Learning from Complementary Labels

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Abstract
Collecting labeled data is costly and thus is a critical bottleneck in real-world classification tasks. To mitigate the problem, we consider a complementary label, which specifies a class that a pattern does not belong to. Collecting complementary labels would be less laborious than ordinary labels since users do not have to carefully choose the correct class from many candidate classes. However, complementary labels are less informative than ordinary labels and thus a suitable approach is needed to better learn from complementary labels. In this paper, we show that an unbiased estimator of the classification risk can be obtained only from complementary labels, if a loss function satisfies a particular symmetric condition. We theoretically prove the estimation error bounds for the proposed method, and experimentally demonstrate the usefulness of the proposed algorithms.

1 Introduction

In ordinary supervised classification problems, each training pattern is equipped with a label which specifies the class the pattern belongs to. Although supervised classifier training is effective, the cost of labeling training patterns is often expensive. For this reason, learning from cheap data has been extensively studied in the last decades, e.g., semi-supervised learning [1], learning from pairwise constraints [16, 11], and classification from positive and unlabeled data [3, 4, 12].

In this paper, we consider another weakly supervised classification scenario: instead of ordinary class labels, only a complementary label which specifies a class the pattern does not belong to is available. If the number of classes is large, choosing a correct class label from many candidate classes is laborious, while choosing one of the incorrect class labels would be much easier and thus less costly. Classification with complementary labels is essentially equivalent to classification with ordinary labels in the binary classification setup, because
complementary label 1 (i.e., not class 1) immediately means ordinary label 2. On the other hand, complementary labels are less informative than ordinary labels in $K$-class problems for $K > 2$, because complementary label 1 only means either of the ordinary labels 2, 3, . . . , $K$.

The complementary classification problem may be solved by the method of learning from partial labels [2], where multiple candidate classes are provided to each training pattern — complementary label $\bar{y}$ can be regarded as an extreme case of a partial label given to all $K - 1$ classes other than class $\bar{y}$. Another possibility to solve the complementary classification problem is to consider a multi-label setup [13], where each pattern can belong to multiple classes — complementary label $\bar{y}$ is translated into a negative label for class $\bar{y}$ and positive labels for the other $K - 1$ classes.

Our contribution in this paper is to give a direct risk minimization framework for the complementary classification problem. More specifically, we consider the complementary loss that incurs a large loss if a predicted complementary label is not correct. We then show that the classification risk can be empirically estimated in an unbiased fashion if the complementary loss satisfies a certain symmetric condition — the sigmoid loss and the ramp loss are shown to satisfy this symmetric condition. Theoretically, we establish the estimation error bounds for the proposed method, showing that learning from complementary labels is also consistent; the order of these bounds is the optimal parametric rate $O_p(1/\sqrt{n})$, where $O_p$ denotes the order in probability and $n$ is the size of training data. Finally, we demonstrate the practical usefulness of the proposed complementary classification methods through experiments.

2 Review of Ordinary Multi-Class Classification

Suppose that $d$-dimensional pattern $x \in \mathbb{R}^d$ and its class label $y \in \{1, \ldots, K\}$ are sampled independently from an unknown probability distribution with density $p(x, y)$. The goal of ordinary multi-class classification is to learn a classifier $f(x) : \mathbb{R}^d \to \{1, \ldots, K\}$ that minimizes the classification risk with multi-class loss $L(f(x), y)$:

$$R(f) = \mathbb{E}_{p(x, y)}[L(f(x), y)],$$

where $\mathbb{E}$ denotes the expectation. Typically, a classifier $f(x)$ is assumed to take the following form:

$$f(x) = \arg \max_{y \in \{1, \ldots, K\}} g_y(x).$$

where $g_y(x) : \mathbb{R}^d \to \mathbb{R}$ is a binary classifier for class $y$ versus the rest. Then, together with a binary loss $\ell(z) : \mathbb{R} \to \mathbb{R}$ that incurs a large loss for large $z$, the one-versus-all (OVA) loss or the pairwise-comparison (PC) loss defined as follows are used as the multi-class loss [17]:

$$L_{\text{OVA}}(f(x), y) = \ell(g_y(x)) + \frac{1}{K-1} \sum_{y' \neq y} \ell(-g_{y'}(x)), \quad (3)$$

$$L_{\text{PC}}(f(x), y) = \sum_{y' \neq y} \ell(g_y(x) - g_{y'}(x)). \quad (4)$$

Finally, the expectation over unknown $p(x, y)$ in Eq.(1) is approximated by the empirical average over independent and identically distributed training samples to obtain a practical classification formulation.

\[^{1}\text{We normalize the “rest” loss by } K - 1 \text{ to be consistent with the discussion in the following sections.}\]
3 Classification from Complementary Labels

In this section, we formulate the problem of complementary classification and propose a risk minimization framework.

We consider the situation where, instead of ordinary class label \( y \), we are given only complementary label \( \bar{y} \) which specifies a class pattern \( \bar{x} \) does not belong to. Our goal is to still learn a classifier that minimizes the classification risk (1), but only from complementarily labeled training samples \( \{(x_i, \bar{y}_i)\}_{i=1}^n \). We assume that \( \{(x_i, \bar{y}_i)\}_{i=1}^n \) are drawn independently from an unknown probability distribution with density\(^2\)

\[
\bar{p}(x, \bar{y}) = \frac{1}{K-1} \sum_{y \neq \bar{y}} p(x, y).
\]

Let us consider a complementary loss \( \bar{L}(f(x), \bar{y}) \) for a complementary sample \( (x, \bar{y}) \). Then we have the following theorem:

**Theorem 1.** The classification risk (1) can be expressed as

\[
R(f) = (K - 1)\mathbb{E}_{p(x, y)}[\bar{L}(f(x), \bar{y})] - M_1 + M_2,
\]

if there exist constants \( M_1, M_2 \geq 0 \) such that the complementary loss satisfies for all \( x \) and \( y \)

\[
\sum_{y=1}^K \bar{L}(f(x), \bar{y}) = M_1 \quad \text{and} \quad \bar{L}(f(x), y) + \bar{L}(f(x), \bar{y}) = M_2.
\]

**Proof.** According to (5),

\[
(K - 1)\mathbb{E}_{p(x, \bar{y})}[\bar{L}(f(x), \bar{y})] = (K - 1) \int \sum_{y=1}^K \bar{L}(f(x), \bar{y}) \bar{p}(x, \bar{y}) dx
\]

\[
= (K - 1) \int \sum_{y=1}^K \bar{L}(f(x), \bar{y}) \left( \frac{1}{K-1} \sum_{y \neq \bar{y}} p(x, y) \right) dx = \int \sum_{y=1}^K \sum_{y \neq \bar{y}} \bar{L}(f(x), \bar{y}) \bar{p}(x, y) dx
\]

\[
= \mathbb{E}_{p(x, \bar{y})} \left[ \sum_{y \neq \bar{y}} \bar{L}(f(x), \bar{y}) \right] = M_1 - \mathbb{E}_{p(x, \bar{y})}[\bar{L}(f(x), y)],
\]

where the fifth equality is due to the first equation in (7). Subsequently,

\[
(K - 1)\mathbb{E}_{p(x, \bar{y})}[\bar{L}(f(x), \bar{y})] - \mathbb{E}_{p(x, y)}[\bar{L}(f(x), y)] = M_1 - \mathbb{E}_{p(x, \bar{y})}[\bar{L}(f(x), y) + \bar{L}(f(x), \bar{y})]
\]

\[
= M_1 - M_2,
\]

where the second equality is due to the second equation in (7).

With the expression (6), the classification risk (1) can be naively approximated in an unbiased fashion by the sample average as

\[
\bar{R}(f) = \frac{K-1}{n} \sum_{i=1}^n \bar{L}(f(x_i), \bar{y}_i) - M_1 + M_2.
\]

Let us define the complementary losses for the OVA loss \( \bar{L}_{OVA}(f(x), y) \) and the PC loss \( \bar{L}_{PC}(f(x), \bar{y}) \) as

\[
\bar{L}_{OVA}(f(x), \bar{y}) = \frac{1}{K-1} \sum_{y \neq \bar{y}} \ell(g_y(x)) + \ell(-g_y(x)),
\]

\[
\bar{L}_{PC}(f(x), \bar{y}) = \sum_{y \neq \bar{y}} \ell(g_y(x) - g_y(x)).
\]

Then we have the following theorem:

\(^2\)The coefficient \( 1/(K-1) \) is for the normalization purpose: it is natural to assume \( \bar{p}(x, \bar{y}) = (1/2) \sum_{y \neq \bar{y}} p(x, y) \) since all \( p(x, y) \) for \( y \neq \bar{y} \) contribute to \( \bar{p}(x, \bar{y}) \); in order to ensure that \( \bar{p}(x, \bar{y}) \) is a valid joint density such that \( \mathbb{E}_{\bar{p}(x, \bar{y})}[1] = 1 \), we must take \( Z = K - 1 \).
Proof. From Eq. (10), we have

\[
\sum_{y=1}^{K} \overline{L}_{\text{OVA}}(f(x), \bar{y}) = \frac{1}{K-1} \sum_{y=1}^{K} \sum_{y' \neq y} \ell(g_y(x)) + \sum_{y=1}^{K} \ell(-g_y(x)) \\
= \sum_{y=1}^{K} \ell(g_y(x)) + \ell(-g_y(x)) = K,
\]

\[
\overline{L}_{\text{OVA}}(f(x), y) + \overline{L}_{\text{OVA}}(f(x), y) = \ell(g_y(x)) + \frac{1}{K-1} \sum_{y' \neq y} \ell(-g_y(x)) \\
+ \frac{1}{K-1} \sum_{y' \neq y} \ell(g_{y'}(x)) + \ell(-g_y(x)) = 2,
\]

\[
\sum_{y=1}^{K} \overline{L}_{\text{PC}}(f(x), \bar{y}) = \sum_{y=1}^{K} \sum_{y' \neq y} \ell(g_y(x) - g_{y'}(x)) \\
= \sum_{y=1}^{K-1} \sum_{y'=y+1}^{K} \left( \ell(g_y(x) - g_y(x)) + \ell(g_y(x) - g_{y'}(x)) \right) = \frac{K(K-1)}{2},
\]

\[
\overline{L}_{\text{PC}}(f(x), y) + \overline{L}_{\text{PC}}(f(x), y) = \sum_{y' \neq y} \ell(g_y(x) - g_{y'}(x)) + \sum_{y' \neq y} \ell(g_{y'}(x) - g_y(x)) = K - 1.
\]

For example, the following binary losses satisfy the symmetric condition (10):

- Zero-one loss: \( \ell_{0,1}(z) = \begin{cases} 0 & \text{if } z > 0, \\ 1 & \text{if } z \leq 0, \end{cases} \) (11)
- Sigmoid loss: \( \ell_S(z) = \frac{1}{1+e^{-z}} \), (12)
- Ramp loss: \( \ell_R(z) = \frac{1}{2} \max \left( 0, \min (2, 1-z) \right) \). (13)

Note that these losses are non-convex [3]. In practice, the sigmoid loss or ramp loss may be used for training a classifier, while the zero-one loss may be used for tuning hyper-parameters (see Section 5 for details).

4. Estimation Error Bounds

In this section, we establish the estimation error bounds for the proposed method.

Let \( \mathcal{G} = \{g(x)\} \) be a function class for empirical risk minimization and \( \sigma_1, \ldots, \sigma_n \) be \( n \) Rademacher variables. Then the Rademacher complexity of \( \mathcal{G} \) for \( \mathcal{X} \) of size \( n \) drawn from \( p(x) \) is defined as follows [9]:

\[
\mathcal{R}_n(\mathcal{G}) = E_{\mathcal{X}}E_{\sigma_1, \ldots, \sigma_n} \left[ \sup_{g \in \mathcal{G}} \frac{1}{n} \sum_{x_i \in \mathcal{X}} \sigma_i g(x_i) \right];
\]

define the Rademacher complexity of \( \mathcal{G} \) for \( \mathcal{X} \) of size \( n \) drawn from \( p(x) \) as

\[
\mathcal{R}_n(\mathcal{G}) = E_{\mathcal{X}}E_{\sigma_1, \ldots, \sigma_n} \left[ \sup_{g \in \mathcal{G}} \frac{1}{n} \sum_{x_i \in \mathcal{X}} \sigma_i g(x_i) \right].
\]
Note that \( \hat{p}(x) = p(x) \) and thus \( \mathcal{R}_n(G) = \mathcal{R}_n(G) \), which enables us to express the obtained theoretical results using the standard Rademacher complexity \( \mathcal{R}_n(G) \).

To begin with, let \( \ell'(z) = \ell(z) - \ell(0) \) be the shifted loss such that \( \ell(0) = 0 \), and \( \tilde{L}_{OVA} \) be losses defined following (8) and (9) but with \( \ell' \) instead of \( \ell \) let \( L' \) be any (not necessarily the best) Lipschitz constant of \( \ell \). Define the corresponding function classes as follows:

\[
\mathcal{H}_{OVA} = \{(x, y) \mapsto \tilde{L}_{OVA}(f(x), y) \mid g_1, \ldots, g_K \in \mathcal{G}\},
\]

\[
\mathcal{H}_{PC} = \{(x, y) \mapsto \tilde{L}_{PC}(f(x), y) \mid g_1, \ldots, g_K \in \mathcal{G}\}.
\]

Then we can obtain the following lemmas.

**Lemma 3.** Let \( \mathcal{R}_n(\mathcal{H}_{OVA}) \) be the Rademacher complexity of \( \mathcal{H}_{OVA} \) for \( S \) of size \( n \) drawn from \( \hat{p}(x, y) \) defined as

\[
\mathcal{R}_n(\mathcal{H}_{OVA}) = \mathbb{E}_S \mathbb{E}_{\sigma_1, \ldots, \sigma_n} \left[ \sup_{h \in \mathcal{H}_{OVA}} \frac{1}{n} \sum_{(x, y_i) \in S} \sigma_i h(x_i, y_i) \right].
\]

Then, \( \mathcal{R}_n(\mathcal{H}_{OVA}) \leq K L' \mathcal{R}_n(G) \).

**Proof.** By definition, \( h(x_i, y_i) = \tilde{L}_{OVA}(f(x_i), y_i) \) so that

\[
\mathcal{R}_n(\mathcal{H}_{OVA}) = \mathbb{E}_S \mathbb{E}_\sigma \left[ \sup_{g_1, \ldots, g_K \in \mathcal{G}} \frac{1}{n} \sum_{(x, y_i) \in S} \sigma_i \left( \frac{1}{K-1} \sum_{y \neq y_i} \ell(g_y(x_i)) + \ell(-g_{y_i}(x_i)) \right) \right].
\]

After rewriting \( \tilde{L}_{OVA}(f(x_i), y_i) \), we can know that

\[
\tilde{L}_{OVA}(f(x_i), y_i) = \frac{1}{K-1} \sum_y \ell(g_y(x_i)) + \frac{K-2}{K} \ell(-g_{y_i}(x_i)),
\]

and subsequently,

\[
\mathcal{R}_n(\mathcal{H}_{OVA}) \leq \frac{1}{K-1} \mathbb{E}_S \mathbb{E}_\sigma \left[ \sup_{g_1, \ldots, g_K \in \mathcal{G}} \frac{1}{n} \sum_{(x, y_i) \in S} \sigma_i \sum_y \ell(g_y(x_i)) \right] + \frac{K-2}{K} \mathbb{E}_S \mathbb{E}_\sigma \left[ \sup_{g_1, \ldots, g_K \in \mathcal{G}} \frac{1}{n} \sum_{(x, y_i) \in S} \sigma_i \ell(-g_{y_i}(x_i)) \right]
\]

due to the sub-additivity of the supremum.

The first term is independent of \( y_i \) and thus

\[
\mathbb{E}_S \mathbb{E}_\sigma \left[ \sup_{g_1, \ldots, g_K \in \mathcal{G}} \frac{1}{n} \sum_{(x, y_i) \in S} \sigma_i \sum_y \ell(g_y(x_i)) \right]
\]

\[
= \mathbb{E}_\mathcal{X} \mathbb{E}_\sigma \left[ \sup_{g_1, \ldots, g_K \in \mathcal{G}} \frac{1}{n} \sum_{x, \sigma_i \in \mathcal{X}} \sigma_i \sum_y \ell(g_y(x_i)) \right]
\]

\[
\leq \sum_y \mathbb{E}_\mathcal{X} \mathbb{E}_\sigma \left[ \sup_{g_1, \ldots, g_K \in \mathcal{G}} \frac{1}{n} \sum_{x, \sigma_i \in \mathcal{X}} \sigma_i \ell(g_y(x_i)) \right]
\]

\[
= \sum_y \mathbb{E}_\mathcal{X} \mathbb{E}_\sigma \left[ \sup_{g_1, \ldots, g_K \in \mathcal{G}} \frac{1}{n} \sum_{x, \sigma_i \in \mathcal{X}} \sigma_i \ell(g_y(x_i)) \right] = K \mathcal{R}_n(\ell \circ G),
\]

which means the first term can be bounded by \( K/(K - 1) \cdot \mathcal{R}_n(\ell \circ G) \). The second term is
more involved. Let $I(\cdot)$ be the indicator function and $\alpha_i = 2I(y = \hat{y}_i) - 1$, then

$$
\mathbb{E}_S \mathbb{E}_\sigma \left[ \sup_{g_1, \ldots, g_K \in \mathcal{G}} \frac{1}{n} \sum_{(x_i, y_i) \in S} \sigma_i \ell_i (-g_{\hat{y}_i}(x_i)) \right] = \mathbb{E}_S \mathbb{E}_\sigma \left[ \sup_{g_1, \ldots, g_K \in \mathcal{G}} \frac{1}{n} \sum_{(x_i, y_i) \in S} \alpha_i \sum_y \ell_i (-g_y(x_i)) I(y = \hat{y}_i) \right]
$$

$$
\leq \mathbb{E}_S \mathbb{E}_\sigma \left[ \sup_{g_1, \ldots, g_K \in \mathcal{G}} \frac{1}{n} \sum_{(x_i, y_i) \in S} \alpha_i \sum_y \ell_i (-g_y(x_i)) \right] + \mathbb{E}_S \mathbb{E}_\sigma \left[ \sup_{g_1, \ldots, g_K \in \mathcal{G}} \frac{1}{n} \sum_{(x_i, y_i) \in S} \alpha_i \sum_y \ell_i (-g_y(x_i)) \right]
$$

where we used that $\alpha_i, \sigma_i$ has exactly the same distribution as $\alpha_i$. This can be similarly bounded by $\mathcal{R}_n(\ell \circ \mathcal{G})$ and the second term can be bounded by $K(K - 2)/(K - 1) \cdot \mathcal{R}_n(\ell \circ \mathcal{G})$.

As a result,

$$
\mathcal{R}_n(\mathcal{HOVA}) \leq \left( \frac{K}{K - 1} + \frac{K(K - 2)}{K - 1} \right) \mathcal{R}_n(\ell \circ \mathcal{G}) = K \mathcal{R}_n(\ell \circ \mathcal{G}) \leq K L_l \mathcal{R}_n(\mathcal{G}) = K L_l \mathcal{R}_n(\mathcal{G}),
$$

according to Talagrand’s contraction lemma [7].

\textbf{Lemma 4.} Let $\mathcal{R}_n(\mathcal{HPC})$ be the Rademacher complexity of $\mathcal{HPC}$ defined similarly to $\mathcal{R}_n(\mathcal{HOVA})$. Then, $\mathcal{R}_n(\mathcal{HPC}) \leq 2K(K - 1)L_l \mathcal{R}_n(\mathcal{G})$.

\textbf{Proof.} By definition,

$$
\mathcal{R}_n(\mathcal{HPC}) = \mathbb{E}_S \mathbb{E}_\sigma \left[ \sup_{g_1, \ldots, g_K \in \mathcal{G}} \frac{1}{n} \sum_{(x_i, y_i) \in S} \sigma_i \left( \sum_{y' \neq y_i} \ell_i (g_{y'}(x_i) - g_{\hat{y}_i}(x_i)) \right) \right].
$$

Using the proof technique for handling the second term in the proof of Lemma 3, we have

$$
\mathcal{R}_n(\mathcal{HPC}) \leq \mathbb{E}_S \mathbb{E}_\sigma \left[ \sup_{g_1, \ldots, g_K \in \mathcal{G}} \frac{1}{n} \sum_{(x_i, y_i) \in S} \sigma_i \sum_{y' \neq y_i} \ell_i (g_{y'}(x_i) - g_{\hat{y}_i}(x_i)) \right]
$$

$$
\leq \sum_y \sum_{y' \neq y} \mathbb{E}_S \mathbb{E}_\sigma \left[ \sup_{g_1, g_2 \in \mathcal{G}} \frac{1}{n} \sum_{x_i \in \mathcal{X}} \sigma_i \ell_i (g_{y'}(x_i) - g_{\hat{y}_i}(x_i)) \right]
$$

due to the sub-additivity of the supremum. Let $\mathcal{G}_{y, y'} = \{ x \mapsto g_{y'}(x) - g_y(x) \mid g_y, g_{y'} \in \mathcal{G} \}$, then by Talagrand’s contraction lemma [7],

$$
\mathbb{E}_S \mathbb{E}_\sigma \left[ \sup_{g_1, g_2 \in \mathcal{G}} \frac{1}{n} \sum_{x_i \in \mathcal{X}} \sigma_i \ell_i (g_{y'}(x_i) - g_y(x_i)) \right] = \mathcal{R}_n(\ell \circ \mathcal{G}_{y, y'}) \leq L_l \mathcal{R}_n(\mathcal{G}_{y, y'})
$$

$$
= L_l \mathbb{E}_S \mathbb{E}_\sigma \left[ \sup_{g_1, g_2 \in \mathcal{G}} \frac{1}{n} \sum_{x_i \in \mathcal{X}} \sigma_i (g_{y'}(x_i) - g_y(x_i)) \right]
$$

$$
\leq L_l \mathbb{E}_S \mathbb{E}_\sigma \left[ \sup_{g_y \in \mathcal{G}} \frac{1}{n} \sum_{x_i \in \mathcal{X}} \sigma_i g_y(x_i) \right] = 2 L_l R_n(\mathcal{G}) = 2 L_l R_n(\mathcal{G}).
$$

This proves that $\mathcal{R}_n(\mathcal{HPC}) \leq 2K(K - 1)L_l \mathcal{R}_n(\mathcal{G})$.

Based on Lemmas 3 and 4, we can derive the uniform deviation bounds of $\tilde{R}(f)$. \hfill \Box
Lemma 5. For any $\delta > 0$, with probability at least $1 - \delta$,
\[
\sup_{g_1, \ldots, g_K \in \mathcal{G}} \left| \hat{R}(f) - R(f) \right| \leq 2K(K - 1)L_\ell\mathcal{R}_n(\mathcal{G}) + (K - 1)\sqrt{\frac{2\ln(2/\delta)}{n}},
\]
where $\hat{R}(f)$ is w.r.t. $\hat{L}_{OVA}$, and
\[
\sup_{g_1, \ldots, g_K \in \mathcal{G}} \left| \hat{R}(f) - R(f) \right| \leq 4K(K - 1)^2L_\ell\mathcal{R}_n(\mathcal{G}) + (K - 1)^2\sqrt{\frac{2\ln(2/\delta)}{n}},
\]
where $\hat{R}(f)$ is w.r.t. $\hat{L}_{PC}$.

Proof. We prove the case of $\hat{L}_{OVA}$; the other case is similar. We consider a single direction
\[
\sup_{g_1, \ldots, g_K \in \mathcal{G}} (\hat{R}(f) - R(f))
\]
with probability at least $1 - \delta/2$; the other direction is similar too.

Given the symmetric condition (10), it must hold that $\|\hat{L}_{OVA}\|_\infty = 2$ when $g_1, \ldots, g_K$
can be any measurable functions. Let a single $(x_i, y_i)$ be replaced with $(x'_i, y'_i)$, then the
change of $\sup_{g_1, \ldots, g_K \in \mathcal{G}} (\hat{R}(f) - R(f))$ is no greater than $2(K - 1)/n$. Apply
McDiarmid’s inequality [8] to the single-direction uniform deviation $\sup_{g_1, \ldots, g_K \in \mathcal{G}} (\hat{R}(f) - R(f))$ to get that
with probability at least $1 - \delta/2$,
\[
\sup_{g_1, \ldots, g_K \in \mathcal{G}} (\hat{R}(f) - R(f)) \leq \mathbb{E} \left[ \sup_{g_1, \ldots, g_K \in \mathcal{G}} (\hat{R}(f) - R(f)) \right] + (K - 1)\sqrt{\frac{2\ln(2/\delta)}{n}}.
\]
Substituting from $R(f) = \mathbb{E}[\hat{R}(f)]$, it is a routine work to show by symmetrization that [9]
\[
\mathbb{E} \left[ \sup_{g_1, \ldots, g_K \in \mathcal{G}} (\hat{R}(f) - R(f)) \right] \leq 2K(K - 1)\mathcal{R}_n(H_{OVA}) \leq 2K(K - 1)L_\ell\mathcal{R}_n(\mathcal{G}),
\]
where the last line is due to Lemma 3.

Let $(g_1^*, \ldots, g_K^*)$ be the true risk minimizer and $(\hat{g}_1, \ldots, \hat{g}_K)$ be the empirical risk mini-
mimizer, i.e.,
\[
(g_1^*, \ldots, g_K^*) = \arg\min_{g_1, \ldots, g_K \in \mathcal{G}} R(f) \quad \text{and} \quad (\hat{g}_1, \ldots, \hat{g}_K) = \arg\min_{g_1, \ldots, g_K \in \mathcal{G}} \hat{R}(f).
\]
Let also $f^*(x) = \arg\max_{y \in \{1, \ldots, K\}} g_y^*(x)$ and $\hat{f}(x) = \arg\max_{y \in \{1, \ldots, K\}} \hat{g}_y(x)$. Finally, based
on Lemma 5, we can establish the estimation error bounds.

Theorem 6. For any $\delta > 0$, with probability at least $1 - \delta$,
\[
R(\hat{f}) - R(f^*) \leq 4K(K - 1)L_\ell\mathcal{R}_n(\mathcal{G}) + (K - 1)\sqrt{\frac{8\ln(2/\delta)}{n}},
\]
if $(\hat{g}_1, \ldots, \hat{g}_K)$ is trained by minimizing $\hat{R}(f)$ w.r.t. $\hat{L}_{OVA}$, and
\[
R(\hat{f}) - R(f^*) \leq 8K(K - 1)^2L_\ell\mathcal{R}_n(\mathcal{G}) + (K - 1)^2\sqrt{\frac{2\ln(2/\delta)}{n}},
\]
if $(\hat{g}_1, \ldots, \hat{g}_K)$ is trained by minimizing $\hat{R}(f)$ w.r.t. $\hat{L}_{PC}$.

Proof. Based on Lemma 5, the estimation error bounds can be proven through
\[
R(\hat{f}) - R(g^*) = \left( \hat{R}(f) - \hat{R}(f^*) \right) + \left( R(\hat{f}) - \hat{R}(f) \right) + \left( \hat{R}(f^*) - R(f^*) \right) \leq 0 + 2\sup_{g_1, \ldots, g_K \in \mathcal{G}} \left| \hat{R}(f) - R(f) \right|,
\]
where we used that $\hat{R}(f) \leq \hat{R}(f^*)$ by the definition of $\hat{f}$. \hfill $\square$
Theorem 6 guarantees learning from complementary labels is also consistent: as $n \to \infty$, $R(\hat{f}) \to R(f^*)$. Consider linear-in-parameter models defined by

$$
\mathcal{G} = \{ g(x) = \langle w, \phi(x) \rangle_{\mathcal{H}} \mid \|w\|_{\mathcal{H}} \leq C_w, \|\phi(x)\|_{\mathcal{H}} \leq C_\phi \},
$$

where here $\mathcal{H}$ is a Hilbert space with an inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$, $w \in \mathcal{H}$ is a normal, $\phi : \mathbb{R}^d \to \mathcal{H}$ is a feature map, and $C_w > 0$ and $C_\phi > 0$ are constants [14]. It is known that $\mathcal{R}_n(\mathcal{G}) \leq C_w C_\phi / \sqrt{n}$ [9] and thus $R(\hat{f}) \to R(f^*)$ in $\mathcal{O}_p(1/\sqrt{n})$ if this $\mathcal{G}$ is used, where $\mathcal{O}_p$ denotes the order in probability. This order is already the optimal parametric rate and cannot be improved without additional strong assumptions on $\tilde{p}(x, y)$, $\ell$ and $\mathcal{G}$ jointly.

5 Experiments

In this section, we experimentally evaluate the performance of the proposed method.

Comparison between proposed methods: Here we first compare the performance between four variations of the proposed approach: The two formulations, OVA (8) and PC (9), each with the sigmoid loss (12) and ramp loss (13). We used the MNIST hand-written digit dataset (with all patterns standardized to have zero mean and unit variance), with different number of classes: 3 classes (digits “1” to “3”) to 10 classes (digits “1” to “9” and “0”). From each class, we selected 500 samples for training and 500 samples for testing, and generated complementary labels by randomly selecting one of the complementary classes. From the training dataset, we left out 25% for validation for hyper-parameter tuning based on the zero-one loss objective version of (8) or (9).

For all the methods, we used a linear-in-input model $g_k(x) = w_k^\top x + b_k$ as the binary classifier, where $\top$ denotes the transpose, $w_k \in \mathbb{R}^d$ is the weight parameters, and $b_k \in \mathbb{R}$ is a bias parameter in class $k \in \{1, \ldots, K\}$. We added an $\ell_2$-regularization term, with hyper-parameter candidates $\lambda \in \{10^{-4}, 10^{-3}, \ldots, 10^4\}$. Adam [6] was used for optimization with 5,000 iterations.

We reported the mean and standard deviation of the classification accuracy over five trials in Table 1. From the results, we can see that PC tends to outperform OVA. A possible explanation for this is that the PC formulation is a more direct approach for classification [15] — it takes the sign of the difference of the classifiers, instead of the sign of each classifier as in OVA. When we compare the sigmoid loss and the ramp loss in PC, the sigmoid loss tends to outperform the ramp loss and hence we use only PC with sigmoid loss for the following experiments.

Benchmark experiments: Next, we compare our proposed method, PC with the sigmoid loss, with two baseline methods. The first baseline is one of the state-of-the-art partial label (PL) methods [2] with the squared hinge loss $\ell(z) = (\max(0, 1 - z))^2$. The second baseline method is a multi-label (ML) formulation, where complementary label $\bar{y}$ is translated into a negative label for class $\bar{y}$ and positive labels for the other $K - 1$ classes. This formulation yields the loss $L_{\text{ML}}(f(x), \bar{y}) = \sum_{y \neq \bar{y}} \ell(g_y(x)) + \ell(-g_{\bar{y}}(x))$, where we used the squared loss $\ell(z) = (z - 1)^2$ as the binary loss.

Another interesting comparison is between learning from complementary labels and ordinary labels. For the ordinary-label (OL) method, we used the unnormalized version of (3) with the squared loss. For better comparison of the two settings, we gave only $1/k_{\text{OL}}$ times as many samples to OL since one ordinary label can be regarded as $K - 1$ complementary labels.
Table 1: Mean and standard deviation of classification accuracy over five trials in percentage, when the number of classes is changed. “PC” is (9), “OVA” is (8), “sigmoid” is (12), and “ramp” is (13). Best and equivalent methods (with 5% t-test) are bold.

| Method | 3 cls | 4 cls | 5 cls | 6 cls | 7 cls | 8 cls | 9 cls | 10 cls |
|--------|-------|-------|-------|-------|-------|-------|-------|--------|
| OVA Sigmoid | 96.2 (0.4) | 91.5 (1.2) | 90.2 (0.9) | 79.2 (4.2) | 75.2 (2.7) | 68.4 (2.5) | 61.9 (5.2) | 52.4 (5.4) |
| OVA Ramp | 95.9 (0.5) | 90.5 (1.1) | 89.9 (1.0) | 77.0 (5.3) | 73.2 (1.5) | 62.9 (5.0) | 54.1 (5.8) | 48.9 (3.3) |
| PC Sigmoid | 95.9 (1.1) | 90.8 (0.6) | 89.3 (1.3) | 80.8 (2.0) | 76.9 (3.2) | 72.2 (2.2) | 66.4 (3.9) | 60.4 (0.6) |
| PC Ramp | 95.9 (1.1) | 90.6 (1.2) | 88.2 (1.2) | 80.1 (2.4) | 74.7 (3.2) | 70.0 (2.6) | 62.3 (4.5) | 55.1 (3.5) |

We used a one-hidden-layer neural network (d-3-1) with rectified linear units (ReLU) [10] as activation functions, and weight decay candidates were chosen from \{10^{-7}, 10^{-4}, 10^{-1}\}.

We evaluated the classification performance with the following benchmark datasets: WAVEFORM1 (d = 21), WAVEFORM2 (d = 40), SATIMAGE (d = 36), SHUTTLE (d = 9), SEGMENTATION (d = 19), PENDIGITS (d = 16), MNIST (d = 784), DRIVE (d = 48), LETTER (d = 16), VOWEL (d = 12), and USPS (d = 256). MNIST and USPS can be downloaded from the website of the late Sam Roweis\(^3\), and all other datasets can be downloaded from UCI machine learning repository.\(^4\) For datasets with 10 or more classes, we chose five classes with an equal number of samples. In Table 2, the specification of the datasets as well as the mean and standard deviation of the classification accuracy over 20 trials is reported. From the results, we can see that the proposed method is either competitive or outperforms the baseline methods in many of the datasets. It is also interesting that the proposed classification method from complementary labels can be competitive with classification from ordinary labels in many of the datasets.

6 Conclusion

We proposed a novel problem setting and algorithm for learning from complementary labels, and showed that an unbiased estimator of the classification risk can be obtained only from complementary labels, if a loss function satisfies a particular symmetric condition. We theoretically proved the estimation error bounds for the proposed method, and experimentally demonstrated the usefulness of the proposed method.

The complementary classification formulation may also be useful in the context of privacy-aware machine learning [5]: a subject needs to answer private questions such as psychological counseling which can make him/her hesitate to answer directly. In such a situation, providing a complementary label, i.e., one of the incorrect answers to the question, would be mentally less demanding. We will investigate this issue in our future work.

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\(^3\)See http://cs.nyu.edu/~roweis/data.html.

\(^4\)See http://archive.ics.uci.edu/ml/.
**Table 2:** Mean and standard deviation of classification accuracy over 20 trials in percentage. “PC/S” is the proposed method for pairwise comparison formulation with sigmoid loss, “PL” is partial label with squared hinge loss, “ML” is multi-label, and “OL” is classification from ordinary labels. Best and equivalent methods (with 5% t-test excluding “OL”) are bold. # train denotes the total number of training and validation samples in each class. # test denotes the number of test samples in each class.

| Dataset     | Class | # train | # test | PC/S    | PL       | ML       | OL       |
|-------------|-------|---------|--------|---------|----------|----------|----------|
| WAVEFORM1   | 1 ~ 3 | 1230    | 406    | 85.7(0.9) | 84.1(1.5) | 84.7(1.6) | 85.8(0.9) |
| WAVEFORM2   | 1 ~ 3 | 1221    | 400    | 84.4(1.3) | 83.1(2.7) | 81.8(2.3) | 86.7(1.8) |
| SATIMAGE    | 1 ~ 7 | 415     | 211    | 67.2(7.0) | 54.8(6.8) | 51.6(6.0) | 67.9(4.2) |
| SHUTTLE     | 1, 4, 5 | 2458   | 809    | 94.9(9.7) | 97.5(0.7) | 90.4(11.8) | 97.5(0.8) |

| SEGMENTATION | 1 ~ 7 | 29     | 299    | 36.1(6.8) | 31.7(5.8) | 26.6(5.4) | 38.6(4.5) |

| PENDIGITS   | 1 ~ 5  | 719    | 336    | 79.4(9.5) | 73.2(6.4) | 75.9(7.7) | 78.8(2.9) |
| 6 ~ 10      | 719    | 335    | 77.7(3.8) | 65.5(6.4) | 72.0(8.6) | 74.7(4.6) |
| even #      | 719    | 335    | 74.6(7.3) | 58.5(9.9) | 65.7(6.3) | 74.8(5.5) |
| odd #       | 719    | 336    | 88.5(5.9) | 74.6(4.4) | 79.1(6.1) | 84.0(8.8) |

| MNIST       | 1 ~ 5  | 5842   | 980    | 88.4(4.2) | 71.5(7.4) | 56.6(12.4) | 77.9(0.4) |
| 6 ~ 10      | 5421   | 892    | 83.4(2.6) | 67.4(8.1) | 50.5(13.7) | 77.0(4.5) |
| even #      | 5421   | 892    | 85.3(2.2) | 70.4(6.7) | 61.7(11.1) | 76.7(1.4) |
| odd #       | 5842   | 958    | 85.0(3.7) | 67.3(8.6) | 57.3(13.0) | 76.5(0.7) |

| DRIVE       | 1 ~ 5  | 3931   | 1280   | 87.6(5.9) | 72.7(7.0) | 64.2(12.6) | 79.3(5.1) |
| 6 ~ 10      | 3958   | 1318   | 84.9(5.7) | 73.1(5.8) | 69.7(9.3) | 81.6(2.9) |
| even #      | 3932   | 1295   | 82.4(5.6) | 72.9(6.6) | 63.2(12.8) | 83.5(5.3) |
| odd #       | 3931   | 1310   | 76.9(8.0) | 60.0(6.9) | 51.6(9.3) | 65.4(3.3) |

| LETTER      | 1 ~ 5  | 565    | 171    | 79.6(5.5) | 67.6(6.0) | 71.0(9.3) | 82.2(4.3) |
| 6 ~ 10      | 550    | 178    | 73.2(6.3) | 63.9(6.1) | 61.2(10.6) | 75.9(5.6) |
| 11 ~ 15     | 556    | 177    | 73.3(5.9) | 66.6(3.4) | 59.0(10.1) | 75.4(5.0) |
| 16 ~ 20     | 550    | 184    | 71.5(5.9) | 64.9(5.2) | 63.5(7.0) | 73.9(5.3) |
| 21 ~ 25     | 585    | 167    | 78.2(6.0) | 68.3(8.1) | 63.1(11.2) | 77.1(5.1) |

| VOWEL       | 1 ~ 5  | 48     | 42     | 35.6(9.0) | 37.0(9.3) | 31.5(6.7) | 54.9(6.7) |
| 6 ~ 10      | 48     | 42     | 32.6(7.5) | 34.1(7.7) | 30.0(9.8) | 53.0(4.4) |
| even #      | 48     | 42     | 36.6(9.0) | 39.9(10.5) | 33.3(7.8) | 62.1(5.6) |
| odd #       | 48     | 42     | 28.2(9.0) | 28.8(7.2) | 23.2(4.8) | 54.0(5.5) |

| USPS        | 1 ~ 5  | 652    | 166    | 70.1(5.2) | 62.8(7.2) | 45.8(5.9) | 76.2(3.3) |
| 6 ~ 10      | 542    | 147    | 64.3(4.7) | 61.4(5.9) | 41.7(5.3) | 76.9(5.1) |
| even #      | 556    | 147    | 70.6(5.4) | 63.7(7.2) | 48.4(5.3) | 75.7(2.7) |
| odd #       | 542    | 166    | 63.1(4.3) | 57.8(6.8) | 37.8(5.7) | 73.6(3.4) |
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