij} \mid x_{ij})} \right]
\]

Taking expectation with respect to PDF \( p(z_{ij} \mid x_{ij}) \) yields

\[
\sum_{i=1}^{2} \sum_{j=1}^{n_i} E_{p(z_{ij} \mid x_{ij})} \alpha_i \left[ \log \frac{\ell_c(\Theta \mid x_{ij}, z_{ij})}{p(z_{ij} \mid x_{ij})} - \log \frac{f_1(z_{ij} \mid x_{ij}, \Theta)}{p(z_{ij} \mid x_{ij})} \right]
\]

\[
= \sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i L(p_{ij}, \Theta) - \sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i KL \{ p_{ij} \mid f_1(z_{ij} \mid x_{ij}, \Theta) \},
\]

8
where \( p_{ij} \equiv p(z_{ij} | x_{ij}) \), \( \sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i L(p_{ij}, \Theta) = E_{p_{ij}}[\alpha_i \log \ell_c(\Theta | x_{ij}, z_{ij}) / p_{ij}] \), and KL\{p \mid\mid f\} is the Kullback-Leibler divergence between \( p \) and \( f \). Our algorithm proceeds by iteratively increasing \( \sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i L(p_{ij}, \Theta) \), a surrogate function for \( \ell_w(\Theta | x) \). In Section 4.2, we show that our algorithm will maximize \( \ell_w(\Theta | x) \) thereby giving the MWLE we desire. Note that Neal and Hinton (1998) developed the necessary theory for the maximization of (15) within the EM framework for the single population case, i.e., for the traditional EM algorithm. The next section (Section 4.2) presents the EM algorithm for \( i = 2 \).

4.2 Theorems and Proofs

In this section, we aim to show that if \( L \) has global (or local) maximum at \( p^* \) and \( \Theta^* \), then \( L_w(\Theta^*) \) is a global (or local) maximum. We note that the monotonic improvement of (13), guaranteed in the regular EM framework, also holds when the relevance weights are constant. As such, we investigate the case when \( \alpha_1 = c \) and \( \alpha_2 = 1 - c \), for \( c \in [0, 1] \). In a fashion similar to that of Neal and Hinton (1998), start with an initial estimate \( \Theta^{(0)} \) for \( \Theta \), and the EM algorithm for the optimization problem in (13) can be summarized as:

\[
\text{E-step} \quad \text{Find } \hat{p}_{ij} = \arg\max_{p_{ij}} \sum_{i=1}^{2} \alpha_i L(p_{ij}, \Theta^{(t)}) \quad (16a)
\]

\[
\text{M-step} \quad \text{Find } \Theta^{(t+1)} = \arg\max_{\Theta} \sum_{i=1}^{2} \alpha_i L(\hat{p}_{ij}, \Theta^{(t)}) \quad (16b)
\]

If converged, stop. Otherwise, set \( t \leftarrow t + 1 \) and repeat, \( (16c) \)

where \( L \) is as given in (15). Following Neal and Hinton (1998), we assume \( \ell_c(\Theta | x_{ij}, z_{ij}) \) is never zero to ensure finite values for \( L \). Moreover, we assume \( \ell_c(\Theta | x_{ij}, z_{ij}) \) is a continuous function of \( \Theta \); accordingly, \( L(p_{ij}, \Theta) \) is a continuous function of \( \Theta \) and \( p_{ij} \).

**Lemma 1.** For fixed \( \Theta \), there exist unique distributions \( p_{ij0} \) that maximize \( \sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i L(p_{ij}, \Theta) \) with respect to \( p_{ij} \), and they are given by

\[
\frac{f_1(x_{ij}, z_{ij} | \Theta)}{\sum_{z_{ij}} f_1(x_{ij}, z_{ij} | \Theta)} = f_1(z_{ij} | x_{ij}, \Theta). 
\]

**Proof.** It follows from the independence of \( X_{2j} \) and \( X_{2k} \), that \( Z_{2j} \) and \( Z_{2k} \) are independent for \( j \neq k \). Therefore, we can individually find the \( p_{ij} \) that minimize \( \alpha_i L(p_{ij}, \Theta) \) for all
\[ j = 1, \ldots, n_i \text{ and } i \in \{1, 2\}. \]

\[
\sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i L(p_{ij}, \Theta) = \sum_{i=1}^{2} \sum_{j=1}^{n_i} E_{p_{ij}} \left[ \alpha_i \log \frac{f_c(\Theta|x_{ij}, z_{ij})}{p_{ij}} \right]
\]

\[= \sum_{i=1}^{2} \sum_{j=1}^{n_i} E_{p_{ij}} \left[ \alpha_i \log f_c(\Theta|x_{ij}, z_{ij}) \right] - \sum_{i=1}^{2} \sum_{j=1}^{n_i} E_{p_{ij}} \left[ \alpha_i \log p_{ij} \right]
\]

\[= \sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i Q(p_{ij}, \Theta) - \sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i H(p_{ij}, | \Theta), \quad (17)\]

where \( \sum_{j=1}^{n_i} \alpha_i Q(p_{ij}, \Theta) = \sum_{i=1}^{2} \sum_{j=1}^{n_i} E_{p_{ij}} [\alpha_i \log f_c(\Theta|x_{ij}, z_{ij})] \) and \( \sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i H(p_{ij}, | \Theta) = \sum_{i=1}^{2} \sum_{j=1}^{n_i} E_{p_{ij}} [\alpha_i \log p_{ij}] \) is the negative entropy of distribution \( p_{ij} \). Based on the constraint \( \sum_{z_{ij}} p(z_{ij}|x_{ij}) = 1 \), we form the Lagrangian

\[
\frac{\partial}{\partial p_{ij}} \left[ \sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i Q(p_{ij}, \Theta) - \sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i H(p_{ij}, | \Theta) - l_0 \left( \sum_{z_{ij}} p_{ij} - 1 \right) \right] = 0.
\]

For each \( z_{ij}, j = 1, \ldots, n_i \) and \( i \in \{1, 2\} \), we have

\[
\alpha_i \log p_{ij} = \alpha_i \log f_1(x_{ij}, z_{ij} | \Theta) - 1 - l_0
\]

i.e.,

\[
\log p_{ij} = \log f_1(x_{ij}, z_{ij} | \Theta) - 1/\alpha_i - l_0/\alpha_i
\]

i.e.,

\[
p_{ij} = f_1(x_{ij}, z_{ij} | \Theta)e^{-1/\alpha_i}e^{-l_0/\alpha_i}
\]

i.e.,

\[
e^{-l_0/\alpha_i} = \frac{e^{1/\alpha_i}}{\sum_{z_{ij}} f_1(x_{ij}, z_{ij} | \Theta)}
\]

i.e.,

\[
1 = \frac{e^{1/\alpha_i}}{\sum_{z_{ij}} f_1(x_{ij}, z_{ij} | \Theta)}
\]

and so

\[
p_{ij} = f_1(x_{ij}, z_{ij} | \Theta) \frac{f_1(x_{ij}, z_{ij} | \Theta)}{f_1(x_{ij} | \Theta)} = f_1(z_{ij} | x_{ij}, \Theta).
\]

\[ \square \]

**Lemma 2.** If \( p_{ij} = p_{ij0} \), then

\[
\sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i L(p_{ij0}, \Theta) = \ell_w(\Theta \mid x).
\]

10
Proof. If \( p_{ij} = p_{ij0} = f_1(z_{ij} \mid x_{ij}, \Theta) \), then

\[
\ell_w(\Theta \mid x) = \sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i L(p_{ij0}, \Theta) - \sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i KL\left(f_1(z_{ij} \mid x_{ij}, \Theta) \mid\mid f_1(z_{ij} \mid x_{ij}, \Theta)\right) \\
= \sum_{i=1}^{2} \alpha_i L(p_{ij0}, \Theta).
\]

\[\square\]

Lemma 3. Maximizing \( \sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i L(p_{ij}, \Theta) \) with respect to \( \Theta \) is equivalent to maximizing \( \sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i Q(p_{ij}, \Theta) \) with respect to \( \Theta \).

Proof. Recall (17),

\[
\sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i L(p_{ij}, \Theta) = \sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i Q(p_{ij}, \Theta) - \sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i H(p_{ij}, \mid \Theta).
\]

The result follows from the fact that the second term, i.e.,

\[
\sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i H(p_{ij}, \mid \Theta) = \sum_{i=1}^{2} \sum_{z} p_{ij} \alpha_i \log p_{ij},
\]

does not depend on \( \Theta \).

\[\square\]

Starting with an initial \( \Theta^{(0)} \), our weighted version of the EM algorithm can be summarized as

**E-step** Find \( \hat{p}_{ij} = f_1(z_{ij} \mid x_{ij}, \Theta^{(t)}) \) for \( j = 1, \ldots, n_i, i = 1, 2 \) \hspace{1cm} (19a)

**M-step** Find \( \Theta^{(t+1)} = \arg\max_{\Theta} \sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i Q(\hat{p}_{ij}, \Theta) \) \hspace{1cm} (19b)

If converged, stop. Otherwise, set \( t \leftarrow t + 1 \) and repeat. \hspace{1cm} (19c)

**Theorem 1.** The algorithm (19) is equivalent to the algorithm (16).

Proof. Result follows directly from Lemmata 1, 2, and 3.

**Theorem 2.** If \( L \) has local (global) maximum at \( p^* = (p^*_1, p^*_2) \) and \( \Theta^* \), where \( p^*_i = (p^*_i1, \ldots, p^*_in_i) \), then \( \ell_w(\Theta \mid x) \) has local (global) maximum at \( \Theta^* \).
Proof. By Lemmata [1] and [2], if \( p^* \) maximizes \( L \), then
\[
\sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i L(p^*_ij, \Theta) = \ell_w(\Theta|\mathbf{x})
\]
for any \( \Theta \). In particular if \( \Theta^* \) is a local maximum of \( L \), then \( L(p^*ij, \Theta^*) > L(p^*_ij, \Theta) \) and \( \ell_x(\Theta|\mathbf{x}) > \ell_x(\Theta^*|\mathbf{x}) \) for all \( \Theta \) near \( \Theta^* \). Suppose that there exists a \( \hat{\Theta} \) near \( \Theta^* \) such that \( \ell_w(\hat{\Theta}|\mathbf{x}) > \ell_w(\Theta^*|\mathbf{x}) \). From Lemmata [1] and [2], this implies that \( L(p^*_ij, \hat{\Theta}) > L(p^*_ij, \Theta^*) \). However, \( L \) is a continuous function of \( \Theta \) and \( p^*ij \), thus contradicting the supposition that \( p^* = (p^*_1, p^*_2) \) and \( \Theta^* \) are a local maximum for \( L \). Therefore \( \ell_w(\Theta | \mathbf{x}) \) must attain a local maximum at \( \Theta^* \). An analogous argument proves the result for a global maximum.

4.3 Parameter Updates

Here we provide the updates required in EM algorithm established in the previous section. 

**Estep:** At the iteration \( t \), compute
\[
\hat{z}^{(i)}_{jg} = f_1(z_{ij} | x_{ij}, \Theta) = \frac{\pi_g \phi_g(x_{ij} | \theta^{(t)}_g)}{\sum_{g=1}^{G} \pi_g \phi_g(x_{ij} | \theta^{(t)}_g)},
\]
for \( i = 2 \). Note the values for \( z^{(1)}_{jg} \) are the observed indicator functions defined in [2]. For ease of notation, we define \( \hat{z}^{(i)}_{jg} = z^{(i)}_{jg} \). The parameter estimates used in the M-step are found by maximizing
\[
\sum_{i=1}^{2} \sum_{j=1}^{n_i} \sum_{g=1}^{G} \alpha_i \hat{z}^{(i)}_{jg} \log \left\{ \pi_{1g} \phi_{1g}(x_{ij} | \theta^{(t)}_{1g}) \right\}.
\]  

**(Mstep 1):** The estimate for \( \pi_g \), found by maximizing [20], is given by
\[
\hat{\pi}_g = \frac{\sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i \hat{z}^{(i)}_{jg}}{\sum_{i=1}^{2} \sum_{j=1}^{n_i} \sum_{g=1}^{G} \alpha_i \hat{z}^{(i)}_{jg}}.
\]

**(Mstep 2):** The estimate for \( \mu_g \), found by maximizing [20], is given by
\[
\hat{\mu}_g = \frac{\sum_{i=1}^{2} \sum_{j=1}^{n_i} x_{ij} \alpha_i \hat{z}^{(i)}_{jg}}{\sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i \hat{z}^{(i)}_{jg}}.
\]

**(Mstep 3):** The estimate for \( \Sigma_g \), found by maximizing [20], is given by
\[
\hat{\Sigma}_g = \frac{\sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i \hat{z}^{(i)}_{jg} (x_{ij} - \hat{\mu}_g)(x_{ij} - \hat{\mu}_g)^\top}{\sum_{i=1}^{2} \sum_{j=1}^{n_i} \alpha_i \hat{z}^{(i)}_{jg}}.
\]
4.4 Choice of weights

Thus far, we have assumed constant weights but have given no direction on how to choose them. In practice, there is no definitive way of defining the weights in the weighted likelihood. Some guidance towards their construction has been presented in a number of articles. For example, Hu (1997) offers several choices for $\alpha_i$, including a scheme that generalizes the smoothing model and an adaptive approach that balances variance and bias; the term ‘adaptive’ in this case indicates that the weights are dependent on the data. Wang (2001) and Wang and Zidek (2005) offer an adaptive approach that relies on a cross-validation technique, and Plante (2008) presents a non-parametric procedure based on minimizing the averaged mean squared error weights. In the general formulation of the REWL approach, Hu (1997) has suggested that the weights, which may best be determined by the user within the context of the problem at hand, should reflect the similarity between the PDF $f_i$ and the target population.

We selected a judicious choice for the weights stemming from the motivating arguments made in Section 2.6. Specifically, we choose the relevance weights $\alpha_1 = c$ and $\alpha_2 = 1 - c$, where

$$c = \frac{n_1}{n_1 + n_2} = \frac{n_1}{n}.$$

In accordance with the special cases presented in Section 4.1, FSC with this choice of weight will be equivalent to one particular species of classification in specific circumstances; however, this will not be the case in general. It is easy to heuristically justify our weights when one considers their meaning in the context of the weighted likelihood, i.e., the more labeled data we have, the less we need to borrow from the unlabelled data (cf. Section 2.6).

5 Applications

In this section, we demonstrate how FSC compares with the three species of classification when applied to real data. We preform model-based discriminant analysis, classification, and clustering as well as FSC on three benchmark data sets. The first data set is the swiss bank notes data (Flury and Riedwyl [1988]), which consists of six measurements on 200 Swiss bank notes, half of which are counterfeit. We also analyze the crabs data set (Campbell and Mahon [1974]), which contain measurements on the frontal lobe size, rear width, carapace length, carapace width, and body depth of four different types of crab. The third data set is the famous iris data set, which contains the length and width in centimetres of the sepal and petal of three species of irises (Anderson, 1935; Fisher, 1936). These data sets are available in the gclus (Hurley, 2012), HDclassif (Bergé et al., 2012), and base packages, respectively, in R (R Core Team, 2013). To carry out model-based clustering we use the gpcm() function with unconstricted covariance structure (i.e., the “VVV” model). The gpcm() function is available in the mixture package (Browne and McNicholas, 2013b), which carries out model-based clustering using methodology outlined in Celeux and Govaert (1995) and Browne and
McNicholas (2013a). The remaining methods are implemented by assigning the appropriate weight in our FSC algorithm, which we implement in R, using the same initialization strategy and stopping criterion presented in Russell et al. (2012).

For each data set, 500 random subsets are considered with varying proportions labelled, e.g., for the iris data, the labelled proportions are the $x$-axis of Figure 1. The results for the iris data indicate that model-based classification performs better than model-based discriminant analysis when less than half of the labels are known, and worse once more are known. Model-based clustering does not perform as well as either of the other species, unless the proportion of labelled data drops below 0.4, in which case it outperforms model-based discriminant analysis. FSC gives comparable performance to the best classification species for all considered proportions of labelled data.

![Figure 1](image.png)

Figure 1: A plot of ARI against the proportion of labelled observations depicting the classification performances of model-based discriminant analysis (QDA), model-based classification, model-based clustering, and FSC for the iris data.

For the crabs data (Figure 2), model-based classification consistently outperforms model-based discriminant analysis, and FSC gives comparable performance to model-based classification. Note that model-based clustering gives very poor performance on the crabs data (ARI=0.145) and so it was omitted from Figure 2.

For the bank data (Figure 3), we observe an interesting phenomenon whereby model-based clustering returns slightly better classification performance than all other methods when the proportion of labelled data is less than 0.5. For all proportions of labelled data, the performance of model-based classification and FSC is identical; however, the performance of model-based discriminant analysis is slightly inferior when less than 70% of the data are labelled. The fact that FSC cannot perform quite as well as model-based clustering when
Figure 2: A plot of the average ARI against the proportion of labelled observations depicting the classification performance of model-based discriminant analysis (QDA), model-based classification, and FSC for the crabs data.

less than half of data are labelled is an artifact of how our relevance weights are chosen — we would need $\alpha_1$ at or close to zero (with $x_1$ taken as empty) for FSC to return similar results. That said, the classification performance of model-based clustering was only very slightly superior to FSC in those cases, with the difference in ARI never exceeding 0.03 (Figure 3).

6 Discussion

A flexible classification paradigm, FSC, has been introduced and contains the three common species of classification as special cases. A weighted likelihood approach is used, wherein relevance weights determine the relative influence of labelled and unlabelled observations. The FSC approach was illustrated using Gaussian mixture models applied to three data sets. In our analyses, we used relevance weights that reflected the number of observations that were labelled and unlabelled respectively, i.e., $\alpha_1 = n_1/n$. This choice of relevance weights can be justified on intuitive grounds based on its interpretation within the weighted likelihood framework. However, the relevance weights could be chosen to take any positive values such that $\alpha_1 + \alpha_2 = 1$; therefore, our FSC framework for classification can be fixed to sit anywhere between unsupervised and supervised classification.

For each of the three data sets that we analyzed, our FSC approach with $\alpha_1 = n_1/n$ performed comparably to the best of the three species of classification. Therefore, using FSC consistently over all three analyses would have led to a smaller overall classification error than sticking with any one species. FSC removes the burden of species choice — especially
between model-based classification or model-based discriminant analysis — which can be significant in real applications. Consider our analysis of the iris data: model-based classification or model-based discriminant analysis performed better depending on the proportion of labelled observations; however, FSC performed similarly to the best species regardless of the proportion of labelled observations. All results support our conjecture that FSC can be used as an automated way of choosing between model-based classification and model-based discriminant analysis in situations where some of the data are labelled. In this way, the FSC approach introduced herein may pave the way for a different approach to classification, one based upon the weighted likelihood.

There are many possible avenues for future research. Our analysis of the bank note data illustrates that it can be better to proceed in an unsupervised classification framework even when up to 50% of the data are labelled. This phenomenon, and specifically a way to detect it \textit{a priori}, deserves further attention. On a related note, alternative approaches to finding optimal choices for the relevance weights are being explored — recall that our approach will work for any positive relevance weights such that $\alpha_1 + \alpha_2 = 1$. The constraint $H = G$ in (1) could be relaxed, thereby allowing multiple components per class. Applying our FSC paradigm beyond Gaussian mixture models is also a topic of ongoing work; considering non-Gaussian mixtures or families of mixtures models is a natural beginning but our paradigm is more broadly applicable.
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