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A Flexible Procedure for Mixture Proportion Estimation in Positive–Unlabeled Learning

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Abstract

Positive-unlabeled (PU) learning considers two samples, a positive set P with observations from only one class and an unlabeled set U with observations from two classes. The goal is to classify observations in U. Class mixture proportion estimation (MPE) in U is a key step in PU learning. Blanchard et al. [2010] showed that MPE in PU learning is a generalization of the problem of estimating the proportion of true null hypotheses in multiple testing problems. Motivated by this idea, we propose reducing the problem to one dimension via construction of a probabilistic classifier trained on the P and U data sets followed by application of a one-dimensional mixture proportion method from the multiple testing literature to the observation class probabilities. The flexibility of this framework lies in the freedom to choose the classifier and the one-dimensional MPE method. We prove consistency of two mixture proportion estimators using bounds from empirical process theory, develop tuning parameter free implementations, and demonstrate that they have competitive performance on simulated waveform data and a protein signaling problem.

Keywords: mixture proportion estimation; PU learning; classification; empirical processes; local false discovery rate; multiple testing

Short title: Mixture Proportion Estimation for PU Learning

1 Introduction

Let

$$X_1, \dots, X_n \sim F = \alpha F_0 + (1 - \alpha) F_1,$$

$$X_{L,1}, \dots, X_{L,m} \sim F_1,$$
(1)

all independent, where F_0 and F_1 are distributions on \mathbb{R}^p with densities f_0 and f_1 with respect to measure μ . The goal is to estimate α and the classifier

$$C_{01}(x) = \frac{(1-\alpha)f_1(x)}{\alpha f_0(x) + (1-\alpha)f_1(x)},$$
(2)

which can be used to separate the unlabeled data $\{X_i\}_{i=1}^n$ into the classes 0 and 1. The above problem has been termed *Learning from Positive and Unlabeled Examples, Presence Only Data, Partially Supervised Classification*, and the *Noisy Label Problem* in the machine learning literature [Elkan and Noto, 2008, Liu et al., 2002, Ramaswamy et al., 2016, Scott, 2015, Scott et al., 2013, Ward et al., 2009]. In this work, we use the term PU learning to refer to Model (1). Here we denote the positive set $P := \{X_{L,i}\}_{i=1}^m$ and the unlabeled set $U := \{X_i\}_{i=1}^n$. This setting is more challenging than the traditional classification framework where one possesses labeled training data belonging to both classes. In particular α and C_{01} are not generally identifiable from the P and U data. PU learning has been applied to text analysis [Liu et al., 2002], time series [Nguyen et al., 2011], bioinformatics [Yang et al., 2012], ecology [Ward et al., 2009], and social networks [Chang et al., 2016].

Several strategies have been proposed for solving the PU problem. Ward et al. [2009] assumes α is known and uses logistic regression to classify U. The SPY method of Liu et al. [2002] classifies U directly by identifying a "reliable negative set." The SPY method has practical challenges including choosing the reliable negative set. Other strategies estimate α directly. Ramaswamy et al. [2016] estimate α via kernel embedding of distributions. Scott [2015] and Blanchard et al. [2010] estimate α using the ROC curve produced by a classifier trained on P and U.

Blanchard et al. [2010] showed that MPE in the PU model is a generalization of estimating the proportion of true nulls in multiple testing problems. Specifically, suppose that F_0 and F_1 are one-dimensional distributions and F_1 is known. Then the unlabeled set X_1, \ldots, X_n may be interpreted as test statistics with the hypotheses:

$$H_0: X_i \sim F_1,$$
$$H_a: X_i \sim F_0.$$

In this context, $1 - \alpha$ is the proportion of true null hypotheses and the classifier C_{01} is the local FDR [Efron et al., 2001]. There are many works on addressing identifiability and estimation of α and C_{01} in this simpler setting [Efron, 2012, Genovese et al., 2004, Meinshausen and Rice, 2006, Patra and Sen, 2016, Robin et al., 2007].

FDR α estimation methods have been developed for one-dimensional MPE problems and are not directly applicable on the multidimensional PU learning problem in which $X_i \in \mathbb{R}^p$. In this work, we show that the PU MPE problem can be reduced to dimension one by constructing a classifier on the P versus U data sets followed by transforming observations to class probabilities. One dimensional MPE methods from the FDR literature can then be applied to the class probabilities. Computer implementation of this approach is straightforward because one can use existing classifier and one-dimensional MPE algorithms. We prove consistency for adaptations of two one-dimensional MPE methods: Storey [2002] based on empirical processes and Patra and Sen [2016] based on isotonic regression. These proofs use results from empirical process theory. We show that the ROC method used in Blanchard et al. [2010] and Scott [2015] in the machine learning literature is a variant of the method proposed by Storey Storey [2002] in the multiple testing literature. These results strengthen connections between the PU learning and multiple testing communities.

The rest of the paper is organized as follows. In Section 2 we give a sketch of the proposed procedure, which includes two proposed estimators C-PS and C-ROC. This section consists of three parts. First, a motivation of the procedure from the hypothesis testing perspective is explained. Second, identifiability of α is addressed. Third, a workflow is provided to explain how to implement the proposed procedure. In Section 3 we show that Model (1) can be reduced to one-dimension with a classifier. In Section 4 we show consistency of two α estimators. In Section 5 we numerically show that the estimators perform well in various settings. A conclusion is made in Section 6. Appendix A.1 gives proofs of theorems in the paper. Supporting lemmas can be found in Appendix A.2.

2 Background and Proposed Procedure

2.1 Multiple Testing, FDR, and Estimating the Proportion of True Nulls

Suppose one conducts n tests of null hypothesis $H_0: X_i \sim F_1$ versus alternative hypothesis $H_a: X_i \sim F_0$, i = 1, ..., n. The X_i are typically test statistics or p-values and the null distribution F_1 is assumed known (usually Unif[0, 1] in the case of X_i being p-values). The distribution of the X_i are $F = \alpha F_0 + (1 - \alpha)F_1$, where $1 - \alpha$ is the proportion of true null hypotheses. The *false discovery rate* (FDR) is the expected proportion of false rejections. If R is the number of rejections and V is the number of false rejections then $FDR \equiv \mathbb{E}[\frac{V}{R}\mathbf{1}_{R>0}]$. Benjamini and Hochberg [1995] developed a linear step-up procedure which bounds the FDR at a user specified level β . In fact, this procedure is conservative and results in an FDR $\leq \beta(1-\alpha) \leq \beta$. This conservative nature causes the procedure to have less power than other methods which control FDR at β . Adaptive FDR control procedures first estimate $1 - \alpha$ and then use this estimate to select a β which ensures control at some specified level while maximizing power. Many estimators of α have been proposed [Benjamini and Hochberg, 2000, Benjamini et al., 2006, Blanchard and Roquain, 2009, Langaas et al., 2005, Patra and Sen, 2016, Storey, 2002].

There are two reasons why these procedures cannot be directly applied to the PU learning problem. First, many of the methods have no clear generalization to dimension greater than one because they require an ordering of the test statistics or p-values. Second, the distribution F_1 is assumed known where as in the PU learning problem we only have a sample from this distribution. The classifier dimension reduction procedure we outline in Section 2.3 addresses the first point by transforming the PU learning problem to 1-dimension. The theory we develop in Sections 3 and 4 addresses the second issue.

2.2 Identifiability of α and C_{01}

Many works in both the PU learning and multiple testing literature have discussed the non-identifiability of the parameters α and F_0 . For any given (α, F_0) pair with $\alpha < 1$, one can find a $\gamma > 0$ such that $\alpha' \equiv \alpha + \gamma \leq 1$. Define $F'_0 \equiv \frac{\alpha F_0 + \gamma F_1}{\alpha + \gamma}$. Then

$$F = \alpha' F_0' + (1 - \alpha') F_1,$$

which implies (α', F_0') and (α, F_0) result in the same distributions for P and U.

To address this issue, we follow the approach taken by Blanchard et al. [2010] and Patra and Sen [2016]

and estimate a lower bound on α defined as

$$\alpha_0 := \inf\left\{\gamma \in (0,1] : \frac{F - (1-\gamma)F_1}{\gamma} \text{ is a c.d.f.}\right\}.$$
(3)

The parameter α_0 is identifiable. Recall the objective is to estimate

$$C_{01}(x) = \frac{(1-\alpha)f_1(x)}{\alpha f_0(x) + (1-\alpha)f_1(x)}.$$

Let $\pi = m/(m+n)$ be the proportion of labeled data. The classifier

$$C(x) = \frac{\pi f_1(x)}{\pi f_1(x) + (1 - \pi)f(x)}$$

outputs the probability an observation is from the labeled data set at a given x. We can approximate C by training a model on the P versus U data sets. The classifiers C and C_{01} are related through α . To see this, note that after some algebra

$$\frac{f_1(x)}{f(x)} = \frac{C(x)}{1 - C(x)} \frac{1 - \pi}{\pi}.$$

Thus

$$C_{01}(x) = \frac{(1-\alpha)f_1(x)}{f(x)} = \frac{1-\pi}{\pi} \frac{C(x)}{1-C(x)}(1-\alpha).$$

Since α is not generally identifiable, neither is C_{01} . However the plug-in estimator, using C_n (a classifier trained on P versus U) and $\hat{\alpha}_0$ (some estimator of α_0),

$$\widehat{C}_{01}^{0}(x) \equiv \frac{1-\pi}{\pi} \frac{C_{n}(x)}{1-C_{n}(x)} (1-\widehat{\alpha}_{0})$$

is an estimated upper bound for C_{01} . We can classify an unlabeled observation X_i as being from F_1 if $\widehat{C}_{01}^0(X_i) > \frac{1}{2}$. The problem has now been reduced to estimation of α_0 . The classifier C_n plays an important role in estimation of α_0 as well, as shown in the following section.

2.3 Workflow for α_0 Estimation

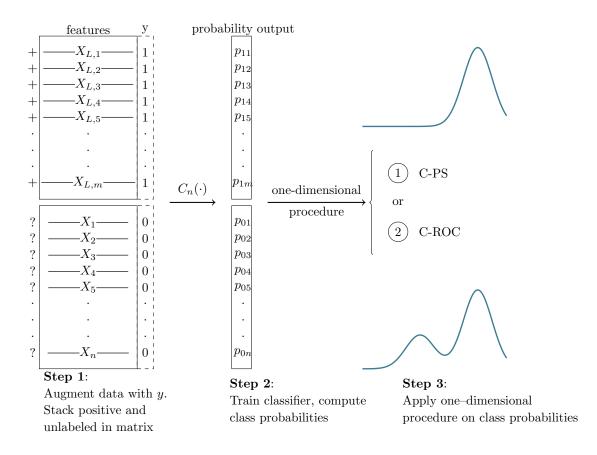


Figure 1: Workflow of proposed procedure. In **Step 1**, "+" denotes the positive samples, and "?" denotes the unlabeled samples of unknown class (can be "+" or "-"). Stack the set P and the set U together as a large matrix, and add a new column y to manually impose pseudo labels on observations: "1" for $X_{L,i}$ and "0" for X_i . In **Step 2**, a classifier $C_n(\cdot)$ is trained on the stacked matrix and the probability predictions (y = 1 as reference) are obtained. In **Step 3**, a one-dimensional procedure is applied to the probability output from Step 2. In this paper, two methods C-PS and C-ROC are proposed. The upper density curve is used to demonstrate that the $\mathbf{p}_1 := \{p_{1i}\}_{i=1}^m$ are from one population, while the bottom density curve shows that $\mathbf{p}_0 := \{p_{0i}\}_{i=1}^n$ are from mixture of two populations.

The proposed procedure to estimate α_0 in Model (1) is summarized in Figure 1. The key idea of this procedure is to reduce the dimension of PU learning problem via the classifier C_n trained on P versus U and then apply a one-dimensional MPE method on the transformed data to estimate α_0 . The procedure consists of three steps:

• Step 1. Label the *P* samples with pseudo label (Y = 1) and label the *U* samples with pseudo label (Y = 0). Hence we have $\tilde{P} := \{(X_{L,i}, Y_i = 1), i = 1, ..., m\}$ and $\tilde{U} := \{(X_i, Y_i = 0), i = 1, ..., n\}$.

- Step 2. Train a probabilistic classifier $C_n(\cdot) = \widehat{P}(Y = 1 | X = \cdot)$ on \widetilde{P} versus \widetilde{U} . Compute probabilistic predictions: $\mathbf{p}_1 := \{p_{1i}, i = 1, \dots, m\}$ and $\mathbf{p}_0 := \{p_{0i}, i = 1, \dots, n\}$, where $p_{1i} := C_n(X_{L,i})$ and $p_{0i} := C_n(X_i)$.
- Step 3. Apply a one-dimensional MPE method to \mathbf{p}_1 and \mathbf{p}_0 to estimate α_0 .

We augment the original data with pseudo labels in Step 1, in order to use a supervised learning classification algorithm. In Step 2 we use Random Forest [Breiman, 2001]. However in principle any classifier can be used. Note that the p_{0i} and p_{1i} are scalars. Hence in Step 3 we can utilize any one-dimensional method to estimate α_0 . In this work we adapt two methods – one from Storey [2002] and Scott [2015], another from Patra and Sen [2016]. Note that the original theory developed for these methods assumed that the null distribution is known, but in the PU problem we need to estimate it from $\mathbf{p_1}$. Since this setting is more complex, new theory is needed. In Section 4, we prove the consistency of two estimators in the PU setting, using Theorems 1 and 2.

3 Dimension Reduction via Classifier

Using the P and U samples we can make probabilistic predictions, i.e. compute the probability that the observation is from distribution F_1 versus from distribution F. The true classifier is

$$C(x) = \frac{f_1(x)\pi}{f_1(x)\pi + f(x)(1-\pi)},$$

where $\pi = \frac{m}{m+n}$ is the proportion of labeled sample within the entire data. We treat π as a known constant.

Denote the distribution of probabilistic predictions for P and U, respectively, as

$$G_L(t) = P(C(X) \le t | X \sim F_1),$$

$$G(t) = P(C(X) \le t | X \sim F).$$

One can consider the two-component mixture model

$$G = \alpha^G G_s + (1 - \alpha^G) G_L, \tag{4}$$

for α^G and G_s , which are again potentially non-identifiable. Define

$$\alpha_0^G := \inf\left\{\gamma \in (0,1] : \frac{G - (1-\gamma)G_L}{\gamma} \text{ is a c.d.f.}\right\}.$$
(5)

<u>Theorem</u> 1. $\alpha_0^G = \alpha_0$.

See Section A.1.1 for a proof. Theorem 1 shows one can solve the p-dimensional MPE problem (3) by solving the 1-dimensional MPE problem (5). In what follows we use α_0 instead of α_0^G to simplify notation.

In practice, the classifier C(X) is approximated by a trained model $C_n(X)$ on a given sample. For convenience, we assume the classifier $C_n(X)$ is trained using another independent sample \mathcal{D}'_n . The \mathcal{D}'_n is omitted in the following to lighten notation. We require the approximated classifier to be a consistent estimator of the true classifier.

Assumptions A. We assume

$$\mathbb{E}|C_n(X) - C(X)| = O\left(n^{-\tau}\right),\tag{6}$$

for some $\tau > 0$.

Such convergence results have been proven for a variety of probabilistic classifiers, including variants of Random Forest [Biau, 2012]. Define

$$G_{L,n}(t) := \frac{1}{m} \sum_{i=1}^{m} \mathbb{1}_{C_n(X_{L,i}) \le t}$$
$$G_n(t) := \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}_{C_n(X_i) \le t}.$$

Intuitively, $G_{L,n}$ and G_n are approximate empirical distribution functions of G_L and G respectively. The approximation is due to the fact that C is estimated with C_n . Thus we would expect Glivenko-Cantelli and Donsker properties for $G_n(t)$ and $G_{L,n}(t)$. However problems can arise when C(X) is not continuous. Essentially convergence in probability for C(X), implied by Assumptions A, only implies convergence of distribution functions at points of continuity. By assuming G_L and G possess densities, we can obtain uniform convergence of distribution functions.

Assumptions B. We assume that G and G_L are absolutely continuous and have bounded density functions g and g_L .

Theorem 2. Under Assumption A and B, for $\beta = min(\tau/3, 1/2)$

$$n^{\beta}(G_{L,n}(t) - G_{L}(t))$$
 is $O_{P}(1)$,
 $n^{\beta}(G_{n}(t) - G(t))$ is $O_{P}(1)$,

where both $O_P(1)$ are uniform in t.

See Section A.1.2 for a proof. The result from Theorem 2 is the key step in showing consistency of our α_0 estimators in the following sections.

4 Estimation of α_0

We generalize a one-dimensional MPE method of Patra and Sen Patra and Sen [2016] to the PU learning problem. We term the method C-PS to emphasize the fact that the method developed by Patra and Sen is applied to the output of a classifier. Then we generalize a one-dimensional method of Storey Storey [2002] to the PU learning problem. We term the method C-ROC because the ROC method developed in Blanchard et al. [2010] and Scott [2015] can be viewed as a variant of the Story's Storey [2002] original idea.

4.1 C-PS

Patra and Sen [2016] remove as much of the $G_{L,n}$ distribution from G_n as possible, while ensuring that the difference is close to a valid cumulative distribution function. We briefly review the idea and provide theoretical results to support use of this procedure in the PU learning problem. See Patra and Sen [2016] for a fuller description of the method in the one-dimensional case.

For any $\gamma \in (0, 1]$ define

$$\widehat{G}_{s,n}^{\gamma} = \frac{G_n - (1 - \gamma)G_{L,n}}{\gamma}.$$

If $\gamma \geq \alpha_0$, $\widehat{G}_{s,n}^{\gamma}$ will be a valid c.d.f. (up to sampling uncertainty) while the converse is true if $\gamma < \alpha_0$. Find the closest valid c.d.f. to $\widehat{G}_{s,n}^{\gamma}$ defined as

$$\check{G}_{s,n}^{\gamma} = \underset{\text{all c.d.f. }W(t)}{\operatorname{argmin}} \int \left(\widehat{G}_{s,n}^{\gamma}(t) - W(t)\right)^2 dG_n(t).$$
(7)

Isotonic regression is used to solve Equation 7. Measure the distance between two c.d.f W_1 and W_2 as

$$d_n(W_1, W_2) = \sqrt{\int (W_1(t) - W_2(t))^2 dG_n(t)}.$$

If $d_n(\widehat{G}_{s,n}^{\gamma}, \check{G}_{s,n}^{\gamma}) \approx 0$, then $\alpha_0 \leq \gamma$ where the level of approximation is a function of the estimation uncertainty and thus the sample size. Given a sequence c_n define

$$\widehat{\alpha}_{0}^{c_{n}} = \inf\left\{\gamma \in (0,1]: \gamma d_{n}(\widehat{G}_{s,n}^{\gamma},\check{G}_{s,n}^{\gamma}) \leq \frac{c_{n}}{n^{\beta-\eta}}\right\}$$

where $\eta \in (0, \beta)$ is a constant and the rate β is from Theorem 2.

<u>Theorem</u> 3. Under Assumptions A and B, if $c_n = o(n^{\beta-\eta})$ and $c_n \to \infty$, then $\widehat{\alpha}_0^{c_n} \xrightarrow{p} \alpha_0$.

The proof, contained in Section A.1.4, is a generalization of results in Patra and Sen [2016] which accounts for the fact that both G_n and $G_{L,n}$ are estimators. While Theorem 3 provides consistency, there are a wide range of choices of c_n . Patra and Sen [2016] showed that $\gamma d_n(\hat{G}_{s,n}^{\gamma}, \check{G}_{s,n}^{\gamma})$ is convex, non-increasing and proposed letting $\hat{\alpha}_0$ be the γ that maximizes the second derivative of $\gamma d_n(\hat{G}_{s,n}^{\gamma}, \check{G}_{s,n}^{\gamma})$. We use this implementation in our numerical work in Section 5.

4.2 C-ROC

Recalling the definitions of G, G_s , and G_L from Section 3, note

$$G(t) = \alpha G_s(t) + (1 - \alpha)G_L(t) \le \alpha + (1 - \alpha)G_L(t)$$

for all t. Thus for any t such that $G_L(t) \neq 1$ we have

$$k(t) \equiv \frac{G(t) - G_L(t)}{1 - G_L(t)} \le \alpha.$$

In the FDR literature, G_L is the distribution of the test statistic or p-value under the null hypothesis and is generally assumed known. Thus only G must be estimated, usually with the empirical cumulative distribution function. Storey [2002] proposed an estimator for k(t) at fixed t (Equation 6) and determined a bootstrap method to find the t which produces the best estimates of the FDR.

The PU problem is more complicated in that one must estimate G and G_L . However the structure of Gand G_L enables one to estimate the identifiable parameter α_0 . Specifically with $t^* = \inf\{t : G_L(t) \ge 1\}$ we have

$$\lim_{t\uparrow t^*} k(t) = \alpha_0. \tag{8}$$

See Lemma 1 for a proof. This result suggests estimating α_0 by substituting the empirical estimators of G_n and $G_{L,n}$ into Equation 8 along with a sequence \hat{t} which is converging to the (unknown) t^* . Such a sequence \hat{t} must be chosen so that the estimated denominator $1 - \hat{G}_{L,n}(\hat{t})$ is not converging to 0 too fast (and hence too variable). For \hat{t} we use a quantile of the empirical c.d.f. which is converging to 1, but at a rate slower than the convergence of the empirical c.d.f.. For some $q \in (0, \beta)$, define

$$\widehat{t} = \inf\{t: G_{L,n}(t) \ge 1 - n^{-q}\} - n^{-1}.$$

The n^{-1} term in \hat{t} avoids technical complications.

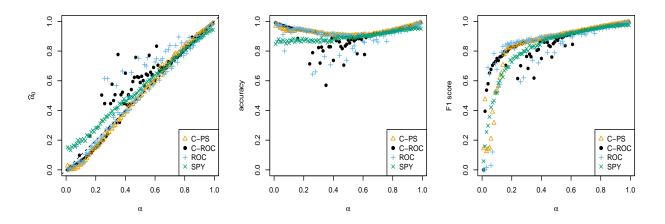


Figure 2: Comparison of methods with different α values. On the x-axis, α varies from 0.01 to 0.99 by step size 0.01. The left plot displays the estimates of the lower bound α_0 . The middle plot displays the accuracy of classifying observations in U. The right plot displays the F1 score of the classifications.

Theorem 4. Under Assumptions A and B

$$k_n(\hat{t}) \equiv \frac{G_n(\hat{t}) - G_{L,n}(\hat{t})}{1 - G_{L,n}(\hat{t})} \xrightarrow{P} \alpha_0$$

See Section A.1.3 for a proof.

4.2.1 Connection with ROC Method

The ROC method of Scott [2015] solves a generalization of the PU learning problem in which the positive set contains mislabeled data. When this method is specialized to the case of no misclassification in the labeled data i.e. the PU learning problem, it becomes a variant of the Storey [2002] method with a particular cutoff value t. Specifically, define the true ROC curve by the parametric equation

$$\{(G_L(t), G(t)) : t \in [0, 1]\}.$$

Scott [2015] (Proposition 2) showed that α_0 is the supremum of one minus the slope between (1,1) and any point on the ROC curve.¹ This is equivalent to the Storey method of Storey [2002] because

$$\alpha_0 = \sup_t 1 - \frac{1 - G(t)}{1 - G_L(t)}$$
$$= \sup_t \frac{G(t) - G_L(t)}{1 - G_L(t)}$$
$$= \sup_t k(t).$$

¹Scott [2015] estimated $\kappa = 1 - \alpha$. We have modified the ROC method notation to reflect the α notation used in this work.

The true ROC curve is not known, so α_0 cannot be computed directly from this expression. Blanchard et al. [2010] found a consistent estimator and Scott [2015] determined rates of convergence using VC theory. For application to data, Scott [2015] splits the labeled and unlabeled data sets in half, constructs a kernel logistic regression classifier on half the data, and estimates the slope between (1,1) and a discrete set of points on the ROC curve. The α_0 estimate is the supremum of 1 minus each of these slopes. Thus we see that the ROC method and earlier methods developed in the FDR literature are in the same family of α estimation strategies. Choosing a t in the Storey approach is equivalent to choosing a point on the ROC curve.

4.2.2 Practical Implementation

We consider two implementations of these ideas. The method of Scott [2015], using a kernel logistic regression classifier and a PU training–test set split to estimate tuning parameters, is referred to as "ROC." To facilitate comparison with C-PS, we consider another version with a Random Forest classifier using out–of–bag probabilities to construct the ROC curve. We call this method C-ROC.

5 Numerical Experiments

To illustrate the proposed methods we carry out numerical experiments on simulated *waveform* data and a real protein signaling data set *TCDB-SwissProt*. We compare the performance of the three methods (C-PS, C-ROC and ROC) discussed in Section 4 and the SPY method. With the SPY method, once the classifications ("positive" or "negative") in set U are made, we use the proportion of "negative" cases as an approximation of α_0 . For the C-ROC and C-PS methods [Breiman, 2001], we use Random Forest to construct $C_n(\cdot)$.

5.1 Waveform Data

We simulate observations from the *waveform* data set using the R-package *mlbench* [Leisch and Dimitriadou, 2010]. The *waveform* data is a binary classification problem with 21 features. We fix $\pi = 0.5$ for all simulations.

5.1.1 Varying α

We vary α from 0.01 to 0.99 in Model (1) in increments of 0.01. For each α the sample sizes are fixed at m = n = 3000. At each α we run the methods described to estimate α and classify observations in U. Results are shown in Figure 2. SPY produces inflated α estimates at low α (left panel) and has the the

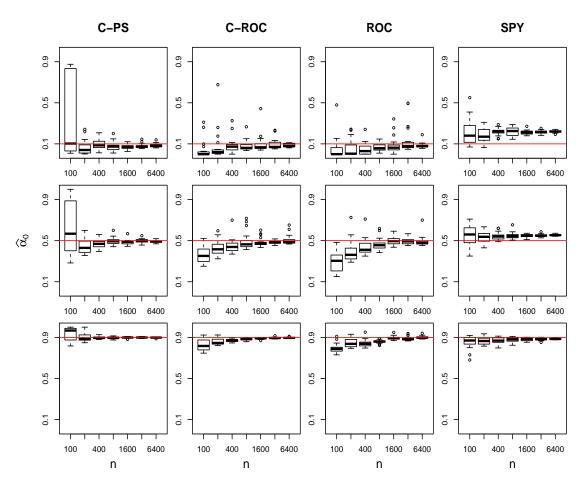


Figure 3: Comparison of methods with different sample sizes. The red solid horizontal lines represent the true α (0.1,0.5,0.9). The range for all y-axes is [0, 1] from bottom to top. The unlabeled sample size n varies with 100×2^{j} (j = 0, ..., 6). Each boxplot summarizes 20 repeated estimates $\hat{\alpha}_{0}$ for each (n, α) pair.

worst overall classification performance (center panel). Both C-ROC and ROC have substantial variability for α near 0.5. Overall, C-PS appears to be the best method.

5.1.2 Varying Sample Size

We empirically examine consistency and convergence rates of the methods by estimating α at increasing sample sizes, keeping the number of labeled and unlabeled observations equal, i.e. n = m. In Figure 3, every method is repeated 20 times for each (n, α) pair. The 20 α_0 estimates are displayed as a boxplot, which show estimator bias and variance. We see that all methods, except SPY, appear consistent under different settings ($\alpha = 0.1, 0.5, 0.9$). The estimators may have substantial bias at small n. C-PS struggles at n = 100, but has the best overall performance, followed by C-ROC and ROC.

5.1.3 Single Feature α_0 Estimation

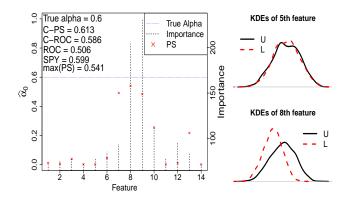


Figure 4: Estimation of α_0 using individual features. In the left panel the horizontal blue dash line is the true α (= 0.6), the vertical black dashed lines are the feature importances (right y-axis), and the red cross symbol are the α_0 estimate using the Patra/Sen procedure on a single feature (left y-axis). The right panels are kernel density estimates of unlabeled (U) and labeled (L) data for features 5 and 8.

One approach to solving the multidimensional PU learning problem is to estimate α separately using each feature. If $X_i \in \mathbb{R}^p$, this results in p estimates $\hat{\alpha}_0^1, \ldots, \hat{\alpha}_0^p$ of the parameter α . Each of these is an estimated lower bound on α . Thus a naive estimate of α_0 is $\max(\hat{\alpha}_0^1, \ldots, \hat{\alpha}_0^p)$. This approach ignores the correlation structure among features.

Using the *waveform* data, we compare this strategy to the multi-dimensional classifier approach. To make the problem challenging we select the 14 weakest features, defined as having the lowest Random Forest importance scores. We apply the Patra–Sen one–dimensional method to obtain individual feature α_0 estimates. The results are summarized in Figure 4. Feature importance matches well with the performance of the α estimates. On the right panels of Figure 4, we see that feature 5 is not useful because there is little difference between the unlabeled and labeled samples, leading to a feature based α estimate of approximately 0.012. In contrast, feature 8 is better in that it gives an alpha estimate of approximately 0.542. The SPY, C-ROC, and C-PS methods all perform better than the individual feature estimates (upper left of Figure 4).

5.2 Protein Signaling

The transporter classification database (TCDB) [Saier et al., 2006], here the P set, consists of 2453 proteins involved in signaling across cellular membranes. It is desirable to add proteins to this database from unlabeled databases which contain a mixture of membrane transport and non-transport proteins. Elkan and Noto [2008] and Das et al. [2007] manually identified 348 of the 4906 proteins as being related to transport in the SwissProt [Boeckmann et al., 2003] database. We treat the SwissProt data as the unlabeled set U for which we have ground truth $\alpha = (4906 - 348)/4906 \approx 0.929$. Information from protein description documents are used as features including function, subcellular location, alternative products, and disease. In total there are p = 741 features. We fit models with both the original feature set and with 2p and 10p features where all additional features are simulated by randomly selecting one of the original p features and permuting its values among the observations. So for 10p, p features are original (and potentially useful for classifying observations) while 9p of the features are simulated noise. Since 10p > n + m (total training set size), this represents a high dimensional setting for estimating α .

We compare C-PS with single feature PS for p, 2p, and 10p features. A common strategy in high dimensional classification problems is to perform feature screening prior to classifier construction. Since the features are all binary, we screen features based on p-values from univariate chi-squared tests (Fisher exact when any 2×2 table cell counts are less than 10). We test the methods after screening for the top k = 500, 200, 100, 50, 10, 1 features with smallest p-values. The C-PS method is applied directly as described earlier on the k best features. For the single feature PS method, after screening for k features, the PS method is applied to all k features individually and the largest estimate is taken as an estimate of α . As explained in Section 5.1.3, for each feature the PS method is an estimate of a lower bound on α , thus taking the maximum of these estimated lower bounds is sensible.

Table 1 shows α estimates for each number of features and each k. First consider the two p feature columns representing the C-PS and single feature PS methods. C-PS with p features produces estimates which are high for k = 50 to 500 features, nearly correct for k = 10 features, and biased quite low for k = 1feature. There appears to be some overfitting with large k, but extreme screening to k = 1 results in a loss of information and a poor lower bound on α . Single feature PS produces estimates that are too high for k = 500 through 10 and too low for p = 1. It is either worse or no better than C-PS at each k. Single feature PS with k = 1 represents choosing the best feature (based on p-values) and then applying the PS method. There is not sufficient information in this single best feature to obtain a good lower bound on α . The behavior of PS overestimating α at k = 10 through 500 features is due to the sensitivity of taking the maximum of single feature PS estimates. Even a single large estimate on one feature results in an overall estimate which is too high. The natural way to correct this is to choose a smaller set of k features, but with k = 1 there is not sufficient information in this single feature to obtain a good lower bound. In contrast, C-PS effectively pools information across multiple features to produce improved estimates. The results are quite consistent across p, 2p and 10p. This is due to the fact that feature screening retains a very similar set of features regardless of the number of noisy features added to the data set. For example, with k = 500, the p and 10p feature models retain 316/500 of the same features while for k = 10 they retain 10/10 of the same features. Thus the estimation methods (C-PS and PS) produce similar α estimates with p and 10p features. This suggests that feature prescreening combined with C-PS can be an effective α estimation strategy in high-dimensional settings with many pure noise features.

	р		$2\mathrm{p}$		10p	
k	C-PS	\mathbf{PS}	C-PS	\mathbf{PS}	C-PS	\mathbf{PS}
500	0.97	1.00	0.96	1.00	0.97	1.00
200	0.97	1.00	0.97	1.00	0.97	1.00
100	0.96	0.99	0.96	0.99	0.96	0.99
50	0.95	0.99	0.95	0.99	0.95	0.99
10	0.93	0.98	0.93	0.98	0.93	0.98
1	0.77	0.77	0.77	0.77	0.77	0.77

Table 1: α estimates from C-PS and single feature PS with p, 2p, and 10p features when prescreening the top k features. True $\alpha \approx 0.93$.

6 Conclusion

In this paper we proposed a framework for estimating the mixture proportion and classifier in the PU learning problem. We implemented this framework using two estimators from the FDR literature, C-PS and C-ROC. The framework has the power to incorporate other one-dimensional MPE procedures, such as Meinshausen and Rice [2006], Genovese et al. [2004], Langaas et al. [2005], Efron [2007], Jin [2008], Cai and Jin [2010] or Nguyen and Matias [2014]. More generally we have strengthened connections between the classification-machine learning literature and the multiple testing literature by constructing estimators using ideas from both communities. Potential directions for future research include generalizing results to the case where the labeled data contains some mislabeling of observations, relaxing Assumption A, and developing methods to handle cases where labeled and unlabeled data sets sizes are substantially different (class imbalance).

Supplementary Materials

R-code and data needed for reproducing results in this work are available online at github.com/zflin/PU_learning.

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Conflict of interest

The authors declare no potential conflict of interests.

Supporting information

The following supporting information is available as part of the online article: **Technical Notes** Proofs of all Theorems in this work.

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Technical Notes for A Flexible Procedure for Mixture Proportion Estimation in Positive–Unlabeled Learning

A.1 Proof of Theorems

A.1.1 Proof of Theorem 1

Equivalently, we are trying to prove

$$\frac{G - (1 - \gamma)G_L}{\gamma} \text{ is a c.d.f.} \Leftrightarrow \frac{F - (1 - \gamma)F_1}{\gamma} \text{ is a c.d.f.}$$
(A.1)

Sufficient to show

$$G - (1 - \gamma)G_L$$
 non-decreasing $\Leftrightarrow f - (1 - \gamma)f_1 \ge 0$ (A.2)
with probability 1.

First we show \Leftarrow . Consider any $t_2 > t_1$. Then

$$(G(t_2) - (1 - \gamma)G_L(t_2)) - (G(t_1) - (1 - \gamma)G_L(t_1))$$

= $\int_{\{x:C(x)\in(t_1,t_2]\}} \underbrace{f(x) - (1 - \gamma)f_1(x)}_{\geq 0 \text{ by assumption}} d\mu(x)$
 $\geq 0.$

Now we show \Rightarrow by proving the contrapositive. By assumption there exists

$$A = \{x : f(x) - (1 - \gamma)f_1(x) < 0\}$$

such that P(A) > 0. Further we have

$$A = \left\{ x : (1 - \gamma) \frac{(1 - \pi)}{\pi} > \frac{f(x)}{f_1(x)} \frac{(1 - \pi)}{\pi} \right\}$$
$$= \left\{ x : \underbrace{\frac{1}{1 + (1 - \gamma) \frac{(1 - \pi)}{\pi}}}_{\equiv t^*} < C(x) \right\}.$$

 So

$$(G(1) - (1 - \gamma)G_L(1)) - (G(t^*) - (1 - \gamma)G_L(t^*))$$

= $\int_{A = \{x: C(x) > t^*\}} f(x) - (1 - \gamma)f_1(x)d\mu(x)$
< 0.

A.1.2 Proof of Theorem 2

$$n^{\beta}(G_n(t) - G(t)) = \frac{n^{\beta}}{n^{1/2}} \underbrace{n^{1/2} \left(G_n(t) - \mathbb{E}[\mathbb{1}_{C_n(X) \le t} | C_n] \right)}_{\equiv \mathbb{R}_n(t)}$$
$$+ n^{\beta} \underbrace{\left(\mathbb{E}[\mathbb{1}_{C_n(X) \le t} | C_n] - G(t) \right)}_{\equiv \mathbb{Q}_n(t)}$$

We now show that $\mathbb{R}_n(t)$ and $\mathbb{Q}_n(t)$ are $O_P(1)$ uniformly in t. Together these facts show the expression is $O_P(1)$ uniformly in t. $\mathbb{R}_n(t)$: Note

$$\mathbb{R}_n(t) = \sqrt{n} \left(\frac{1}{n} \sum_{i=1}^n \mathbb{1}_{C_n(X_i) \le t} - \mathbb{E}[\mathbb{1}_{C_n(X) \le t} | C_n] \right).$$

By the DKW inequality

$$P(||\mathbb{R}_n||_{\infty} > x | C_n) \le 2e^{-2x^2}.$$

Thus $||\mathbb{R}_n||_{\infty}$ is $O_P(1)$. $\underline{\mathbb{Q}}_n(t)$: We have

$$\mathbb{Q}_{n}(t) = \mathbb{E}\left[\underbrace{\mathbb{I}_{C_{n}(X) \leq t} - \mathbb{1}_{C(X) \leq t}}_{B_{1}} | C_{n}\right]$$

$$\leq \underbrace{|E[T_{n}\mathbb{1}_{|C(X)-t| \leq \epsilon_{n}} | C_{n}]|}_{B_{1}}$$

$$+ \underbrace{|E[T_{n}\mathbb{1}_{|C(X)-t| > \epsilon_{n}}\mathbb{1}_{|C(X)-C_{n}(X)| < \epsilon_{n}} | C_{n}]|}_{B_{2}}$$

$$+ \underbrace{|E[T_{n}\mathbb{1}_{|C(X)-t| > \epsilon_{n}}\mathbb{1}_{|C(X)-C_{n}(X)| > \epsilon_{n}} | C_{n}]|}_{B_{3}}$$

Noting that $|T_n| \leq 1$ and C_n is independent of C(X), we have

$$B_1 \le P(|C(X) - t| \le \epsilon_n) \le 2\epsilon_n \sup_t g(t)$$

where g is the density of C(X), which exists and is bounded by Assumptions B. B_2 is 0 because $T_n = 0$ whenever the indicator functions in B_2 are both 1. Finally noting $B_3 \leq \mathbb{E}[\mathbb{1}_{|C(X)-C_n(X)|>\epsilon_n}|C_n]$ and using Markov's inequality twice, we have

$$P(B_3 > r_n) \leq P(\mathbb{E}[\mathbb{1}_{|C(X) - C_n(X)| > \epsilon_n} | C_n] > r_n)$$

$$\leq \frac{P(|C(X) - C_n(X)| > \epsilon_n)}{r_n}$$

$$\leq \frac{E[|C_n(X) - C(X)|]}{\epsilon_n r_n}.$$

Setting $\epsilon_n = n^{-\tau/3}$, $r_n = n^{-\tau/3}$, and $\beta = \tau/3$ achieves the desired result. Identical arguments hold for showing $n^{\beta}(G_{L,n}(t) - G_L(t))$ is $O_P(1)$ uniform in t.

A.1.3 Proof of Theorem 4

Since $\hat{t} = \inf\{t : G_{L,n}(t) \ge 1 - n^{-q}\} - n^{-1}$ and $0 < q < \beta$, we have

$$(n^{\beta}(1-G_{L,n}(\widehat{t})))^{-1} = \frac{n^{q}}{n^{\beta}} = o(1).$$

Recall by Theorem 2 we have

$$n^{\beta}(G_{L,n}(t) - G_L(t)) \equiv d_L(t) = O_P(1)$$
$$n^{\beta}(G_n(t) - G(t)) \equiv d(t) = O_P(1)$$

where this and subsequent O_P and o_P are uniform in t. We have

$$\begin{split} \frac{G_n(\hat{t}) - G_{L,n}(\hat{t})}{1 - G_{L,n}(\hat{t})} &= \frac{G(\hat{t}) - G_L(\hat{t})}{1 - G_{L,n}(\hat{t})} + \frac{n^{-\beta}(d_L(\hat{t}) - d(\hat{t}))}{1 - G_{L,n}(\hat{t})} \\ &= \underbrace{\left(\frac{1 - G_L(\hat{t})}{1 - G_{L,n}(\hat{t})}\right)}_{\equiv A} \underbrace{\left(\frac{G(\hat{t}) - G_L(\hat{t})}{1 - G_L(\hat{t})}\right)}_{\equiv k(\hat{t})} \\ &+ \underbrace{\frac{d_L(\hat{t}) - d(\hat{t})}{n^{\beta}(1 - G_{L,n}(\hat{t}))}}_{o_P(1)}. \end{split}$$

Note that

$$A = 1 + \frac{d_L(\hat{t})}{n^{\beta}(1 - G_{L,n}(\hat{t}))} = 1 + o_P(1).$$

Thus it is sufficient to show that $k(\hat{t}) \to \alpha_0$. By Lemma 1, $k(t) \uparrow \alpha_0$ as $t \uparrow t^*$. We show that for any $\epsilon > 0$

$$P(\hat{t} \in (t^* - \epsilon, t^*)) \to 1.$$

Thus by the continuous mapping theorem, the estimator is consistent.

Part 1: We show $P(t^* - \hat{t} > \epsilon) \to 0$. By the definition of t^* , there exists $\gamma > 0$ such that $G_L(t^* - \epsilon/2) = 1 - \gamma$. We have

$$P(t^* - \hat{t} > \epsilon)$$

$$= P(G_{L,n}(t^* - \epsilon + n^{-1}) > G_{L,n}(\hat{t} + n^{-1}))$$

$$\leq P(G_{L,n}(t^* - \epsilon + n^{-1}) > 1 - n^{-q})$$

$$\leq \underbrace{P(G_L(t^* - \epsilon + n^{-1}) > 1 - n^{-q} - \gamma/2)}_{\equiv A}$$

$$+ \underbrace{P(|G_{L,n}(t^* - \epsilon + n^{-1}) - G_L(t^* - \epsilon + n^{-1})| > \gamma/2)}_{\rightarrow 0 \text{ by Theorem 2}}.$$

 $A \to 0$ because for sufficiently large n, $G_L(t^* - \epsilon + n^{-1}) \le G_L(t^* - \epsilon/2) = 1 - \gamma < 1 - n^{-q} - \gamma/2$.

<u>Part 2</u>: We show $P(\hat{t} \ge t^*) \to 0$. We have

$$\begin{split} P(\widehat{t} \ge t^*) &= P(G_{n,L}(\widehat{t} + n^{-1}) \ge G_{n,L}(t^* + n^{-1})) \\ &= P(1 - n^{-q} \ge G_{n,L}(t^* + n^{-1})) \\ &= P(1 - G_{n,L}(t^* + n^{-1}) \ge n^{-q}) \\ &= P(\underbrace{n^{\beta}(G_L(t^* + n^{-1}) - G_{n,L}(t^* + n^{-1}))}_{O_P(1) \text{ by Theorem 2}} \ge n^{\beta - q}). \end{split}$$

Since $\beta > q$ we have the result.

A.1.4 Proof of Theorem 3

Proof. $\forall \epsilon > 0$, we need to show $P(|\hat{\alpha}_0^{c_n} - \alpha_0| > \epsilon) \to 0$. Note

$$P(|\widehat{\alpha}_0^{c_n} - \alpha_0| > \epsilon) = P(\widehat{\alpha}_0^{c_n} < \alpha_0 - \epsilon) + P(\widehat{\alpha}_0^{c_n} > \alpha_0 + \epsilon).$$

First we show that $P(\widehat{\alpha}_0^{c_n} < \alpha_0 - \epsilon) \to 0$. If $\alpha_0 \leq \epsilon$, then

$$P(\widehat{\alpha}_0^{c_n} < \alpha_0 - \epsilon) \le P(\widehat{\alpha}_0^{c_n} < 0) = 0.$$

If $\alpha_0 > \epsilon$, suppose we have $\hat{\alpha}_0^{c_n} < \alpha_0 - \epsilon$, then by Lemma 7,

$$d_n(\widehat{G}_{s,n}^{\alpha_0-\epsilon},\check{G}_{s,n}^{\alpha_0-\epsilon}) \le \frac{c_n}{n^{\beta-\eta}(\alpha_0-\epsilon)}.$$

The LHS of above converges to positive constant by Lemma 6, while the RHS converges to zero by the choice of c_n , hence $P(\hat{\alpha}_0^{c_n} < \alpha_0 - \epsilon) \to 0$.

Now we show that $P(\widehat{\alpha}_0^{c_n} > \alpha_0 + \epsilon) \to 0$. Suppose we have $\widehat{\alpha}_0^{c_n} > \alpha_0 + \epsilon$, then by Lemma 7,

$$n^{\beta-\eta}d_n(\widehat{G}_{s,n}^{\alpha_0+\epsilon},\check{G}_{s,n}^{\alpha_0+\epsilon}) > \frac{c_n}{(\alpha_0-\epsilon)}.$$

The LHS of above converges to zero by Lemmas 6 and 5, while the RHS diverges to infinity by the choice of c_n , hence $P(\hat{\alpha}_0^{c_n} > \alpha_0 + \epsilon) \to 0$.

A.2 Lemmas

<u>Lemma</u> 1. $\lim_{t\uparrow t^*} k(t) = \alpha_0$.

Proof. Define $\alpha'_0 = \lim_{t \uparrow t^*} k(t)$.

Show $\alpha'_0 \leq \alpha_0$: By the definition of α_0 there exists c.d.f. G_{α_0} such that

$$G(t) = \alpha_0 G_{\alpha_0}(t) + (1 - \alpha_0) G_L(t)$$
$$\leq \alpha_0 + (1 - \alpha_0) G_L(t).$$

Thus

$$k(t) = \frac{G(t) - G_L(t)}{1 - G_L(t)} \le \alpha_0$$

for all t. Thus $\alpha'_0 = \lim_{t \uparrow t^*} k(t) \le \alpha_0$.

Show $\alpha'_0 \geq \alpha_0$: Consider any $\gamma < \alpha_0$. We show $\gamma < \alpha'_0$. Since $\gamma < \alpha_0$,

$$\frac{G - (1 - \gamma)G_L}{\gamma}$$

is not a c.d.f. Thus there exists $t_1 < t_2$ such that

$$\frac{G(t_1) - (1 - \gamma)G_L(t_1)}{\gamma} > \frac{G(t_2) - (1 - \gamma)G_L(t_2)}{\gamma}.$$
(A.3)

Case 1: L.H.S. of Equation (A.3) > 1: If $G_L(t_1) = G(t_1)$, L.H.S. $= G_L(t_1) \le 1$. Thus $G_L(t_1) \ne G(t_1)$. By Lemma 3 $G_L(t_1) \leq G(t_1) \leq 1$. Thus $G_L(t_1) < 1$. By assumption

$$\frac{G(t_1) - (1 - \gamma)G_L(t_1)}{\gamma} > 1$$

Rearranging terms

$$\gamma < \frac{G(t_1) - G_L(t_1)}{1 - G_L(t_1)} \tag{A.4}$$

Since $G_L(t^*) = 1$ and $G_L(t) < 1$, $t_1 < t^*$. Thus by Lemma 2 the R.H.S. of Equation (A.4) is bounded by α'_0 . Case 2: L.H.S. of Equation (A.3) ≤ 1 : If $t_2 \geq t^*$, then $G_L(t_2) = 1$. Since $G(t) \geq G_L(t)$ (Lemma 3), $G(t_2) = 1$. Thus the R.H.S. of Equation (A.3) equals 1. This violates the assumption of Case 2, thus $t_2 < t^*$. From Equation (A.3) we have

$$G(t_1) - G(t_2) > (1 - \gamma)(G_L(t_1) - G_L(t_2))$$

which implies (since $G_L(t_1) - G_L(t_2) < 0$) that

$$\frac{G(t_2) - G(t_1)}{G_L(t_2) - G_L(t_1)} < (1 - \gamma).$$
(A.5)

From Lemma 4 we have

$$\frac{1 - G_L(t_2)}{1 - G(t_2)} = \frac{G_L(1) - G_L(t_2)}{G(1) - G(t_2)} \ge \frac{G_L(t_2) - G_L(t_1)}{G(t_2) - G(t_1)}$$

Combining this result with Equation (A.5) we obtain

$$\frac{1-G(t_2)}{1-G_L(t_2)} \le 1-\gamma$$

which implies

$$\gamma \le \frac{G(t_2) - G_L(t_2)}{1 - G_L(t_2)} = k(t_2)$$

Since $k(t) \uparrow$ as $t \uparrow t^*$ (see Lemma 2), we have the result.

Lemma 2. k(t) is increasing on $t \in [0, t^*)$.

Proof. Recall $Q(p) = \inf\{t \in (0,1] : G_L(t) \ge p\}$ and $t^* = Q(1)$. Note that with a, b, c, d > 0 and a/b < c/d,

$$\frac{a+c}{b+d} > \frac{a}{b}.$$

Next note that by Lemma 4, for $t^* > t_2 > t_1$,

$$\frac{G(t_2) - G(t_1)}{G_L(t_2) - G_L(t_1)} > \frac{1 - G(t_2)}{1 - G_L(t_2)}.$$

Thus we have

$$1 - k(t_1) = \frac{1 - G(t_1)}{1 - G_L(t_1)}$$

= $\frac{1 - G(t_2) + G(t_2) - G(t_1)}{1 - G_L(t_2) + G_L(t_2) - G_L(t_1)}$
\ge $\frac{1 - G(t_2)}{1 - G_L(t_2)}$
= $1 - k(t_2).$

<u>Lemma</u> 3.

$$\frac{g_L(t)}{g(t)} = \frac{1-\pi}{\pi} \frac{t}{1-t}$$

 $G(t) \ge G_L(t)$

and

for all t.

Proof. Define
$$A = \{x : \frac{\pi f_L(x)}{\pi f_L(x) + (1-\pi)f(x)} = t\}$$

$$\frac{g_L(t)}{g(t)} = \frac{\int_A f_L(x)}{\int_A f(x)}$$

$$= \frac{1-\pi}{\pi} \frac{\int_A \frac{\pi f_L(x)}{\pi f_L(x) + (1-\pi)f(x)} \pi f_L(x) + (1-\pi)f(x)}{\int_A \frac{(1-\pi)f(x)}{\pi f_L(x) + (1-\pi)f(x)} \pi f_L(x) + (1-\pi)f(x)}$$

$$= \frac{1-\pi}{\pi} \frac{\int_A t(\pi f_L(x) + (1-\pi)f(x))}{\int_A (1-t)(\pi f_L(x) + (1-\pi)f(x))}$$

$$= \frac{1-\pi}{\pi} \frac{t}{1-t}$$

Thus $\frac{g_L(t)}{g(t)} \uparrow$ as $t \uparrow$. Since $\frac{g_L(t)}{g(t)}$ is monotone increasing in t, g_L stochastically dominates g and thus $G(t) \ge G_L(t)$ for all t. Formally this can be shown by considering any $t_2 > t_1$ and noting

$$\frac{g_L(t_2)}{g(t_2)} \ge \frac{g_L(t_1)}{g(t_1)}.$$

Thus

$$g_L(t_2)g(t_1) \ge g_L(t_1)g(t_2).$$
 (A.6)

Integrating (A.6) from 0 to t_2 with respect to t_1 we obtain

$$g_L(t_2)G(t_2) \ge G_L(t_2)g(t_2),$$

which implies

$$\frac{G(t)}{G_L(t)} \ge \frac{g(t)}{g_L(t)}.\tag{A.7}$$

Integrating (A.6) from t_1 to 1 with respect to t_2 we obtain

$$(1 - G_L(t_1))g(t_1) \ge g_L(t_1)(1 - G(t_1)),$$

which implies

$$\frac{g(t)}{g_L(t)} \ge \frac{1 - G(t)}{1 - G_L(t)}.$$
(A.8)

Combining Equations (A.7) and (A.8) we have

$$\frac{G(t)}{G_L(t)} \ge \frac{1 - G(t)}{1 - G_L(t)}$$

which implies the result

$$G(t) \ge G_L(t).$$

Lemma 4 (Ratio). For all $0 \le t_1 < t_2 \le 1$ where $G(t_2) - G(t_1) > 0$ we have

$$\frac{1-\pi}{\pi}\frac{t_1}{1-t_1} < \frac{G_L(t_2) - G_L(t_1)}{G(t_2) - G(t_1)} \le \frac{1-\pi}{\pi}\frac{t_2}{1-t_2}$$

where $1/0 \equiv \infty$.

Proof. The classifier is

$$C(x) = \frac{\pi f_L(x)}{\pi f_L(x) + (1 - \pi)f(x)} = \frac{1}{1 + \frac{1 - \pi}{\pi} \frac{f(x)}{f_L(x)}}$$

Define $A_t = \{x : C(x) \le t\} = \{x : \frac{1-t}{t} \frac{\pi}{1-\pi} f_L(x) \le f(x)\}$. Therefore on the set $A_{t_2} \cap A_{t_1}^C$ we have

$$\frac{1-t_2}{t_2}\frac{\pi}{1-\pi}f_L(x) \le f(x) < \frac{1-t_1}{t_1}\frac{\pi}{1-\pi}f_L(x)$$

 So

$$\frac{G_L(t_2) - G_L(t_1)}{G(t_2) - G(t_1)} = \frac{\int_{A_{t_2} \cap A_{t_1}^C} f_L(x)}{\int_{A_{t_2} \cap A_{t_1}^C} f(x)}$$
$$> \frac{\int_{A_{t_2} \cap A_{t_1}^C} f_L(x)}{\frac{1 - t_1}{t_1} \frac{\pi}{1 - \pi} \int_{A_{t_2} \cap A_{t_1}^C} f_L(x)}$$
$$= \frac{t_1}{1 - t_1} \frac{1 - \pi}{\pi}.$$

We can obtain the upper bound in an identical manner.

Lemma 5.

$$n^{\beta-\eta}d_n(G,G_n) = o_P(1),$$

$$n^{\beta-\eta}d_n(G_L,G_{L,n}) = o_P(1).$$

Proof.

$$n^{\beta-\eta}d_n(G,G_n) = \sqrt{\int \left[\underbrace{n^{-\eta}}_{=o_P(1)} \underbrace{n^{\beta}\left(G_n(t) - G(t)\right)}_{=O_P(1)}\right]^2 dG_n(t)},$$

where $n^{\beta}(G_n(t) - G(t)) = O_P(1)$ uniformly, and then $n^{-\eta}n^{\beta}(G_n(t) - G(t)) = o_P(1)$ uniformly. Therefore

$$n^{\beta-\eta}d_n(G,G_n) \le \sup_t |n^{-\eta}n^\beta (G_n(t) - G(t))| = o_P(1).$$

The G_L , $G_{L,n}$ case can be proven in an identical manner.

<u>Lemma</u> 6. For $1 \ge \gamma \ge \alpha_0$,

$$\gamma d_n(\widehat{G}_{s,n}^{\gamma}, \check{G}_{s,n}^{\gamma}) \le d_n(G, G_n) + (1 - \gamma) d_n(G_L, G_{L,n}).$$

Thus,

$$\gamma d_n(\widehat{G}_{s,n}^{\gamma},\check{G}_{s,n}^{\gamma}) \to \begin{cases} 0 & \text{if } \gamma \ge \alpha_0, \\ > 0 & \text{if } \gamma < \alpha_0. \end{cases}$$

Proof. Let

$$G_s^{\gamma} = \frac{G - (1 - \gamma)G_L}{\gamma}$$

If $\gamma \geq \alpha_0$, then

$$\begin{aligned} \gamma d_n(\widehat{G}_{s,n}^{\gamma}, \check{G}_{s,n}^{\gamma}) &\leq \gamma d_n(\widehat{G}_{s,n}^{\gamma}, G_s^{\gamma}) \\ &\leq d_n(G, G_n) + (1 - \gamma) d_n(G_L, G_{L,n}). \end{aligned}$$

The first inequality holds by the definition of $\check{G}_{s,n}^{\gamma}$ due to the fact that G_s^{γ} is a valid CDF when $1 \ge \gamma \ge \alpha_0$, and the second inequality is due to triangle inequality.

Now we prove the limit property of $\gamma d_n(\hat{G}_{s,n}^{\gamma}, \check{G}_{s,n}^{\gamma})$. If $\gamma \geq \alpha_0$, then $\gamma d_n(\hat{G}_{s,n}^{\gamma}, \check{G}_{s,n}^{\gamma}) \to 0$ since $d_n(G, G_n) \to 0$ and $d_n(G_L, G_{L,n}) \to 0$ by Lemma 5. If $\gamma < \alpha_0$, by the definition of α_0^G , G_s^{γ} is not a valid c.d.f.. Pointwise, $\hat{G}_{s,n}^{\gamma} \to G_s^{\gamma}$. So for large n, $\hat{G}_{s,n}^{\gamma}$ is not valid c.d.f., while $\check{G}_{s,n}^{\gamma}$ is always a c.d.f.. So $\gamma d_n(\hat{G}_{s,n}^{\gamma}, \check{G}_{s,n}^{\gamma})$ would converge to some positive constant.

 $\underline{\text{Lemma}} \text{ 7. } B_n := \{ \gamma \in [0,1] : n^{\beta - \eta} \gamma d_n(\widehat{G}_{s,n}^{\gamma}, \check{G}_{s,n}^{\gamma}) \le c_n \} \text{ is convex. Thus, } B_n = (\widehat{\alpha}_0^{c_n}, 1] \text{ or } B_n = [\widehat{\alpha}_0^{c_n}, 1].$

Proof. Obviously, $1 \in B_n$. Assume $\gamma_1 \leq \gamma_2$ from B_n , let $\gamma_3 = \xi \gamma_1 + (1 - \xi) \gamma_2$, where $\xi \in [0, 1]$. Then by definition of $\widehat{G}_{s,n}^{\gamma}$,

$$\xi \gamma_1 \widehat{G}_{s,n}^{\gamma_1} + (1-\xi)\gamma_2 \widehat{G}_{s,n}^{\gamma_2} = \gamma_3 \widehat{G}_{s,n}^{\gamma_3}$$

Note that $\frac{1}{\gamma_3} \left(\xi \gamma_1 \check{G}_{s,n}^{\gamma_1} + (1-\xi) \gamma_2 \check{G}_{s,n}^{\gamma_2} \right)$ is a valid c.d.f. We have $\gamma_3 \in B_n$ because

$$\begin{split} &d_{n}(\widehat{G}_{s,n}^{\gamma_{3}},\check{G}_{s,n}^{\gamma_{3}}) \\ &\leq d_{n}\left(\widehat{G}_{s,n}^{\gamma_{3}},\frac{1}{\gamma_{3}}\left(\xi\gamma_{1}\check{G}_{s,n}^{\gamma_{1}}+(1-\xi)\gamma_{2}\check{G}_{s,n}^{\gamma_{2}}\right)\right) \\ &= d_{n}\left(\frac{1}{\gamma_{3}}\left(\xi\gamma_{1}\widehat{G}_{s,n}^{\gamma_{1}}+(1-\xi)\gamma_{2}\widehat{G}_{s,n}^{\gamma_{2}}\right),\frac{1}{\gamma_{3}}\left(\xi\gamma_{1}\check{G}_{s,n}^{\gamma_{1}}+(1-\xi)\gamma_{2}\check{G}_{s,n}^{\gamma_{2}}\right)\right) \\ &\leq \frac{\xi\gamma_{1}}{\gamma_{3}}d_{n}(\widehat{G}_{s,n}^{\gamma_{1}},\check{G}_{s,n}^{\gamma_{1}})+\frac{(1-\xi)\gamma_{2}}{\gamma_{3}}d_{n}(\widehat{G}_{s,n}^{\gamma_{2}},\check{G}_{s,n}^{\gamma_{2}}) \\ &\leq \frac{\xi\gamma_{1}}{\gamma_{3}}\frac{c_{n}}{n^{\beta-\eta}\gamma_{1}}+\frac{(1-\xi)\gamma_{2}}{\gamma_{3}}\frac{c_{n}}{n^{\beta-\eta}\gamma_{2}}=\frac{c_{n}}{n^{\beta-\eta}\gamma_{3}}. \end{split}$$