Estimation of Classification Rules from Partially Classified Data

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Abstract We consider the situation where the observed sample contains some observations whose class of origin is known (that is, they are classified with respect to the $g$ underlying classes of interest), and where the remaining observations in the sample are unclassified (that is, their class labels are unknown). For class-conditional distributions taken to be known up to a vector of unknown parameters, the aim is to estimate the Bayes’ rule of allocation for the allocation of subsequent unclassified observations. Estimation on the basis of both the classified and unclassified data can be undertaken in a straightforward manner by fitting a $g$-component mixture model by maximum likelihood (ML) via the EM algorithm in the situation where the observed data can be assumed to be an observed random sample from the adopted mixture distribution. This assumption applies if the missing-data mechanism is ignorable in the terminology pioneered by Rubin (1976). An initial likelihood approach was to use the so-called classification ML approach whereby the missing labels are taken to be parameters to be estimated along with the parameters of the class-conditional distributions. However, as it can lead to inconsistent estimates, the focus of attention switched to the mixture ML approach after the appearance of the EM algorithm (Dempster et al., 1977). Particular attention is given here to the asymptotic relative efficiency (ARE) of the Bayes’ rule estimated from a partially classified sample. Lastly, we consider briefly some recent results in situations where the missing label pattern is non-ignorable for the purposes of ML estimation for the mixture model.

Key words: Bayes’ rule, partially classified data, semi-supervised learning
1 Introduction

We consider the estimation of a classifier from a sample that is not completely classified with respect to the predefined classes. This problem goes back at least to the mid-seventies (McLachlan, 1975), and it received a boost shortly afterwards with the advent of the EM algorithm (Dempster et al., 1977) which could be applied to carry out maximum likelihood (ML) estimation for a partially classified sample. There is now a wide literature on the formation of classifiers on the basis of a partially classified sample or semi-supervised learning (SSL) as it is referred to in the machine learning literature. In the sequel, it is assumed that the features with known class labels are correctly classified, containing no misclassified features as, for example, in McLachlan (1972) and, more recently, Cannings and Samworth (2019).

More specifically, we focus on the case of \( g = 2 \) classes \( C_1 \) and \( C_2 \) in which the \( p \)-dimensional feature vector \( Y \) measured on an entity is distributed as

\[
Y \sim N(\mu_i, \Sigma) \quad \text{in} \quad C_i \quad (i = 1, 2).
\]

We let \( \theta \) contain the \( 1 + 2p + \frac{1}{2}p(p + 1) \) unknown parameters, consisting of the mixing proportion \( \pi_i \), the elements of the class means \( \mu_1 \) and \( \mu_2 \), and the distinct elements of the common class covariance matrix \( \Sigma \). The Bayes’ rule of allocation \( R(y) \) in this case assigns an entity with observed feature vector \( y \) to either \( C_1 \) or \( C_2 \), according as

\[
d(y) = \beta_0 + \beta^T y
\]

is greater or less than zero, where

\[
\beta_0 = -\frac{1}{2}(\mu_1 + \mu_2)^T \Sigma^{-1}(\mu_1 - \mu_2) + \log(\pi_1 / \pi_2),
\]

\[
\beta = \Sigma^{-1}(\mu_1 - \mu_2),
\]

and where \( \pi_i \) denotes the prior probability of membership of \( C_i (i = 1, 2) \); see, for example, McLachlan (1992).

2 History of SSL in Statistics

In his discussion of the paper read to the Royal Statistical Society by Hills (1966), Smith (1966) suggested that in the case of a completely unclassified sample which exhibits bimodality on some feature, a classifier be formed from the unclassified observations on the feature as follows: “One then arbitrarily divides them at the antimode, .... On the basis of this division, we calculate a suitable allocation rule; and, by using this allocation rule, get an improved division, and so on. As far as I know, there is no theoretical research into the effect of ‘lifting oneself by one’s own bootstraps’ in this way.”
This led McLachlan (1975) to consider this approach as suggested by Smith (1966) under the normal homoscedastic model (1). Under the latter assumption, the procedure is equivalent to treating the labels of the unclassified features as unknown parameters to be estimated along with $\theta$. This approach became subsequently known as the classification maximum likelihood (CML) approach as considered by Hartley and Rao (1968) among others; see McLachlan and Basford (1988, Section 1.12). The CML approach gives an inconsistent estimate of $\theta$ except in special cases like $\pi_1 = \pi_2$.

In order to make the problem analytically tractable for the calculation of the expected error rate of the estimated Bayes’ rule, McLachlan (1975) assumed that there were also a limited number $n_c$ of classified features available from $C_i$ in addition to the number of $n_u = n - n_c$ unclassified features, where $n$ denotes the total size of the now partially classified sample and $n_c = n_{1c} + n_{2c}$.

In the sequel, we let $x_{CC} = (x_1^T, \ldots, x_n^T)^T$ denote $n$ independent realizations of $X = (Y^T, Z)^T$ as the completely classified training data, where $Z$ denotes the class membership of $Y$, being equal to 1 if $Y$ belongs to $C_1$, and zero otherwise. We let $m_j$ be the missing-label indicator being equal to 1 if $z_j$ is missing and zero if it is available ($j = 1, \ldots, n$). Accordingly, the unclassified sample $x_{PC}$ is given by those members $x_j$ in $x_{CC}$ for which $m_j = 0$ and only the feature vectors $y_j$ without their class labels $z_j$ for those members in $x_{CC}$ for which $m_j = 1$.

**3 Asymptotic expected error rate of CML approach**

In practice, $\beta$ has to be estimated from available training data. It can be calculated iteratively as described in the previous section. More formally, it can be obtained iteratively by applying the expectation–maximization (EM) algorithm of Dempster et al. (1977) with the following modification (McLachlan, 1982). Namely, the E-step is executed using outright (hard) rather than fractional (soft) assignment of each unclassified feature to a component of the mixture as with the standard application of the EM algorithm. We let $\hat{\beta}_{PC}^{(k)}$ denote the estimator after the $k$th iteration of the vector $\beta = (\beta_0, \beta^T)^T$ of discriminant function coefficients obtained by the classification ML approach applied to the partially classified sample $x_{PC}$. The estimated Bayes’ rule using $\hat{\beta}_{PC}^{(k)}$ for $\beta$ in the Bayes’ rule $R(\beta)$ is denoted by $\hat{R}_{PC}^{(k)}$. The (overall) conditional error rate of $\hat{R}_{PC}^{(k)}$ is denoted by $\text{err}(\hat{\beta}_{PC}^{(k)}; \theta)$.

Then the expected excess error rate of the estimated Bayes’ rule $\hat{R}_{PC}^{(k)}$ is defined after the $k$th iteration by $E\{\text{err}(\hat{\beta}_{PC}^{(k)}; \theta)\} - \text{err}(\theta)$, where $\text{err}(\theta)$ is the optimal error rate.

In the present SSL context, McLachlan (1975) showed in the case of equal, known prior probabilities that the overall expected error rate of this classifier after the $k$th iteration is given as, $n_u \to \infty$, by
\[ E \{ \text{err} (\hat{\beta}^{(k)}_{PC}; \theta) \} = \Phi \left( -\frac{1}{2} \Delta \right) + \{ \phi \left( \frac{1}{2} \Delta \right) / 4 \} a_{1}^{(k)} + O(n^{-2}), \]  
\tag{2} \]
where
\[ a_{1}^{(k)} = h_{1}^{2k} \Delta + h_{2}^{2k} \left( \frac{1}{n_{1c}} + \frac{1}{n_{2c}} \right) + h_{2}^{2k} \left( \frac{p - 1}{n_{c}} \right), \]
\[ h_{1} = \phi \left( \frac{1}{2} \right) \left[ 4 \phi \left( \frac{1}{2} \right) + \Delta \right] \left( 1 - 2 \Phi \left( -\frac{1}{2} \right) \right], \]
\[ h_{2} = \{ \phi \left( \frac{1}{2} \right) \}^{2} \left( 4 + \Delta^{2} \right) / h_{1}, \]
and where \( \Delta = \left( \mu_{1} - \mu_{2} \right)^{T} \Sigma^{-1} \left( \mu_{1} - \mu_{2} \right)^{1/2} \) is the Mahalanobis distance between the class-conditional distributions and \( \text{err}(\theta) = \Phi \left( -\frac{1}{2} \Delta \right) \).

As it can be shown that both \( |h_{1}| \) and \( |h_{2}| \) are always less than one, it follows from (2) that the expected error rate of \( \hat{R}^{(k)}_{PC} \) decreases after each iteration and converges to the optimal error rate as \( k \to \infty \).

4 Asymptotic relative efficiency of ML approach

The construction of classifiers from partially classified data can be undertaken also by the fitting of finite mixture models. The ML estimate of the vector of parameters \( \theta \) can be obtained via the EM algorithm of Dempster et al. (1977). As noted in McLachlan and Peel (2000), it was the publication of this seminal paper that greatly stimulated interest in the use of finite mixture models.

We let
\[ \log L_{C}(\theta) = \sum_{j=1}^{n} (1 - m_{j}) \left[ z_{j} \log \left\{ \pi_{1} \phi \left( y_{j}; \mu_{1}, \Sigma \right) \right\} + (1 - z_{j}) \log \left\{ \pi_{2} \phi \left( y_{j}; \mu_{2}, \Sigma \right) \right\} \right] \]
\[ \log L_{UC}(\theta) = \sum_{j=1}^{n} m_{j} \log \sum_{i=1}^{2} \pi_{i} \phi \left( y_{j}; \mu_{i}, \Sigma \right), \]
\[ \log L_{PC}^{(ig)}(\theta) = \log L_{C}(\theta) + \log L_{UC}(\theta), \]
\[ \log L_{CC}(\theta) = \log L_{C}(\theta) \]
\tag{3} \]
where \( \phi \left( y_{j}; \mu, \Sigma \right) \) denotes the multivariate normal density with mean \( \mu \) and covariance matrix \( \Sigma \). In situations where one proceeds by ignoring the “missingness” of the class labels, \( L_{C}(\theta) \) and \( L_{UC}(\theta) \) denote the likelihood function formed from the classified data and the unclassified data, respectively, and \( L_{PC}^{(ig)}(\theta) \) is the likelihood function formed from the partially classified sample \( x_{PC} \). The log of the likelihood \( L_{CC}(\theta) \) for the completely classified sample \( x_{CC} \) is given by (5) with all \( m_{j} = 0 \).

Situations in the present context where it is appropriate to ignore the missing-data mechanism in carrying out likelihood inference are where the missing labels are missing at random in the framework for missing data pioneered by Rubin (1976).
This will be the case in the present context if the missingness of the labels does not depend on the features nor the labels (missing completely at random) or if the missingness depends only on the features (missing at random), as in McLachlan and Gordon (1989).

We let \( \hat{\theta}_{CC} \) and \( \hat{\theta}_{PC} \) be the estimate of \( \theta \) formed by consideration of \( L_{CC}(\theta) \) and \( L_{PC}(\theta) \), respectively, and we let \( \hat{\beta}_{CC} \) and \( \hat{\beta}_{PC} \) be the estimates of \( \beta \) formed from the elements of \( \hat{\theta}_{CC} \) and \( \hat{\theta}_{PC} \), respectively. The relative efficiency of the estimated Bayes’ rule \( \hat{R}_{PC}^{(ig)} \) compared to the rule \( \hat{R}_{CC} \) using \( \hat{\beta}_{CC} \) for \( \beta \) based on the completely classified sample \( x_{CC} \) is defined by

\[
\text{ARE}(\hat{R}_{PC}^{(ig)}) = \frac{E\{\text{err}(\hat{\beta}_{CC} ; \theta)\} - \text{err}(\theta)}{E\{\text{err}(\hat{\beta}_{PC}^{(ig)} ; \beta)\} - \text{err}(\theta)}, \tag{6}
\]

where the expectation in the numerator and denominator of the right-hand side of (6) is taken over the distribution of the estimators of \( \beta \) and is expanded up to terms of the first order.

Under the assumption that the class labels are missing always completely at random, (that is, the missingness of the labels does not depend on the data), Ganesalingam and McLachlan (1978) derived the ARE of \( \hat{R}_{PC}^{(ig)} \) compared to \( \hat{R}_{CC} \) in the case of a completely unclassified sample \( (\gamma = n_u/n = 1) \) for univariate features \( (p = 1) \). Their results are listed in Table 1 for \( \Delta = 1, 2, 3, \) and 4. O’Neill (1978) extended their result to multivariate features and for arbitrary \( \gamma \) using the result of Efron (1975) for the information matrix of \( \beta \) in applying logistic regression. His results showed that this ARE was not sensitive to the values of \( p \) and does not vary with \( p \) for equal class prior probabilities. Not surprisingly, it can be seen from Table 1 that the ARE of \( \hat{R}_{PC}^{(ig)} \) for a totally unclassified sample is low, particularly for classes weakly separated as represented by \( \Delta = 1 \) in Table 1.

Table 1 Asymptotic relative efficiency of \( \hat{R}_{PC}^{(ig)} \) compared to \( \hat{R}_{CC} \)

| \( \pi_1 \) | \( \Delta = 1 \) | \( \Delta = 2 \) | \( \Delta = 3 \) | \( \Delta = 4 \) |
|----------------|----------------|----------------|----------------|----------------|
| 0.1            | 0.0036         | 0.0591         | 0.2540         | 0.5585         |
| 0.2            | 0.0025         | 0.0668         | 0.2972         | 0.6068         |
| 0.3            | 0.0027         | 0.0800         | 0.3289         | 0.6352         |
| 0.4            | 0.0038         | 0.0941         | 0.3509         | 0.6522         |
| 0.5            | 0.0051         | 0.1008         | 0.3592         | 0.6580         |

In other work on the ARE of \( \hat{R}_{PC}^{(ig)} \) compared to \( \hat{R}_{CC} \), McLachlan and Scot (1995) evaluated it where the unclassified univariate features had labels missing always at random due to truncation of the features.
5 Modelling missingness for unobserved class labels

In many practical applications class labels will be assigned by experts. Manual annotation of the dataset can induce a systematic missingness mechanism. This led Ahfock and McLachlan (2019a,b) to pursue the idea that the probability that a particular feature is unlabelled is related to the difficulty of determining its true class label. As an example, suppose medical professionals are asked to classify each image from a set of MRI scans into three groups, tumour present, no tumour present, or unknown. It seems reasonable to expect that the unassigned images will correspond to those that do not present clear evidence for the presence or absence of a tumour. The unlabelled images will exist in regions of the feature space where there is class overlap. In these situations, the unlabelled features carry additional information that can be used to improve the efficiency of parameter estimation.

The missing-data mechanism of Rubin (1976) is specified in the present context by the conditional distribution

$$\Pr\{M_j = m_j | y_j, z_j; \kappa\} \quad (j = 1, \ldots, n),$$

(7)

where $\kappa$ is a vector of parameters. Ahfock and McLachlan (2019a,b) proposed that

$$\Pr\{M_j = 1 | y_j, z_j\} = \Pr\{M_j = 1 | y_j\} = q(y_j; \theta, \xi),$$

(8)

where the parameter $\xi$ is distinct from $\theta$. On putting $\Psi = (\theta^T, \xi^T)^T$, an obvious choice for the function $q(y_j; \Psi)$ is the logistic model

$$q(y_j; \Psi) = \frac{\exp\{\xi_0 + \xi_1 e_j\}}{1 + \exp\{\xi_0 + \xi_1 e_j\}},$$

(9)

where

$$e_j = -\sum_{i=1}^2 \tau_i(y_j; \theta) \log \tau_i(y_j; \theta)$$

(10)

denotes the entropy for $y_j$, and where $\tau_i(y_j; \theta)$ is the posterior probability that the $j$th entity with observed feature $y_j$ belongs to Class $C_i (i = 1, 2)$.

The log of the full likelihood function for $\Psi$ is given by

$$\log L^{(\text{full})}_{\text{PC}}(\Psi) = \log L^{(\text{ig})}_{\text{PC}}(\theta) + \log L^{(\text{miss})}_{\text{PC}}(\Psi),$$

(11)

where

$$\log L^{(\text{miss})}_{\text{PC}}(\Psi) = \sum_{j=1}^n [(1 - m_j) \log \{1 - q(y_j; \Psi)\} + m_j \log q(y_j; \Psi)]$$

(12)

is the log likelihood function for $\Psi$ formed on the basis of the missing-label indicators $m_j (j = 1, \ldots, n)$. 


Under the model for the missingness of the class labels Ahfock and McLachlan (2019a,b) showed for the normal homoscedastic model that the ARE of the Bayes’ rule using the full ML estimate of $\beta$ can not only be improved but, rather surprisingly, can be greater than one.

6 Fractionally supervised classification

In this section we make use of the model to examine the potential usefulness of fractionally supervised classification (FSC) as proposed by Vrbik and McNicholas (2015) and considered further by Gallaugher and McNicholas (2019). With this approach, the parameter $\theta$ is estimated by consideration of the objective function $L^{(\alpha)}_{PC}(\theta)$ defined for a given $\alpha$ in [0,1] by

$$\log L^{(\alpha)}_{PC}(\theta) = \alpha \log L_C(\theta) + (1 - \alpha) \log L_{UC}(\theta).$$

One suggestion for the choice of $\alpha$ in practice is to use BIC (Schwarz, 1978).

We report here a simulation experiment undertaken by Ahfock and McLachlan (2019a) in which a partially classified sample of size $n = 500$ was generated on each of $N = 100$ replications. Bivariate features were generated from a mixture of two normal bivariate distributions in equal proportions ($\pi_1 = \pi_2 = 0.5$) with unequal covariance matrices, where the two components correspond to $g = 2$ classes. The component means were given by $\mu_1 = (0,0)^T$ and $\mu_2 = (0,3)^T$ with the component-covariance matrices having unit variances for both variables with correlation 0.7 in the first component and zero correlation in the second component. The conditional distribution of the missing-label indicators $M_j$ was specified by the model with $\xi_0 = -5$ and $\xi_1 = 100$. For each partially classified sample $x_{PC}$ generated, the estimate $\hat{\theta}^{(\alpha)}_{PC}$ of $\theta$ was calculated via maximization of the objective function $L^{(\alpha)}_{PC}$ for a grid of values of $\alpha$, along with the estimate $\hat{\theta}^{(full)}_{PC}$ using the full likelihood function $L^{(full)}_{PC}(\Psi)$. On each replication the adjusted Rand index (ARI) for the estimated Bayes’ rule was obtained by applying it to 2,000 data points in a test set. The average values of these ARI’s are displayed in Figure. They show that as $\alpha$ moves away from a small neighbourhood of $\alpha = 0.5$, the performance of the rule using the fractionally supervised estimate falls dramatically. The horizontal line in Figure is the simulated value of the ARI for the use of $\hat{\theta}^{(full)}_{PC}$.

References

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Fig. 1 Plot of simulated ARI for various values of $\alpha$