Bridging Ordinary-Label Learning and Complementary-Label Learning

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Abstract
Unlike ordinary supervised pattern recognition, in a newly proposed framework namely complementary-label learning, each label specifies one class that the pattern does not belong to. In this paper, we propose the natural generalization of learning from an ordinary label and a complementary label, specifically focused on one-versus-all and pairwise classification. We assume that annotation with a bag of complementary labels is equivalent to providing the rest of all the labels as the candidates of the one true class. Our derived classification risk is in a comprehensive form that includes those in the literature, and succeeded to explicitly show the relationship between the single and multiple ordinary/complementary labels. We further show both theoretically and experimentally that the classification error bound monotonically decreases corresponding to the number of complementary labels. This is consistent because the more complementary labels are provided, the less supervision becomes ambiguous.

1. Introduction
In the most common problem setting in supervised learning, the class to which the training data belong is provided as a label, namely an ordinary label. There is increasing interest in generalizing the concept of ordinary labels (Chapelle et al., 2010; Natarajan et al., 2013; Ishida et al., 2018; Cour et al., 2011; Luo & Orabona, 2010). In this paper, we consider a problem setting where each training data is provided with a label, that is, a complementary label, which specifies one class that the pattern does not belong to. The ordinary and complementary labels respectively reflect the information regarding a class to which the training data are likely and unlikely to belong.

The learning framework was first proposed by (Ishida et al., 2017). Assuming that a single complementary label is provided to each training data, the corresponding loss function considering one-versus-all and pairwise classification was defined, and also the classification risk and error were analyzed. The classification risk studied by (Ishida et al., 2019) depends on a more generalized loss function where the classification strategy is not necessarily restricted to be one-versus-all or pairwise classification.

Although choosing the correct class of a pattern involves considerable work for the annotators, the use of complementary labels can alleviate the annotation cost. However, in this framework, loss of generalities can occur if annotators choose only one class as a complementary label. In other words, it is reasonably assumed that multiple labels can be chosen as classes to which a pattern does not belong.

In (Feng & An, 2019), the authors analyzed the classification risk and error in cases involving an arbitrary number of complementary labels provided to each training data. However, in this problem setting, the number of complementary labels provided to the training data is variable. Therefore, the problem setting itself is not a generalization of that defined by (Ishida et al., 2017) and ordinary supervised learning, in which the number of provided labels is fixed.

To overcome the limitation, in this work, we performed a detailed theoretical analysis to generalize the learning framework where a single ordinary/complementary label is provided; that is, we formulated learning from training data provided with multiple complementary labels. In particular, we (1) formulated the data-generation probability model, (2) extended the definition of the loss functions for one-versus-all and pairwise classification, and (3) derived the classification risk and error for the defined loss function, assuming that each training data is provided with fixed number of multiple complementary labels.

The introduced loss function is a natural generalization of those pertaining to the one-versus-all and pairwise classification from a single ordinary/complementary label. We focus on the additivity and duality of such loss functions, allowing a straightforward comparison of the proposed approach and those shown in the existing literature. The properties also allow our classification risk to be in a more simple form than that of (Ishida et al., 2017; 2019). Further, the derived classification error monotonically decreases corresponding to the number of complementary labels.
labels. This property is in agreement with the fact that effective learning becomes challenging as supervised information from provided labels becomes more ambiguous. The error bound for one-versus-all classification derived in our work is significantly tighter than those shown in (Ishida et al., 2017; 2019). The formulation is validated by experiment demonstrated with real-world dataset. In the experiment, we show that the corresponding tightness of error bound for one-versus all and pairwise classification are almost the same.

The remaining paper is organized as follows. Section 2 provides a review of the existing work regarding the generalization of supervised learning from ordinary labels. Section 3 introduces several key formulations pertaining to ordinary-label and complementary-label learning. Section 4 presents the generation probability model of data provided with multiple complementary labels and the loss functions for the learning conducted from such data. Furthermore, this section describes the natural generalization of the proposed loss function from those for one-versus-all and pairwise classification defined by (Ishida et al., 2017) and the evaluation of the classification risk. The error bound of the one-versus-all and pairwise classification is derived in Section 5. Section 6 describes the experimental investigation performed considering real-world data to validate the classification error, and Section 7 presents the conclusions.

2. Related Work

This section provides a review of the existing work regarding the generalization of supervised learning from the ordinary labels provided to training data.

Semi-supervised learning, in which the classification algorithm is provided with some training data labeled but not necessarily for all, has been extensively investigated (Chapelle et al., 2010; Grandvalet & Bengio, 2005; Mann & McCallum, 2007; Niu et al., 2013; Kipf & Welling, 2017; Laine & Aila, 2017). Although the prediction accuracy of such learning is less than that of fully supervised learning, this technique requires less labeled training data, thereby reducing the annotation cost.

As another type of generalization, there exists a method of learning from training data, in which each data is provided with multiple labels, only one of which specifies the one true class. Such labels are generally known as partial labels (or candidate labels) (Cour et al., 2011; Luo & Orabona, 2010; Cid-sueiro, 2012; Raykar et al., 2010). This approach can potentially be applied when the true class of a given training data is not clear or when the label information requires to be kept confidential.

Framework of learning from labels, namely complementary labels, specifying classes that the pattern does not belong to has been also formulated. Providing a complementary label to a training data is equivalent to considering the other labels as candidate labels. In other words, a set of candidate labels is a comprehensive concept involving both ordinary and complementary labels as special cases. (Ishida et al., 2017) provided the complementarily labeled data-generation probability model and classification risk, which was not realized in (Cour et al., 2011). In addition, when learning from noisy labels, which stochastically represent incorrect information (Natarajan et al., 2013; Kim et al., 2019; Liu & Dietterich, 2012), providing complementary label to prevent the specification of a noisy label as a true label has been noted to be effective.

However, the problem setting in (Ishida et al., 2017) encounters a limitation in cases in which only one complementary label is provided to each training data, leading to a loss of generality. To this end, theoretical analysis of learning from multiple complementary labels is performed by (Feng & An, 2019). It was assumed that an arbitrary number of complementary labels were provided to the training data; in other words, the number of labels provided to the data varied with each data. Consequently, the considered problem setting is considerably different from that of (Ishida et al., 2017), in which the number of labels is fixed. Furthermore, in fact, when assuming that only one complementary label is provided to each data, the data-generation probability model, classification risk, and error bound described in (Feng & An, 2019) do not have the same form as those shown in (Ishida et al., 2017). For the same reason, the problem setting in (Feng & An, 2019) is different from that of ordinary supervised learning, in which a single label is provided to each training data. Furthermore, because the analysis in (Feng & An, 2019) was performed considering only one-versus-all classification, the theoretical behavior in pairwise classification is not clarified.

To overcome these limitations, we addressed the problem by using an approach different from that of (Feng & An, 2019). Assuming that a fixed number of multiple ordinary/complementary labels are provided to each training data, we studied the generalized formulation, which involves a comprehensive form of learning from a single ordinary/complementary label. Although the generalization of complementary learning has been recently investigated (Cao & Xu, 2020), our proposed approach is different from that of (Cao & Xu, 2020). In particular, we focused on the fact that both the loss functions of one-versus-all and pairwise classification satisfy the additivity and duality. Our theoretical analysis regarding the classification risk and error is based on the generalization of the loss functions satisfying these properties. Consequently, our results clarified the theoretical relationship of learning from ordinary label and complementary label.
3. Background

This section presents the data-generation probability model and loss functions shown in the existing literature. All these formulations were on the assumption that a single ordinary label or complementary label is provided.

3.1. Supervised Learning from Ordinary Label

In the $K$ ($\geq 2$) classification problem, supervised learning concerns the efficiency of a classifier $f : \mathcal{X} \rightarrow \mathcal{Y}$, which maps a pattern $x \in \mathcal{X}$ to the class to which it belongs, that is, $y \in \mathcal{Y}$, where $|\mathcal{Y}| = K$. Given the discriminant function $g_y : \mathcal{X} \rightarrow \mathbb{R}$, which represents the confidence on the 2 class classification about $y$, the classifier $f$ can be defined as $f(x) = \arg \max_{y \in \mathcal{Y}} g_y(x)$.

Given a pair $(x, y)$, in which $x$ is the pattern and $y$ is an ordinary label representing the belonging class of $x$, the prediction by $f$ can be evaluated using a loss function $\ell : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}$. For example, the loss functions for one-versus-all and pairwise classification, $\mathcal{L}_{\text{OVA}}$ and $\mathcal{L}_{\text{PC}}$, respectively, can be defined as (Zhang, 2004):

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

(1)

$$\mathcal{L}_{\text{PC}}(f(x), y) = \sum_{y' \neq y} \ell(g_y(x) - g_{y'}(x))$$

(2)

Note that the function $\ell : \mathbb{R} \rightarrow \mathbb{R}_+$ monotonically decreases corresponding to the input.

The 0-1 loss, $\ell_{0,1}(z) := I(z \leq 0)$, is a standard type of function $\ell$, where $I$ is an indicator function. The 0-1 loss is unsuitable for loss optimization, as it is undifferentiable at $z = 0$, and its gradient is always 0 for all other inputs. Consequently, the 0-1 loss is usually surrogated by other functions, such as the sigmoid and ramp losses, all of which satisfy the following condition:

$$\ell(z) + \ell(-z) = a$$

(3)

where $a \in \mathbb{R}$ is constant. In the remaining study, we assume $\ell$ to satisfy (3) but not its differentiability.

In addition, we assume that $(x, y)$, involving the pattern $x$ and its belonging class $y$, is generated from a probabilistic distribution $P(x, y)$. The classification risk $R(f)$ of a classifier $f$ can be defined as follows:

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

(4)

where $\mathbb{E}_{P(x,y)}$ represents the expectation for $P(x, y)$.

3.2. Supervised Learning from Complementary Label

(Ishida et al., 2017) discussed the formulation considering a label specifying a class that a pattern does not belong to. Given a pair $(x, \overline{y})$ of a pattern $x \in \mathcal{X}$ and a class $\overline{y} \in \mathcal{Y}$ to which the pattern does not belong, the prediction by $f : \mathcal{X} \rightarrow \mathcal{Y}$ can be evaluated by the loss function $\mathcal{L} : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}$. (Ishida et al., 2017) defined the loss functions for one-versus-all and pairwise classification as follows:

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

(5)

$$\mathcal{L}_{\text{PC}}(f(x), \overline{y}) = \sum_{y' \neq \overline{y}} \ell(g_y(x) - g_{\overline{y}}(x))$$

(6)

Compared to (1) and (2), the loss functions defined in (5) and (6) are in natural forms to deal with the training data provided a label $\overline{y}$. The extended form of the loss functions in (5) and (6) is as follows (Ishida et al., 2019):

$$\mathcal{L}(f(x), \overline{y}) = -(K-1)\mathcal{L}(f(x), y) + \sum_{y \in \mathcal{Y}} \mathcal{L}(f(x), y)$$

(7)

Considering (3), the function in (7) involves both one-versus-all and pairwise classification losses.

Given a pattern $x$ and its complementary label $\overline{y} \in \mathcal{Y}$, the generation probability $\overline{P}(\overline{y}|x)$ of the labeled data is as follows:

$$\overline{P}(\overline{y}|x) = \frac{1}{K-1} \sum_{y \neq \overline{y}} P(y|x)$$

(8)

Here, $\overline{P}(\overline{y}|x)$ is proportional to the sum of probabilities regarding all the other labels.

Subsequently, $(x, \overline{y})$ is assumed to be stochastically generated from the distribution $\overline{P}(x, \overline{y}) = \overline{P}(\overline{y}|x)P(x)$. The $R(f)$ defined in (4) can be expressed as:

$$R(f) = (K-1)\mathbb{E}_{\overline{P}(x, \overline{y})} [\mathcal{L}(f(x), \overline{y})] - \overline{m}_1 + m_2$$

(9)

such that $\overline{m}_1$ and $m_2$ are constants, where $\overline{m}_1 := \sum_{y \in \mathcal{Y}} \mathcal{L}(f(x), y)$ and $m_2 := \mathcal{L}(f(x), y) + \mathcal{L}(f(x), y)$.

4. Formulation

The formulation in (Ishida et al., 2017) assumes that a single complementary label is provided to the training data. We generalize this formulation, assuming that $M$ ($1 \leq M \leq K-1$) complementary labels are provided to each training data. This section describes the data-generation probability model of the data provided with multiple complementary labels. Next, the loss functions for learning from multiple complementary labels are defined, and the classification risk is evaluated.
4.1. Generalization of Generation Probability

The labels specifying the incorrect classes are equally informative as the remaining labels that specify the classes to which a pattern likely belongs. The latter labels are termed as candidate labels and the set of these labels is defined as $\mathcal{Y} = \mathcal{Y}_N(\mathcal{Y})$, where $\mathcal{Y}_N(\mathcal{Y})$ denotes the set of all the $N$-size subsets of $\mathcal{Y}$. From now on we make the assumption that providing $M (= K - N)$ complementary labels to a training data is equivalent to providing $N (= |\mathcal{Y}| = K - M)$ candidate labels.

As stated in Section 3, (8) represents the probability of $\mathcal{Y}$ not being a true label. This aspect can be interpreted in the context of a candidate label; $\mathcal{P}(\mathcal{Y}|x)$ represents the probability with which a true label is included in $\mathcal{Y}$. In contrast to (8), which can only be applied when $M = 1$ (or $N = |\mathcal{Y}| - 1 = K - 1$), our generalized data-generation probability model is defined as:

$$P_N(\mathcal{Y}|x) = \frac{1}{K-1} \sum_{y \in \mathcal{Y}} P(y|x)$$ (10)

where $P_N(\mathcal{Y}|x)$ represents the probability of the true label being included in $\mathcal{Y}$. Note that (10) is the same as (8) if $N = K - 1$. An equation equivalent to (10) was defined in (Cao & Xu, 2020); the significant difference is that the distribution, in contrast to (10), represents the probability of a true label not being included in a set of $K - N$ complementary labels $\mathcal{Y} = \mathcal{Y}\setminus\mathcal{Y}$. Thus, the expression proposed in (Cao & Xu, 2020) does not express the relationship between learning from ordinary and complementary labels. In the remaining work, we assume that $\mathcal{Y}$ is generated from $P_N(\mathcal{Y}|x)$ independently.

4.2. Generalization of Loss Function

For one-versus-all and pairwise classification from a set of multiple candidate labels $\mathcal{Y}$, the corresponding loss functions $L_{\text{OVA}}$ and $L_{\text{PC}}$ can be defined as:

$$L_{\text{OVA}}(f(x), \mathcal{Y}) = \frac{K - N}{K - 1} \sum_{y \in \mathcal{Y}} \ell(g_y(x)) + \frac{N}{K - 1} \sum_{\bar{y} \notin \mathcal{Y}} \ell(-g_{\bar{y}}(x))$$ (11)

$$L_{\text{PC}}(f(x), \mathcal{Y}) = \sum_{y \in \mathcal{Y}} \sum_{\bar{y} \notin \mathcal{Y}} \ell(g_y(x) - g_{\bar{y}}(x))$$ (12)

Note that (11) and (12) are the same as (1) and (2), respectively, if $N = 1$. Similarly, the newly defined equations are the same as (5) and (6) if $N = K - 1$.

As a generalization of (11) and (12), we introduce a loss function $L : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}$, which is defined as the additive form of loss functions for ordinary-label learning:

$$L(f(x), \mathcal{Y}) = \xi_1 \sum_{y \in \mathcal{Y}} L(f(x), y) + \xi_2$$ (13)

where $\xi_1 \in \mathbb{R}^+$ and $\xi_2 \in \mathbb{R}$ are constants. Assuming $L(f(x), y) = L_{\text{OVA}}(f(x), y)$, $\xi_1 = 1$, and $\xi_2 = -aN(\mathcal{N} - 1)$, (13) becomes the same expression as (11) if $\ell$ satisfies (3). Under the same condition on $\ell$, by assuming $L(f(x), y) = L_{\text{PC}}(f(x), y)$, $\xi_1 = 1$, and $\xi_2 = -a \cdot N C_2$, (13) and (12) have the same expression (see supplementary materials for complete proofs).

Similar to the loss functions defined in (7), $L$ in (13) is defined from the ordinary loss function $L$. In contrast to the loss function defined in (7), which can be applied only if a single complementary label is provided, the loss function pertaining to (13) can be applied for any number of complementary (or candidate) labels. Consequently, $L$ in (13) can be considered as a generalized form of (5) and (6).

Furthermore, for any $x$, let the loss function $L$ satisfy the following condition:

$$\sum_{y \in \mathcal{Y}} L(f(x), y) = m_1$$

where $m_1 \in \mathbb{R}$ is a constant. Both $L_{\text{OVA}}$ and $L_{\text{PC}}$ satisfy this condition, where $m_1 = aK$ and $m_1 = a \cdot K C_2$, respectively. For any $x$ and $y$, we then define a function $\tilde{L}$, which satisfies the following condition:

$$L(f(x), y) + \tilde{L}(f(x), y) = m_2$$

where $m_2 \in \mathbb{R}$ is a constant. This condition is satisfied by $L_{\text{OVA}}$ and $\tilde{L}_{\text{OVA}}$ and also by $L_{\text{PC}}$ and $\tilde{L}_{\text{PC}}$, where $m_2 = 2a$ and $a(K - 1)$ respectively.

Now, the following equation holds:

$$L(f(x), Y) = \xi_1 \sum_{\bar{y} \in \mathcal{Y}} \tilde{L}(f(x), \bar{y}) + \xi_2$$ (14)

where $\mathcal{Y} \cup \bar{Y} = \mathcal{Y}$ and $\mathcal{Y} \cap \bar{Y} = \emptyset$. Note that $\xi_2 = \xi_1 m_1 \bar{Y} + \xi_2 - \xi_1 m_2 (K - N)$, and it can be expressed as $\xi_2 = \xi_2$ if $m_1 = m_2 = 0$. (13) and (14) express the duality of the loss function $L$.

To the best of our knowledge, this is the first study of the additivity and duality commonly found in loss functions for one-versus-all and pairwise classification. This property is critical to study the classification risk and error, and it has not been discussed in any of the existing studies (Ishida et al., 2019; Cao & Xu, 2020).

4.3. Classification Risk with Multiple Complementary Labels

If we define loss function $L$ as in (13), the following theorem holds for any type of $L$. Similar to (4) and (9), the the-
orem allows the expression of the classification risk from multiple complementary labels in terms of the expectation of loss. The complete proof is available in the supplementary materials.

**Theorem 1.** Given a pattern \( x \), a set of candidate labels \( Y \), and loss function \( L \) defined by (13), the classification risk \( R(f) \) can be expressed as follows:

\[
R(f) = \frac{K-1}{\xi_1 (K-N)} \mathbb{E}_{P_n(x,Y)} [L(f(x), Y)] + C \tag{15}
\]

where

\[
C = - \frac{N-1}{K-N} \sum_{y \in Y} \mathcal{L}(f(x), y) - \frac{\xi_2}{\xi_1} \frac{(K-1)}{(K-N)} \tag{16}
\]

Some conditions can be used to simplify the expression in (15) for one-versus-all and pairwise classification, without losing generalities. Note that redefining (3) as \( \ell(z) := \ell(z) - \ell(0) = \ell(z) - \frac{y}{2} \) does not affect the loss minimization when learning. If we shift \( \ell \) to satisfy \( a = 0, n_1 = 0 \) holds for both \( \mathcal{OVA} \) and \( \mathcal{PC} \); therefore, the first term in (16) can be eliminated.

Similarly, \( \xi_1 \) and \( \xi_2 \) in (13) do not affect the loss minimization. Considering \( \xi_1 = 1 \) and \( \xi_2 = 0 \), we can simplify (15) as follows without loss of generalities:

\[
\mathcal{L}(f(x), Y) = \sum_{y \in Y} \mathcal{L}(f(x), y) \tag{17}
\]

Consequently, by assuming that \( a = 0, \xi_1 = 1, \) and \( \xi_2 = 0 \), the following expression holds for the classification risk.

\[
R(f) = \frac{K-1}{K-N} \mathbb{E}_{P_n(x,Y)} [L(f(x), Y)] \tag{18}
\]

**5. Statistical Analysis**

This section discusses the error bound for one-versus-all and pairwise classification. For simplicity, we assume that \( \ell \) satisfies (3) with \( a = 0 \), and the conditions \( \inf \ell(z) = -1/2 \) and \( \sup \ell(x) = 1/2 \). Further, we assume that \( \ell \) is Lipschitz continuous. In addition, we assume \( \xi_1 = 1 \) and \( \xi_2 = 0 \). For the rest of this paper, we define \( \mathcal{L} \) and \( R(f) \) by using (17) and (18), respectively.

**5.1. Notations**

Let us consider that a set of \( n \) training data \( \mathcal{S} = \{(x_i, Y_i)\}_{i=1}^n \) is given, and each training data is generated with a probability of \( P_n(x, Y) \) independently. Based on (18), the empirical classification risk \( \hat{R}(f) \) for the set \( \mathcal{S} \) is:

\[
\hat{R}(f) = \frac{K-1}{n (K-N)} \sum_{i=1}^n \mathcal{L}(f(x_i), Y_i) \]

We define the ideal classifier that minimizes the generalization error (Bayes classifier) and the empirically ideal classifier as \( f^* := \arg \min f R(f) \) and \( f := \arg \min f \hat{R}(f) \), respectively. We define the classification error \( \mathcal{E}_N \) for the classifier \( f \) as follows.

\[
\mathcal{E}_N = R(f) - R(f^*) \tag{19}
\]

In the literature, the Rademacher complexity for a set of discriminant functions \( \mathcal{G} \) over the input space \( X \) is usually defined as follows:

\[
\mathcal{R}_n(\mathcal{G}) = \mathbb{E}_s \mathbb{E}_\sigma \left[ \sup_{g \in \mathcal{G}} \frac{1}{n} \sum_{i=1}^n \sigma_i g(x_i) \right]
\]

where \( \sigma = \{\sigma_1, \cdots, \sigma_n\} \) is a set of independent stochastic variables, which take one value of \( \{-1, +1\} \) with the same probability. In addition, \( \mathbb{E}_s \) and \( \mathbb{E}_\sigma \) represent the expectation for each element of \( \mathcal{S} \) and \( \sigma \), respectively.

**5.2. Evaluation of Error Bound**

The following lemmas are introduced to derive the classification error bound.

**Lemma 1.** We express the supremum of the difference in loss \( \|\mathcal{L}\|_\infty \) in accordance with the change in a set of candidate labels, i.e., given any \( Y, Y' \in \mathcal{Y} \),

\[
\|\mathcal{L}\|_\infty = \sup_{g_1, \cdots, g_K \in \mathcal{G}} \left( \sum_{y \in Y} \mathcal{L}(f(x), y) - \sum_{y' \in Y'} \mathcal{L}(f(x), y') \right)
\]

Then, the following holds for one-versus-all classification.

\[
\|\mathcal{L}_{\mathcal{OVA}}\|_\infty = \begin{cases} \frac{K N}{K-1}, & \text{if } N \leq \frac{K}{2} \\ \frac{K(K-N)}{K-1}, & \text{otherwise} \end{cases}
\]

Similarily, for pairwise classification,

\[
\|\mathcal{L}_{\mathcal{PC}}\|_\infty = N(K-N)
\]

**Lemma 2.** Define a function set \( \mathcal{H}_{\mathcal{OVA}}, \mathcal{H}_{\mathcal{PC}} \) as follows:

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

\[
\mathcal{H}_{\mathcal{PC}} = \{(x,Y) \mapsto \mathcal{L}_{\mathcal{PC}}(f(x), Y) \mid g_1, \cdots, g_K \in \mathcal{G}\}
\]

Then, if \( \ell \) is \( L_\ell \) \( (\geq 0) \) Lipschitz continuous, the following holds for \( \mathcal{H}_{\mathcal{OVA}} \).

\[
\mathcal{R}_n(\mathcal{H}_{\mathcal{OVA}}) \leq \begin{cases} \frac{K(K+N)}{K-1} L_\ell \mathcal{R}_n(\mathcal{G}), & \text{if } N \leq \frac{K}{2} \\ \frac{K(2K-N)}{K-1} L_\ell \mathcal{R}_n(\mathcal{G}), & \text{otherwise} \end{cases}
\]

Similarly, for \( \mathcal{H}_{\mathcal{PC}} \),

\[
\mathcal{R}_n(\mathcal{H}_{\mathcal{PC}}) \leq 2K(K-1)L_\ell \mathcal{R}_n(\mathcal{G})
\]
Based on these lemmas, the error bounds for the one-versus-all and pairwise classification can be defined as follows. The complete proofs are provided in the supplementary materials.

**Theorem 2.** Assume that function $\ell$ satisfies the stated condition in the beginning of this section, and is $L_\ell$ Lipschitz continuous. Then, for any $\delta > 0$, the following equation for one-versus-all classification holds with a probability of at least $1 - \delta$.

$$
\mathcal{E}_N \leq \begin{cases} 
\frac{4K(K+N)}{K-N} L_\ell \mathfrak{R}_{n_0} (g) + \frac{KN}{K-N} \sqrt{\frac{2\ln(2/\delta)}{n}} 
& \text{(if } N \leq \frac{K}{2} \text{)} \\
\frac{4K(2K-N)}{K-N} L_\ell \mathfrak{R}_n (g) + K \sqrt{\frac{2\ln(2/\delta)}{n}} 
& \text{(otherwise)} 
\end{cases}
$$

(20)

Similarly, for pairwise classification, the following equation holds with a probability of at least $1 - \delta$.

$$
\mathcal{E}_N \leq \frac{8K(K-1)^2}{K-N} L_\ell \mathfrak{R}_n (g) + N(K-1) \sqrt{\frac{2\ln(2/\delta)}{n}}
$$

(21)

We now focus on the error bounds in Theorem 2 assuming $N = K - 1$, which implies a single complementary label is provided. Because $K \geq 2$, it is obvious that $N > K/2$; therefore, the error bound for the one-versus-all classification according to (20) is:

$$
\mathcal{E}_N \leq 4K(K+1)L_\ell \mathfrak{R}_{n_0} (g) + K \sqrt{\frac{2\ln(2/\delta)}{n}}
$$

The error bound shown in (Ishida et al., 2017) is derived as the following$^1$.

$$
\mathcal{E}_N \leq 4K(K+1)L_\ell \mathfrak{R}_n (g) + 2(K-1) \sqrt{\frac{2\ln(2/\delta)}{n}}
$$

Comparing the second terms in the above equations, the error bound derived in this paper is tighter than that of (Ishida et al., 2017), because the $\|\mathcal{L}\|_\infty$ derived in Lemma 1 is evaluated strictly. In practice, although $\|\mathcal{L}_{OVA}\|_\infty = 2$ holds in (Ishida et al., 2017), $\|\mathcal{L}_{OVA}\|_\infty = K/(K-1) \leq 2$ holds in this paper if $N = K - 1$, which is more precise than the former case. Considering the above-mentioned analysis, the error bound of the one-versus-all classification in Theorem 2 is a comprehensive form of that shown in (Ishida et al., 2017), and it is also consequently tighter. Note that if $N = K - 1$, the pairwise classification error bound shown in (21) is the same as that of (Ishida et al., 2017). In other words, the error bound of the pairwise classification in Theorem 2 is also a comprehensive form of that shown in (Ishida et al., 2017).

Furthermore, the upper-bound of $\mathcal{E}_N$ increases monotonically corresponding to $N$ in accordance with (20) and (21). This aspect is in agreement with the fact that a decrease in the number of candidate labels leads to less ambiguous supervision of the training data.

### 6. Experiment

This section describes the evaluation of the accuracy of one-versus-all and pairwise classification and the validation of the formulation discussed in Section 5.2. Understanding the exact behavior of the classification error only from the derived equations in Theorem 2 is difficult. Therefore, we attempt to quantitively discuss the error in a real-world classification problem. The source code for the described experiment is available online$^2$.

#### 6.1. Dataset Generation

The generation probability model of the training data provided with multiple candidate labels is as defined in (10). We generate the experimental dataset according to this definition, and the annotation of the training data is performed as follows. First, we prepare pretrained $K$ class classifiers, namely, annotators, for the ordinarily labeled training data. The annotators are multi-layer perceptrons (MLP) with softmax as the output layer activation function. The annotators are trained on the MNIST$^3$, Fashion-MNIST$^4$, Kuzush-MNIST$^5$, and CIFAR-10$^6$ datasets. Table 1 summarizes the datasets. Because all these cases correspond to the 10 class ($y \in \{0, \ldots, 9\}$) classification problem, the data belonging to $y = 5, \ldots, 9$ is eliminated when we assume $K = 5$ in the following experiment. Because the discriminant functions of the annotators $g_1, \ldots, g_K$ are normalized using softmax, each of the functions can be treated as having a data generation probability $P(y|x)$. Therefore, assuming that the number of candidate labels is $N$, we generate $Y$ in accordance with $P_N (f(x), Y)$, calculated using the discriminant functions. Similarly, for the test dataset, the true label $y \in Y$ is provided in accordance with $g_1, \ldots, g_K$ of the annotators.

In the experiment, we pretrained the annotators for $K = 10$ and $K = 5$. When $K = 10$, the classification accuracy for the MNIST, Fashion-MNIST, Kuzush-MNIST, and CIFAR-10 datasets are 99.17%, 92.67%, 95.1%, and 81.62%, respectively. For $K = 5$, the corresponding accuracies are 99.90%, 95.16%, 96.56%, and 85.60%. As all the accuracies are reasonably high, the generation probabil-

$^1$In (Ishida et al., 2017), the first term in the right-hand side is expressed as $4K(K+1)L_\ell \mathfrak{R}_{n_0} (g)$; however, this is a wrong computation caused by a simple miscalculation.

$^2$https://github.com/YasuhiroKatsura/ord-comp

$^3$http://yann.lecun.com/exdb/mnist/

$^4$https://github.com/zalandoresearch/fashion-mnist

$^5$https://github.com/rois-codh/kmnist

$^6$https://www.cs.toronto.edu/~kriz/cifar.html
Bridging Ordinary-Label Learning and Complementary-Label Learning

Figure 1: Error for 10 and 5 classification for different numbers of complementary labels $N$. The red and blue closed plots represent the experimental results for the one-versus-all and pairwise classification, respectively. The red and blue open plots represent the theoretical error bounds for the one-versus-all and pairwise classification, respectively.

Table 1: Datasets used in the experiment.

|                  | MNIST | Fashion | Kuzushi | CIFAR-10 |
|------------------|-------|---------|---------|----------|
| Number of classes| 10    | 10      | 10      | 10       |
| Number of dimensions| 28×28 | 28×28   | 28×28   | 3×32×32  |
| (gray)           | (gray)| (gray)  | (RGB)   |          |
| Number of data   | 60,000| 60,000  | 60,000  | 60,000   |

6.2. Evaluation of Classification Error Bound

Experimental Setup: Assuming that the number of classes $K$ is 10 or 5, the classification accuracy is compared under different numbers of candidate labels $N \in \{1, \cdots, K-1\}$. The loss functions $L_{\text{OVa}}$ and $L_{\text{PC}}$ are defined using (17), and the function $\ell$ is an origin-symmetric sigmoid loss, i.e., $\ell(z) = (1 + e^z)^{-1} - 1/2$. We set the number of training data for each class as 1,000, and the data were randomly selected from the complete dataset. We conducted the experiment using MLP for the MNIST, Fashion-MNIST, and Kuzushi-MNIST datasets. The number of epochs was 300, weight decay was $10^{-4}$, learning rate was $10^{-4}$, and Adam was used as the optimization algorithm (Kingma & Ba, 2015). For CIFAR-10, the experiment was performed using Dense Net (Huang et al., 2016). The number of epochs was 300, weight decay was $5 \times 10^{-4}$, momentum was 0.9, and the optimization algorithm was the stochastic gradient descent. The initial learning rate was set as $10^{-2}$, and it was halved every 30 epochs. The range of discriminant functions $g_y$ was $[-1/2, 1/2]$ for both MLP and Dense Net.

Error Computation: The classification error was calculated according to (19). Because the exact $\hat{f}$ defined in Section 5.1 was not available, we surrogated it with a classifier that could minimize the loss of the training data in the experiment. Similarly, we substituted $f^*$ with a classifier that could minimize the loss of the test data. Additionally, we computed the theoretical classification error bounds according to (20) and (21). We set $\delta = 0.1$ because Theorem 2 holds with a high probability if $\delta$ is relatively small. Furthermore, we set $L_\ell$ as 1.0 because it is the minimum Lipschitz constant of the shifted sigmoid loss. Assuming that both MLP and Dense Net in the experiment had adequate capacity, we set $R_n(G) = 0.5$.

Results: We performed 5 trials for each experiment and observed the classification accuracy, that is, rate of correct classification for the test dataset estimated by a classifier which minimizes loss for training data. The mean and standard deviation for the accuracy are listed in Table 2. The results indicate that the mean of the accuracy tends to monotonically decrease corresponding to $N$. That is, increase in the number of complementary labels leads to a better performance than the case of $N = K - 1$ ($M = 1$).
Table 2: Experimental classification accuracies for 10 and 5 class classification (%). The experiments were performed 5 times for each case; the mean accuracy and standard deviation are presented by the upper and lower values, respectively. The highest accuracy is boldfaced.

|          | N            | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  |
|----------|--------------|----|----|----|----|----|----|----|----|----|
| **K = 10** |              |    |    |    |    |    |    |    |    |    |
| MNIST    | 92.28        | 68.22 | 89.44 | 86.86 | 80.72 | 85.99 | 77.28 | 72.27 | 62.13 |
| (OVA)    | (±0.45)      | (±6.97) | (±4.23) | (±4.16) | (±6.05) | (±4.82) | (±5.02) | (±6.42) | (±11.03) |
| MNIST    | 92.38        | 91.58 | 85.94 | 87.38 | 84.93 | 83.93 | 84.79 | 71.73 | 67.07 |
| (PC)     | (±0.42)      | (±3.57) | (±6.57) | (±4.26) | (±6.53) | (±3.57) | (±3.94) | (±4.63) | (±6.66) |
| Fashion  | 81.07        | 80.66 | 80.43 | 80.62 | 79.64 | 78.99 | 75.10 | 74.89 | 71.41 |
| (OVA)    | (±0.09)      | (±0.32) | (±1.05) | (±1.15) | (±1.03) | (±1.49) | (±5.58) | (±2.61) | (±2.59) |
| Fashion  | 81.47        | 81.51 | 80.41 | 81.23 | 79.24 | 79.88 | 78.45 | 75.64 | 73.11 |
| (PC)     | (±0.16)      | (±0.95) | (±0.16) | (±3.12) | (±0.38) | (±1.29) | (±0.88) | (±3.79) | (±2.30) |
| Kuzushii | 64.19        | 60.83 | 58.96 | 57.45 | 52.20 | 51.28 | 49.43 | 41.27 | 37.09 |
| (OVA)    | (±0.24)      | (±3.33) | (±5.90) | (±3.55) | (±2.96) | (±1.60) | (±5.65) | (±3.46) | (±3.76) |
| Kuzushii | 66.15        | 63.67 | 58.53 | 57.20 | 55.96 | 54.28 | 49.74 | 43.62 | 34.82 |
| (PC)     | (±0.48)      | (±2.96) | (±5.92) | (±4.09) | (±3.44) | (±1.95) | (±4.02) | (±0.66) | (±3.07) |
| CIFAR-10 | 57.17        | 53.84 | 51.16 | 43.88 | 37.95 | 34.85 | 25.94 | 24.33 | 24.18 |
| (OVA)    | (±3.30)      | (±4.95) | (±2.01) | (±4.42) | (±5.96) | (±4.39) | (±3.80) | (±3.36) | (±3.63) |
| CIFAR-10 | 58.30        | 49.04 | 41.63 | 35.68 | 33.29 | 27.62 | 22.26 | 22.36 | 17.32 |
| (PC)     | (±2.89)      | (±3.56) | (±6.24) | (±4.64) | (±3.10) | (±3.43) | (±3.58) | (±4.35) | (±1.20) |

|          | N            | 1  | 2  | 3  | 4  | 5  | 6  | 7  | 8  | 9  |
|----------|--------------|----|----|----|----|----|----|----|----|----|
| **K = 5** |              |    |    |    |    |    |    |    |    |    |
| MNIST    | 98.06        | 97.77 | 97.06 | 95.40 | 96.12 | 97.12 | 95.80 | 92.13 | 89.10 |
| (OVA)    | (±0.12)      | (±0.18) | (±0.20) | (±0.18) | (±0.13) | (±0.14) | (±0.16) | (±0.29) |
| MNIST    | 98.12        | 97.61 | 97.12 | 95.80 | 96.12 | 97.12 | 95.80 | 92.13 | 89.10 |
| (PC)     | (±0.13)      | (±0.14) | (±0.16) | (±0.18) | (±0.19) | (±0.17) | (±0.19) | (±0.29) |
| Fashion  | 86.42        | 85.63 | 84.94 | 83.37 | 85.63 | 85.63 | 84.94 | 83.37 | 82.01 |
| (OVA)    | (±0.26)      | (±0.83) | (±0.41) | (±0.37) | (±0.26) | (±0.83) | (±0.41) | (±0.37) |
| Fashion  | 85.52        | 85.74 | 84.74 | 83.14 | 85.74 | 84.74 | 83.14 | 82.01 | 79.97 |
| (PC)     | (±0.33)      | (±0.44) | (±0.37) | (±0.41) | (±0.33) | (±0.44) | (±0.37) | (±0.41) |
| Kuzushii | 80.49        | 79.02 | 75.78 | 76.55 | 80.49 | 79.02 | 75.78 | 76.55 | 75.33 |
| (OVA)    | (±0.33)      | (±0.61) | (±0.25) | (±1.08) | (±0.33) | (±0.61) | (±0.25) | (±1.08) |
| Kuzushii | 80.97        | 78.78 | 76.53 | 70.23 | 80.97 | 78.78 | 76.53 | 70.23 | 68.88 |
| (PC)     | (±0.22)      | (±0.47) | (±0.65) | (±0.79) | (±0.22) | (±0.47) | (±0.65) | (±0.79) |
| CIFAR-10 | 65.32        | 64.76 | 61.30 | 52.65 | 65.32 | 64.76 | 61.30 | 52.65 | 48.91 |
| (OVA)    | (±0.37)      | (±0.36) | (±0.56) | (±0.83) | (±0.37) | (±0.36) | (±0.56) | (±0.83) |
| CIFAR-10 | 69.11        | 66.98 | 62.10 | 56.29 | 69.11 | 66.98 | 62.10 | 56.29 | 55.19 |
| (PC)     | (±2.59)      | (±3.72) | (±1.47) | (±2.36) | (±2.59) | (±3.72) | (±1.47) | (±2.36) |

The mean and standard deviation of the experimental classification error are listed in Table 3. Furthermore, the mean of the experimental error and theoretical error bounds are shown in Figure 1 as a logarithmic graph. The results indicate that the theoretical error bound for one-versus-all and pairwise classification are about equally tight. The experimental error tends to monotonically increase corresponding to N, which is in accordance with the discussion in Section 5.2. The increase in theoretical error bound and experimental error are similar in shape, indicating that the bound reflects qualitative property found in the experimental error.

**7. Conclusion**

A framework of learning where each training data is provided with multiple ordinary/complementary labels was formulated, then investigated theoretically. The approach allows the natural generalization of learning from a single ordinary/complementary label. The data-generation probability model considering multiple complementary labels and the corresponding loss function were defined. Our generalized loss function is based on the common property, addivity and duality, found in both one-versus-all and pairwise classification loss functions, which allow the formulation in a simple expression. Moreover, the classification risk for one-versus-all and pairwise classification was derived. The classification risk was noted to be proportional to the expectation of the loss for data generation probability. This finding suggests that learning by empirical risk minimization can be performed when multiple complementary labels are provided to each training data. Furthermore, it was theoretically and experimentally demonstrated that the error bounds monotonically decrease corresponding to the number of complementary labels. In addition, the error bound for the one-versus-all classification was significantly tighter than that presented in the existing literature.
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A. Proofs of Loss Function Properties

As stated in Section 4, if we define a loss function $\mathcal{L}$ in an additive form by (13), there exist constants $\xi_1$ and $\xi_2$ which satisfy (11) and (12). We first describe proof of (11). The following formulation holds in accordance with $\ell(z) + \ell(-z) = a$.

$$
\sum_{y \in Y} \mathcal{L}_{\text{OVA}} (f(x), y) = \sum_{y \in Y} \left( \ell(g_y(x)) + \frac{1}{K-1} \sum_{y' \neq y} \ell(-g_{y'}(x)) \right)
$$

$$
= \sum_{y \in Y} \left( \frac{K}{K-1} \ell(g_y(x)) - \frac{1}{K-1} \ell(g_y(x)) + \frac{1}{K-1} \sum_{y' \in Y} \ell(-g_{y'}(x)) - \frac{1}{K-1} \ell(-g_y(x)) \right)
$$

$$
= \frac{1}{K-1} \sum_{y \in Y} \left( K \ell(g_y(x)) + \sum_{y' \in Y} \ell(-g_{y'}(x)) - a \right)
$$

$$
= \frac{1}{K-1} \left( (K - N + N) \sum_{y \in Y} \ell(g_y(x)) + N \sum_{y \in Y} \ell(-g_{y'}(x)) + N \sum_{y' \notin Y} \ell(-g_{y'}(x)) - aN \right)
$$

$$
= \frac{1}{K-1} \left( (K - N) \sum_{y \in Y} \ell(g_y(x)) + N \sum_{y' \notin Y} \ell(-g_{y'}(x)) + aN(N-1) \right)
$$

$$
= \frac{K - N}{K-1} \sum_{y \in Y} \ell(g_y(x)) + \frac{N}{K-1} \sum_{y' \notin Y} \ell(-g_{y'}(x)) + \frac{aN(N-1)}{K-1}
$$

$$
= \mathcal{L}_{\text{OVA}} (f(x), Y) + \frac{aN(N-1)}{K-1}
$$

Note that $\ell(z) - \ell(-z) = a$ is incorrectly assumed in (Ishida et al., 2017), which causes miscalculation in proof of Lemma 2.

Next, we describe proof of (12). Similar to the above formulation, in accordance with $\ell(z) + \ell(-z) = a$,

$$
\sum_{y \in Y} \mathcal{L}_{\text{PC}} (f(x), y) = \sum_{y \in Y} \sum_{y' \neq y} \ell(g_y(x) - g_{y'}(x))
$$

$$
= \sum_{y \in Y} \sum_{y' \neq y} \ell(g_y(x) - g_{y'}(x)) - \sum_{y \in Y} \ell(g_y(x) - g_y(x))
$$

$$
= \sum_{y \in Y} \ell(g_y(x) - g_{y'}(x)) + \sum_{y, y' \in Y \ y \neq y'} \ell(g_y(x) - g_{y'}(x)) + \sum_{y, y' \in Y \ y \neq y'} \ell(g_y(x) - g_{y'}(x)) - \frac{aN}{2}
$$

$$
= \sum_{y \in Y} \ell(g_y(x) - g_{y'}(x)) + a \cdot N C_2
$$

$$
= \mathcal{L}_{\text{PC}} (f(x), Y) + a \cdot N C_2
$$

The third and fourth equality hold due to $\ell(0) = a/2$. \hfill \square

B. Proof of Theorem 1

To prove Theorem 1, we introduce the following lemma.

**Lemma 3.** Let any finite sets be $X$ with size of $K$, and any elements of the $N$-size power set $\mathcal{P}_N(X)$ be $A$. Then, the
the following equation holds for any function \(f\) and \(g\) over \(X\).

\[
\sum_{A \in \mathcal{P}_N(X)} \sum_{a_1, a_2 \in A} f(a_1)g(a_2) = K_2C_{N-2} \sum_{x_1, x_2 \in X, x_1 \neq x_2} f(x_1)g(x_2) + K_1C_{N-1} \sum_{x_1, x_2 \in X, x_1 = x_2} f(x_1)g(x_2)
\]  

(22)

Proof. The left-hand side can be formulated as:

\[
\sum_{A \in \mathcal{P}_N(X)} \sum_{a_1, a_2 \in A} f(a_1)g(a_2) = \sum_{A \in \mathcal{P}_N(X)} \sum_{a_1, a_2 \in A} f(a_1)g(a_2) + \sum_{A \in \mathcal{P}_N(X)} \sum_{a_1, a_2 \in A} f(a_1)g(a_2)
\]

For the first term, any \(A\) can be chosen from \(\mathcal{P}_N(X)\) in \(K\) \(C_N\) patterns, and any \(a_1, a_2 (a_1 \neq a_2)\) can be chosen from \(A\) in \(N\) \(P_2\) patterns. Because \(f(a_1)g(a_2)\) with any \(a_1, a_2 (a_1 \neq a_2)\) can be chosen from \(X\) in \(K\) \(P_2\) patterns, the first term in (22) holds due to \(K_2C_{N-2} = \frac{kC_{N-2}}{K}\). Similar for the second term.

Here, we describe proof of Theorem 1 as the following.

We first derive the expectation of the sum of loss for all the ordinary labels.

\[
\mathbb{E}_{P_N(Y|X)} \left[ \sum_{y \in Y} \mathcal{L}(f(x), y) \right] = \sum_{y \in \mathcal{P}_N(Y)} \sum_{y' \in \mathcal{Y}} \sum_{y' \neq y} \mathcal{L}(f(x), y') P_N(y|x)
\]

\[
= \frac{1}{K-1C_{N-1}} \left\{ K_2C_{N-2} \sum_{y \in \mathcal{Y}} \sum_{y' \neq y} \mathcal{L}(f(x), y') P_N(y|x) + K_1C_{N-1} \sum_{y \in \mathcal{Y}} \mathcal{L}(f(x), y) P_N(y|x) \right\}
\]

\[
= \frac{N-1}{K-1} \mathbb{E}_{P_N(Y|X)} \left[ \sum_{y' \in \mathcal{Y}} \mathcal{L}(f(x), y') - \mathcal{L}(f(x), y) \right] + \mathbb{E}_{P_N(Y|X)} [\mathcal{L}(f(x), y)]
\]

The second equality holds due to the definition of \(P_N(Y|X)\). The third equality holds due to Lemma 3. Thus, the following formulation holds due to (13).

\[
\mathbb{E}_{P_N(X, Y)} [\mathcal{L}(f(x), Y)] = \xi_1 \mathbb{E}_{P_N(X, Y)} \left[ \sum_{y \in \mathcal{Y}} \mathcal{L}(f(x), y) \right] + \xi_2
\]

\[
= \frac{\xi_1(K-N)}{K-1} \mathbb{E}_{P_N(X, Y)} [\mathcal{L}(f(x), y)] + \frac{\xi_1(N-1)}{K-1} \sum_{y \in \mathcal{Y}} \mathcal{L}(f(x), y) + \xi_2
\]

\[\square\]

C. Proof of Lemma 1

According to the duality described in (13) and (14), loss function \(\mathcal{L}\) can be formulated by \(\mathcal{L}(f(x), y)\) for \(N\) candidate labels \(y \in Y\), or \(\mathcal{L}(f(x), \overline{y})\) for \(K-N\) complementary labels \(\overline{y} \in \overline{Y}\). Thus, we can redefine loss function \(\mathcal{L}\) as the
following:

\[ \mathcal{L}(f(x), Y) = \sum_{y \in Y} \tilde{\mathcal{L}}(f(x), y) = \begin{cases} \sum_{y \in Y} \mathcal{L}(f(x), y), & \text{if } N \leq \frac{K}{2} \\ \sum_{y \in Y} \mathcal{L}(f(x), y), & \text{otherwise} \end{cases} \]

where \( \tilde{\mathcal{L}} \) and \( \tilde{Y} \) denote \( \mathcal{L} \) and \( Y \) respectively if \( N \leq K/2 \), otherwise \( \mathcal{L}, Y \) respectively. Therefore, given \( \tilde{N} = |\tilde{Y}| \) it always satisfies \( \tilde{N} \leq K/2 \). Note that \( \xi_2 = \tilde{\xi}_2 = 0 \) due to the assumption of \( a = 0 \), as discussed in Section 4.2. Similarly, \( \tilde{\ell}(z) \) denotes \( \tilde{\ell} : z \mapsto \ell(z) \) if \( N \leq K/2 \) otherwise \( \tilde{\ell} : z \mapsto \ell(-z) \). For the rest of this work, we prove Lemma 1 according to those definitions.

First we describe proof for one-versus-all classification. Under the assumption of \( a = 0 \), the following formulation holds.

\[ \sum_{y \in \tilde{Y}} \tilde{\mathcal{L}}_{OVA}(f(x), y) = \sum_{y \in \tilde{Y}} \left( \frac{K}{K-1} \tilde{\ell}(g_y(x)) + \frac{1}{K-1} \sum_{y' \in \tilde{Y}} \tilde{\ell}(-g_{y'}(x)) \right) \]

Thus, the following formulation holds for any \( \tilde{Y}, \tilde{Y}' \in \mathcal{P}_N(Y) \).

\[
\|\mathcal{L}_{OVA}\|_\infty = \sup_{g_1, \ldots, g_K \in G} \left( \sum_{y \in \tilde{Y}} \tilde{\mathcal{L}}_{OVA}(f(x), y) - \sum_{y' \in \tilde{Y}'} \tilde{\mathcal{L}}_{OVA}(f(x), y') \right) \\
= \sup_{g_1, \ldots, g_K \in G} \left\{ \frac{K}{K-1} \left( \sum_{y \in \tilde{Y}} \tilde{\ell}(g_y(x)) - \sum_{y' \in \tilde{Y}'} \tilde{\ell}(g_{y'}(x)) \right) + \frac{1}{K-1} \left( \sum_{y \in \tilde{Y}} \tilde{\ell}(-g_y(x)) - \sum_{y \in \tilde{Y}} \tilde{\ell}(-g_{y'}(x)) \right) \right\} \\
\leq \frac{K}{K-1} \left( \frac{\tilde{N}}{2} + \frac{\tilde{N}}{2} \right) \\
= \frac{K\tilde{N}}{K-1}
\]

The second inequality holds because supremum and infimum of \( \ell \) are 1/2 and \( -1/2 \) respectively.

We further describe proof for pairwise classification. Under the assumption of \( a = 0 \), the following formulation holds.

\[ \sum_{y \in \tilde{Y}} \tilde{\mathcal{L}}_{PC}(f(x), y) = \sum_{y \in \tilde{Y}} \sum_{y' \notin \tilde{Y}} \tilde{\ell}(g_y(x) - g_{y'}(x)) \]

Thus,

\[
\|\mathcal{L}_{PC}\|_\infty = \sup_{g_1, \ldots, g_K \in G} \left( \sum_{y' \in \tilde{Y}} \tilde{\mathcal{L}}_{PC}(f(x), y') - \sum_{y \in \tilde{Y}} \tilde{\mathcal{L}}_{PC}(f(x), y) \right) \\
= \sup_{g_1, \ldots, g_K \in G} \left( \sum_{y \in \tilde{Y}} \sum_{y' \notin \tilde{Y}} \tilde{\ell}(g_y(x) - g_{y'}(x)) - \inf_{g_1, \ldots, g_K \in G} \sum_{y' \in \tilde{Y}'} \sum_{y \notin \tilde{Y}} \tilde{\ell}(g_{y'}(x) - g_y(x)) \right) \\
\leq \frac{\tilde{N}(K-\tilde{N})}{2} - \frac{\tilde{N}(K-\tilde{N})}{2} \\
= \tilde{N}(K-\tilde{N})
\]
D. Proof of Lemma 2

We describe proof for one-versus-all classification. Under the assumption that \( h \in \mathcal{H}_{OVA} \) is equivalent to \( \mathcal{L}_{OVA} \), the following formulation holds due to the definition of \( \mathcal{H}_{OVA} \).

\[
\mathcal{R}_n (\mathcal{H}_{OVA}) = E_S E_\sigma \left[ \sup_{h \in \mathcal{H}_{OVA}} \frac{1}{n} \sum_{i=1}^{n} \sigma_i h(x_i, Y_i) \right]
\]

\[
= E_S E_\sigma \left[ \sup_{g_1, \cdots, g_K \in G} \frac{1}{n} \sum_{i=1}^{n} \sigma_i \sum_{y \in \bar{Y}_i} \bar{\ell}_{OVA} (f(x_i), y) \right]
\]

\[
= E_S E_\sigma \left[ \sup_{g_1, \cdots, g_K \in G} \frac{1}{n} \sum_{i=1}^{n} \sigma_i \sum_{y \in \bar{Y}_i} \left( \frac{K}{K-1} \bar{\ell} (g_y(x_i)) + \frac{1}{K-1} \sum_{y' \in Y} \bar{\ell} (-g_{y'}(x_i)) \right) \right]
\]

\[
\leq \frac{K}{K-1} E_S E_\sigma \left[ \sup_{g_1, \cdots, g_K \in G} \frac{1}{n} \sum_{i=1}^{n} \sigma_i \sum_{y \in \bar{Y}_i} \bar{\ell} (g_y(x_i)) \right]
\]

\[
+ \frac{1}{K-1} E_S E_\sigma \left[ \sup_{g_1, \cdots, g_K \in G} \frac{1}{n} \sum_{i=1}^{n} \sigma_i \sum_{y \in \bar{Y}_i} \sum_{y' \in Y} \bar{\ell} (-g_{y'}(x_i)) \right]
\]

Let \( I(y \in \bar{Y}_i) \) be an indicator function and define \( \alpha_i := 2I(y \in \bar{Y}_i) - 1 \), then for the first term,

\[
E_S E_\sigma \left[ \sup_{g_1, \cdots, g_K \in G} \frac{1}{n} \sum_{i=1}^{n} \sigma_i \sum_{y \in \bar{Y}_i} \bar{\ell} (g_y(x_i)) \right]
\]

\[
= E_S E_\sigma \left[ \sup_{g_1, \cdots, g_K \in G} \frac{1}{n} \sum_{i=1}^{n} \sigma_i \sum_{y \in \bar{Y}_i} \bar{\ell} (g_y(x_i)) I(y \in \bar{Y}_i) \right]
\]

\[
= E_S E_\sigma \left[ \sup_{g_1, \cdots, g_K \in G} \frac{1}{2n} \sum_{i=1}^{n} \sigma_i \sum_{y \in Y} \bar{\ell} (g_y(x_i)) (\alpha_i + 1) \right]
\]

\[
\leq \sum_{y \in Y} \left\{ E_S E_\sigma \left[ \sup_{g_1, \cdots, g_K \in G} \frac{1}{2n} \sum_{i=1}^{n} \sigma_i \sum_{y \in Y} \bar{\ell} (g_y(x_i)) \right] + E_S E_\sigma \left[ \sup_{g_1, \cdots, g_K \in G} \frac{1}{2n} \sum_{i=1}^{n} \sigma_i \sum_{y \in Y} \bar{\ell} (g_y(x_i)) \right] \right\}
\]

\[
= K E_S E_\sigma \left[ \sup_{g \in \mathcal{G}} \frac{1}{n} \sum_{i=1}^{n} \sigma_i \sum_{y \in Y} \bar{\ell} (g(x_i)) \right]
\]

\[
= K \mathcal{R}_n (\bar{\ell} \circ \mathcal{G})
\]

The second equality from the last holds because \( \sigma_i \) and \( \alpha_i \sigma_i \) are drawn from the same probabilistic distribution. For the second term,

\[
E_S E_\sigma \left[ \sup_{g_1, \cdots, g_K \in G} \frac{1}{n} \sum_{i=1}^{n} \sigma_i \sum_{y \in \bar{Y}_i} \sum_{y' \in Y} \bar{\ell} (-g_{y'}(x_i)) \right] \leq \sum_{y \in Y} \left\{ E_S E_\sigma \left[ \sup_{g \in \mathcal{G}} \frac{1}{n} \sum_{i=1}^{n} \sigma_i \bar{\ell} (-g_{y}(x_i)) \right] \right\}
\]

\[
= K \bar{\mathcal{N}} E_S E_\sigma \left[ \sup_{g \in \mathcal{G}} \frac{1}{n} \sum_{i=1}^{n} \sigma_i \bar{\ell} (-g(x_i)) \right]
\]
Thus,

\[ \mathcal{R}_n^2 (\mathcal{H}) \leq \frac{K^2 + K N}{K - 1} \mathcal{R}_n \left( \ell \circ \mathcal{G} \right) \]

The second inequality holds due to \( \mathcal{R}_n \left( \ell \circ \mathcal{G} \right) \leq L_\ell \mathcal{R}_n (\mathcal{G}) \) according to Talagrand’s contraction lemma (Ledoux & Talagrand, 2013).

We further describe proof for pairwise classification. Under the assumption that \( h \) and \( L_{PC} \) are equivalent,

\[
\mathcal{R}_n (\mathcal{H}_{PC}) = \mathbb{E}_{\mathcal{S}} \mathbb{E}_\sigma \left[ \sup_{h \in \mathcal{H}_{PC}} \frac{1}{n} \sum_{i=1}^{n} \sigma_i h (x_i, Y_i) \right] \\
= \mathbb{E}_{\mathcal{S}} \mathbb{E}_\sigma \left[ \sup_{g_1, \ldots, g_K \in \mathcal{G}} \frac{1}{n} \sum_{i=1}^{n} \sigma_i \sum_{y \in Y_i} \ell (g_y (x_i) - g_{y'} (x_i)) \right] \\
= \mathbb{E}_{\mathcal{S}} \mathbb{E}_\sigma \left[ \sup_{g_1, \ldots, g_K \in \mathcal{G}} \frac{1}{n} \sum_{i=1}^{n} \sigma_i \sum_{y \in Y_i, y' \neq y} \ell (g_y (x_i) - g_{y'} (x_i)) I (y \in \bar{Y}_i) \right] \\
\leq \sum_{y \in Y, y' \neq y} \mathbb{E}_{\mathcal{S}} \mathbb{E}_\sigma \left[ \sup_{g_1, \ldots, g_K \in \mathcal{G}} \frac{1}{2n} \sum_{i=1}^{n} \sigma_i \ell (g_y (x_i) - g_{y'} (x_i)) (\alpha_i + 1) \right] \\
\leq \sum_{y \in Y, y' \neq y} \sum_{g_y, g_{y'} \in \mathcal{G}} \mathbb{E}_{\mathcal{S}} \mathbb{E}_\sigma \left[ \frac{1}{n} \sum_{i=1}^{n} \sigma_i \ell (g_y (x_i) - g_{y'} (x_i)) \right]

Let we define \( \mathcal{G}_{g_y, g_{y'}} := \{ x \mapsto g_y (x) - g_{y'} (x) | g_y, g_{y'} \in \mathcal{G} \} \), then:

\[
\mathbb{E}_{\mathcal{S}} \mathbb{E}_\sigma \left[ \sup_{g_y, g_{y'} \in \mathcal{G}} \frac{1}{n} \sum_{i=1}^{n} \sigma_i \ell (g_y (x_i) - g_{y'} (x_i)) \right] = \mathcal{R}_n \left( \ell \circ \mathcal{G}_{g_y, g_{y'}} \right) \\
\leq L_\ell \mathcal{R}_n (\mathcal{G}_{g_y, g_{y'}}) \\
= L_\ell \mathbb{E}_{\mathcal{S}} \mathbb{E}_\sigma \left[ \sup_{g_y, g_{y'} \in \mathcal{G}} \frac{1}{n} \sum_{i=1}^{n} \sigma_i (g_y (x_i) - g_{y'} (x_i)) \right] \\
\leq L_\ell \mathbb{E}_{\mathcal{S}} \mathbb{E}_\sigma \left[ \sup_{g_y \in \mathcal{G}} \frac{1}{n} \sum_{i=1}^{n} \sigma_i g_y (x_i) \right] + L_\ell \mathbb{E}_{\mathcal{S}} \mathbb{E}_\sigma \left[ \sup_{g_{y'} \in \mathcal{G}} \frac{1}{n} \sum_{i=1}^{n} (-\sigma_i) g_{y'} (x_i) \right] \\
= 2L_\ell \mathcal{R}_n (\mathcal{G})
\]

The third equality holds because \( \sigma_i \) and \(-\sigma_i\) are drawn from the same probabilistic distribution. Then,

\[
\mathcal{R}_n (\mathcal{H}_{PC}) \leq 2K (K - 1) L_\ell \mathcal{R}_n (\mathcal{G})
\]
E. Proof of Theorem 2

We only describe proof for one-versus-all classification; proof for pairwise classification is similar. We substitute the jth data \((x_j, Y_j)\) in \(S\) with any data \((x'_j, Y'_j)\), and define the data set as \(S'\). Let a set of empirical discrimination functions and empirical risk for \(S'\) be \(G' := \{g'\}\) and \(\hat{R}'(f)\) respectively. Then the following formulation holds due to Lemma 1.

\[
\sup_{g_1, \cdots, g_K \in G} \left( \hat{R}(f) - R(f) \right) - \inf_{g_1, \cdots, g_K \in G} \left( \hat{R}'(f) - R(f) \right) \\
\leq \frac{K - 1}{n(K - N)} \sup_{g_1, \cdots, g_K \in G} \inf_{g_1, \cdots, g_K \in G'} \left\{ (\mathcal{L}_{OVA}(f(x_j), Y_j) - \mathcal{L}_{OVA}(f(x'_j), Y'_j)) \right\} \\
\leq \frac{K - 1}{n(K - N)} \|\mathcal{L}_{OVA}\|_{\infty} \\
\leq \frac{K \tilde{N}}{n(K - N)}
\]

According to McDiarmid’s inequality (McDiarmid, 1989), for any integer \(\delta > 0\) the following formulation holds with a probability at least \(1 - \delta/2\).

\[
\sup_{g_1, \cdots, g_K} \left( \hat{R}(f) - R(f) \right) - \mathbb{E} \left[ \sup_{g_1, \cdots, g_K} \left( \hat{R}(f) - R(f) \right) \right] \leq \frac{K \tilde{N}}{2(K - N)} \sqrt{\frac{2 \ln(2/\delta)}{n}}
\]

Let \(S' := \{(x_i', Y_i')\}_{i=1}^n\) be any dataset where each data is drawn from the data-generation probability model \(P_N(x, Y)\). Due to \(R(f) = \mathbb{E} \left[ \hat{R}(f) \right]\),

\[
\mathbb{E} \left[ \sup_{g_1, \cdots, g_K} \left( \hat{R}(f) - R(f) \right) \right] = \frac{K - 1}{K - N} \mathbb{E}_S \left[ \sup_{g_1, \cdots, g_K \in G} \left( \frac{1}{n} \sum_{i=1}^n \mathcal{L}_{OVA}(f(x_i), Y_i) - \mathbb{E}_{S'} \left[ \frac{1}{n} \sum_{i=1}^n \mathcal{L}_{OVA}(f(x'_i), Y'_i) \right] \right) \right] \\
\leq \frac{K - 1}{K - N} \mathbb{E}_S \mathbb{E}_{S'} \left[ \sup_{g_1, \cdots, g_K \in G} \left( \frac{1}{n} \sum_{i=1}^n \mathcal{L}_{OVA}(f(x_i), Y_i) - \frac{1}{n} \sum_{i=1}^n \mathcal{L}_{OVA}(f(x'_i), Y'_i) \right) \right] \\
= \frac{K - 1}{K - N} \mathbb{E}_S \mathbb{E}_{S'} \left[ \sup_{g_1, \cdots, g_K \in G} \left( \frac{1}{n} \sum_{i=1}^n \mathcal{L}_{OVA}(f(x_i), Y_i) + \frac{1}{n} \sum_{i=1}^n (-\sigma_i) \mathcal{L}_{OVA}(f(x'_i), Y'_i) \right) \right] \\
\leq \frac{2(K - 1)}{K - N} \mathbb{E}_S \mathbb{E}_{\sigma} \left[ \sup_{g_1, \cdots, g_K \in G} \frac{1}{n} \sum_{i=1}^n \sigma_i \mathcal{L}_{OVA}(f(x_i), Y_i) \right] \\
= \frac{2(K - 1)}{K - N} \mathbb{E}_{\sigma} \left( H_{OVA} \right) \\
\leq \frac{2K(K + \tilde{N})}{K - N} L_{\mathcal{L}} \mathcal{R}_n(G)
\]

The second equality holds because \(\mathcal{L}(f(x_i, Y_i))\) and \(\sigma_i \mathcal{L}(f(x_i, Y_i))\) are drawn from the same probabilistic distribution; similar for \(\mathcal{L}(f(x'_i, Y'_i))\). The last inequality holds due to Lemma 2. \(\hat{R}(f) \leq \hat{R}(f^*)\) holds according to (19), thus,

\[
\mathcal{E}_N = \left( \hat{R}(f) - \hat{R}(f^*) \right) + \left( R(f) - \hat{R}(f) \right) + \left( \hat{R}(f^*) - R(f^*) \right) \\
\leq 2 \sup_{g_1, \cdots, g_K \in G} \left| \hat{R}(f) - R(f) \right| \\
\leq \frac{4K(K + \tilde{N})}{K - N} L_{\mathcal{L}} \mathcal{R}_n(G) + \frac{K \tilde{N}}{K - N} \sqrt{\frac{2 \ln(2/\delta)}{n}}
\]

\(\square\)