
Learning from Aggregate Observations

Yivan Zhang

The University of Tokyo / RIKEN
yivanzhang@ms.k.u-tokyo.ac.jp

Nontawat Charoenphakdee

The University of Tokyo / RIKEN
nontawat@ms.k.u-tokyo.ac.jp

Zhenguo Wu

The University of Tokyo
zhenguo@ms.k.u-tokyo.ac.jp

Masashi Sugiyama

RIKEN / The University of Tokyo
sugi@k.u-tokyo.ac.jp

Abstract

We study the problem of *learning from aggregate observations* where supervision signals are given to *sets* of instances instead of individual instances, while the goal is still to predict labels of unseen individuals. A well-known example is multiple instance learning (MIL). In this paper, we extend MIL beyond binary classification to other problems such as multiclass classification and regression. We present a general probabilistic framework that accommodates a variety of aggregate observations, e.g., pairwise similarity/triplet comparison for classification and mean/difference/rank observation for regression. Simple maximum likelihood solutions can be applied to various differentiable models such as deep neural networks and gradient boosting machines. Moreover, we develop the concept of consistency up to an equivalence relation to characterize our estimator and show that it has nice convergence properties under mild assumptions. Experiments on three problem settings — *classification via triplet comparison* and *regression via mean/rank observation* indicate the effectiveness of the proposed method.

1 Introduction

Modern machine learning techniques usually require a large number of high-quality labels for *individual* instances [26]. However, in the real world, it could be prohibited to obtain individual information while we can still obtain some forms of supervision for *sets* of instances. We give three following motivating use cases. The first scenario is when individual information cannot be released to the public due to *privacy concerns* [24]. One way to avoid releasing individual information is to only disclose some summary statistics of small groups to the public so that individual information can be protected. The second scenario is when individual annotations are *intrinsically unavailable* but group annotations are provided, which arises in a problem such as drug activity prediction problem [16]. The third scenario is when the labeling cost for an individual instance is *expensive* [65].

In classification, one of the most well-known examples of learning from aggregate observations is *multiple instance learning* (MIL) [64] for binary classification, where training instances are arranged in sets and the aggregate information is whether the positive instances exist in a set. MIL has found applications in many areas [61, 11], including aforementioned drug activity prediction [16].

Learning from label proportions (LLP) [30, 44, 62, 40] is another well-studied example where the proportion of positive instances in each set is observed. However, most earlier studies as well as recent work in MIL and LLP only focus on binary classification and the type of aggregation is limited. Recently, *classification from comparison* has gained more attention. Bao et al. [4] considered *learning from pairwise similarities*, where one can obtain a binary value indicating whether two instances belong to the same category or not. Cui et al. [14] considered *learning from triplets com-*

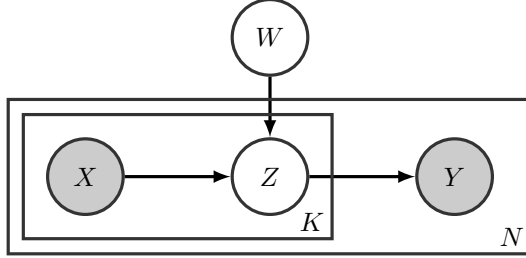


Figure 1: **Graphical representation of the data generating process.** X represents the *feature vector* and Z represents the unobservable *true target* for each X . An *aggregate observation* Y can be observed from a set of Z , $Z_{1:K}$, via an *aggregate function* $T : \mathcal{Z}^K \mapsto \mathcal{Y}$, where $K \geq 2$ is the cardinality of the set. Z follows a parametric distribution $p(Z|\theta)$ parameterized by $\theta = f(X; W)$, which is the output of a deterministic function f , parameterized by W . The goal is to estimate W from $(X_{1:K}, Y)$ -pairs to predict the true target Z from a single feature vector X .

parison. Nevertheless, both works [4, 14] are only applicable to binary classification. For multiclass classification from aggregate observations, we are only aware of a recent work by Hsu et al. [25], where pairwise similarities are used to train a multiclass classifier based on maximum likelihood estimation, although its theoretical understanding is limited.

In regression, learning from aggregate observations has been assessed to only a limited extent. One example is *multiple instance regression* [45, 1], where it is assumed that there is only one instance in each set, called the “primary instance”, that is responsible for the real-valued label. Another example is *learning from spatially aggregated data*, where only spatially summed or averaged values can be observed. Gaussian processes (GP) were proposed to handle this problem [33, 52, 53]. Although uncertainty information can be nicely obtained with a GP-based method, it may not be straightforward to scale it for high-dimensional data.

In general, the concept of drawing conclusions or making predictions about individual-level behavior based on aggregate-level data was also of great interest in other fields, such as ecological inference [47, 28, 49, 19] and preference learning [54, 8, 38, 43], which is also used in psychometrics and econometrics.

The goal of this paper is to provide a versatile framework that can be applied for many types of aggregate observations, both in multiclass classification and regression. We propose a simple yet effective solution to this class of problems based on maximum likelihood estimation, where Hsu et al. [25]’s method is one of our special cases. Note that the maximum likelihood method has been explored for weak supervisions such as classification from noisy labels and coarse-grained labels [41, 63], but only Hsu et al. [25] considered aggregate observations.

Our contributions can be summarized as follows. Firstly, we expand the usage of maximum likelihood to aggregate observations, e.g., classification from triplet comparison and regression from mean/rank observation. Next, we provide a theoretical foundation of this problem by introducing the concept of *consistency up to an equivalence relation* to analyze the characteristics of our estimator. We demonstrate that this concept is highly useful by analyzing the behavior of our estimator and obtain insightful results, e.g., regression from mean observation is consistent but regression from rank observation is only consistent *up to an additive constant*. Finally, experimental results are also provided to validate the effectiveness of our method.

2 Problem setting

In this section, we clarify the notation and assumptions and introduce a probabilistic model for aggregate observations.

Table 1: Examples of Learning from Aggregate Observations

Task	Learning from ...	Aggregate Observation $Y = T(Z_{1:K})$
Classification $Z \in \{1, \dots, C\}$	similarity/dissimilarity ($K = 2$)	if Z_1 and Z_2 are the same or not
	triplet comparison ($K = 3$)	if $d(Z_1, Z_2)$ is smaller than $d(Z_1, Z_3)$, where $d(\cdot, \cdot)$ is a similarity measure between classes
	multiple instance ($K \geq 2$)	if $Z_{1:K}$ contains positive instances ($C = 2$)
Regression $Z \in \mathbb{R}$	mean/sum ($K \geq 2$)	the arithmetic mean or the sum of $Z_{1:K}$
	difference/rank ($K = 2$)	the difference $Z_1 - Z_2$, or the relative order $Z_1 > Z_2$
	min/max ($K \geq 2$)	the smallest/largest value in $Z_{1:K}$
	uncoupled data ($K \geq 2$)	randomly permuted $Z_{1:K}$

2.1 Notation¹

Let $X \in \mathcal{X}$ be the *feature vector*, and $Z \in \mathcal{Z}$ be the unobservable *true target* that we want to predict, where \mathcal{X} and \mathcal{Z} are their support spaces, respectively. The goal is to learn a discriminative model that predicts the true target Z from the feature vector X . We do not have any restrictions on \mathcal{Z} as long as we can model the conditional probability $p(Z|X)$. If \mathcal{Z} is a finite set, e.g., $\{1, \dots, C\}$, the task is C -class classification; and if \mathcal{Z} is \mathbb{R} , the task is regression. However, in the problem setting of learning from aggregate observations, we cannot observe the true target Z directly. Instead, we assume that we can observe some information about *multiple instances*.

Concretely, the supervision signal $Y \in \mathcal{Y}$, called *aggregate observation*, for the set $Z_{1:K}$, can be obtained from $Z_{1:K}$ via an *aggregate function* $T : \mathcal{Z}^K \mapsto \mathcal{Y}$, i.e., $Y = T(Z_{1:K})$. We want to use observations of $(X_{1:K}, Y)$ to predict the true target Z based on features X . Figure 1 illustrates the graphical representation of the data generating process.

2.2 Assumptions

Here, we summarize our assumptions used in learning from aggregate observations as follows.

Assumption 1 (Aggregate observation assumption). $p(Y|X_{1:K}, Z_{1:K}) = p(Y|Z_{1:K})$.

This means that Y and $X_{1:K}$ are conditionally independent given $Z_{1:K}$. This assumption is common in existing studies [11, 25, 60, 14]. It can be implied in the data collection process, e.g., when we first collect (X, Z) -pairs but only disclose some summary statistics of $Z_{1:K}$ for learning due to privacy concerns. It also means that we expect the true target Z to carry enough information about X , so that we do not need to extract more information from $X_{1:K}$ to predict Y .

Further, since we assumed that Y can be determined by $Y = T(Z_{1:K})$, the conditional probability becomes $p(Y|Z_{1:K}) = \delta_{T(Z_{1:K})}(Y)$, where $\delta(\cdot)$ denotes the *Dirac delta function*.

Assumption 2 (Independent observations assumption). $p(Z_{1:K}|X_{1:K}) = \prod_{i=1}^K p(Z_i|X_i)$.

This means that elements in $Z_{1:K}$ are mutually independent. It might be violated if we collect the data group by group, so that instances in a group tend to be similar and have high correlation [11]. In such a case, our formulation and proposed method only serve as a practical approximation and our theoretical implications may not hold. Note that if the independence condition does not hold, aggregate observations could be more informative in some scenarios. For example, spatially aggregated data are aggregated within a specific region rather than randomly collected from many different regions [33]. Thus, one may be able to utilize the dependency in $Z_{1:K}$ to obtain a better estimation of $p(Z_{1:K}|X_{1:K})$.

Combining these two assumptions, we can decompose the joint distribution $p(X_{1:K}, Z_{1:K}, Y)$ as

$$p(X_{1:K}, Z_{1:K}, Y) = p(Y|Z_{1:K}) \prod_{i=1}^K p(Z_i|X_i)p(X_i). \quad (1)$$

¹In this work, we denote uppercase letters X, Y, Z as random variables, lowercase letters x, y, z as instances of random variables, and calligraphic letters $\mathcal{X}, \mathcal{Y}, \mathcal{Z}$ as their support spaces. The subscript such as $Z_{1:K}$ is an abbreviation for the set $\{Z_1, Z_2, \dots, Z_K\}$. The superscript such as $y^{(i)}$ denotes the i -th sample point in a dataset. With abuse of notation, $p(\cdot)$ denotes a distribution and also its probability mass/density function.

2.3 Aggregate function

The aggregate function $T : \mathcal{Z}^K \mapsto \mathcal{Y}$ characterizes different problems within our framework. It induces an *equivalence relation* \sim over the set \mathcal{Z}^K as $z_{1:K}^{(i)} \sim z_{1:K}^{(j)} \iff T(z_{1:K}^{(i)}) = T(z_{1:K}^{(j)})$. The coarseness of \sim influences how hard the problem is. Since \sim is usually much coarser than the equality equivalence relation on \mathcal{Z}^K , the model is not able to distinguish some observationally equivalent $Z_{1:K}$. However, we can analyze this equivalence relation \sim and obtain the characteristics of the solution. In some problems, we are able to recover the conditional distribution $p(Z|X)$, or at least up to some transformation. We show this fact theoretically in Section 4 and experimentally in Section 6. In Table 1, we provide examples of problems that can be accommodated in our framework of learning from aggregate observations, which are categorized by underlying tasks and their aggregate functions.

3 Proposed method

In this section, we describe the proposed method for learning from aggregate observations.

The key idea is to estimate $p(Y|X_{1:K})$ based on $p(Z|X)$ using the aggregate function g . Based on the decomposition of the joint distribution in Equation (1), we can marginalize $p(Y, Z_{1:K}|X_{1:K}) = p(Y|Z_{1:K}) \prod_{i=1}^K p(Z_i|X_i)$ over $Z_{1:K}$ as

$$p(Y|X_{1:K}) = \int_{\mathcal{Z}^K} \delta_{T(z_{1:K})}(Y) \prod_{i=1}^K p(z_i|X_i) dz_{1:K} = \mathbb{E}_{\substack{Z_i \sim p(Z_i|X_i) \\ i=1, \dots, K}} [\delta_{T(Z_{1:K})}(Y)], \quad (2)$$

where $\mathbb{E}[\cdot]$ denotes the expectation.

To model the true target Z , we assume that Z conditioned on X follows a certain parametric distribution, parameterized by $\theta \in \Theta$, i.e., $p(Z_i|X_i) = p(Z_i|\theta = f(X_i; W))$. Here, $f : \mathcal{X} \rightarrow \Theta$ is a deterministic function parameterized by $W \in \mathcal{W}$, which maps the feature vector X to the corresponding parameter θ . Note that we do not restrict the family of f . It can be a deep neural network [35] or a gradient boosting machine [20], as long as the likelihood $p(Z|X)$ is differentiable w.r.t. the model parameter W .

Then, we use the likelihood to measure how likely our model with parameter W can generate observed data. Our learning objective, the *expected log-likelihood*, is defined as

$$\ell(W) = \mathbb{E}[\log p(Y|X_{1:K}; W)]. \quad (3)$$

Approximating $\ell(W)$ based on i.i.d. samples of $(X_{1:K}, Y)$ -pair of size N , $\{x_{1:K}^{(i)}, y^{(i)}\}_{i=1}^N \stackrel{\text{i.i.d.}}{\sim} p(X_{1:K}, Y)$, the *log-likelihood* is defined as

$$\ell_N(W) = \frac{1}{N} \sum_{i=1}^N \log p(y^{(i)}|x_{1:K}^{(i)}; W), \quad (4)$$

which converges to $\ell(W)$ almost surely as $N \rightarrow \infty$ [55]. Then, the *maximum likelihood estimator* (MLE) of W given aggregate observations is defined as $\widehat{W}_N = \arg \max_W \ell_N(W)$.

Although MLE exists for all kinds of aggregate observations in theory, the likelihood can be hard to calculate because of the integral involved in Equation (2). In Section 5, we give three examples where we can obtain an analytical expression of the log-likelihood so that we do not need to resort to numerical integration or approximation methods to optimize the learning objective.

4 Consistency of learning from aggregate observations

In this section, we develop theoretical tools and show that although the estimator may not always converge to the true parameter, it can still capture some important information about the true parameter. In Section 5, we show that our theoretical analysis can elucidate the fact that our estimators can have different types of consistency depending on the given aggregate observations.

Assume that the parameter W is in a metric space (\mathcal{W}, d) with a metric d . Denote the true parameter by W_0 . An estimator \widehat{W}_N based on N sample points is said to be *consistent* if $\widehat{W}_N \xrightarrow{P} W_0$ as $N \rightarrow \infty$, where \xrightarrow{P} means convergence in probability.

The MLE is consistent under mild conditions [55], but the *identifiability* of the model is always necessary. However, in learning from aggregate observations, it is more common that we can only *partially* identify the model. i.e., two parameter W and W' might be *observationally equivalent* and yield the same likelihood, which is defined as follows:

Definition 3 (Equivalence). An *equivalence relation* \sim on \mathcal{W} induced by the likelihood is defined according to $W \sim W' \iff \ell(W) = \ell(W')$. The equivalence class of W is denoted by $[W]$.

Then, *consistency up to an equivalence relation* is defined as follows:

Definition 4 (Consistency up to \sim). An estimator \widehat{W}_N is said to be *consistent up to an equivalence relation* \sim , if $d(\widehat{W}_N, [W_0]) \xrightarrow{P} 0$ as $N \rightarrow \infty$, where $d(W, [W_0]) = \inf_{W'_0 \in [W_0]} d(W, W'_0)$.

That is to say, an estimator converges in probability to a set of values that is at least observationally equivalent to the true parameter. Then, following Wald [57] and Van der Vaart [55], we can confirm that the MLE given aggregate observations has the desired behavior under mild assumptions:

Proposition 5. The MLE \widehat{W}_N based on Equation (4) is consistent up to \sim if the following conditions hold:

- (A) The parameter space \mathcal{W} is compact;
- (B) $\forall W \in \mathcal{W}$, the log-likelihood $\ell(W|x_{1:K}, y) = \log p(x_{1:K}, y; W)$ is upper-semicontinuous for almost all $(x_{1:K}, y)$;
- (C) \forall sufficiently small ball $U \subset \mathcal{W}$, the function $\ell^U(W|x_{1:K}, y) = \sup_{W \in U} \ell(W|x_{1:K}, y)$ is measurable and satisfies $\mathbb{E}[\ell^U(W|X_{1:K}, Y)] < \infty$;
- (D) $\exists W'_0 \in [W_0]$ s.t. $\ell_N(\widehat{W}_N) \geq \ell_N(W'_0) - \delta_N$, where δ_N is a sequence of random variables such that $\delta_N \xrightarrow{P} 0$.

Definitions 3, 4 and Proposition 5 provide a foundation to analyze the behavior of an MLE for learning from aggregate observations. The key difference between an analysis of the traditional MLE and ours is that due to limited supervision, the concept of *consistency* can be too strict. Although an MLE is not consistent for some aggregate observation (see Sections 5.2 and 5.4), we can show that an MLE is still useful by using the concept of *consistency up to an equivalence relation*.

5 Realizations of learning from aggregate observations

In this section, we illustrate three novel realizations of the proposed maximum likelihood approach to learning from aggregate observations where the integral in Equation (2) can be solved analytically. Furthermore, we demonstrate how to use the theoretical tools we developed in Section 4 to provide a better understanding of the behavior of the estimator given different kinds of aggregate observations.

Here, we will drop $\theta = f(X; W)$ from expressions to keep the notation uncluttered. Any parameter of the distribution of Z is either determined from X in this way or just kept fixed. We defer the proofs of propositions in this section to Appendix A.

5.1 Classification via pairwise similarity

In classification, the true target is categorical: $Z \in \{1, \dots, C\}$, where C is the number of classes. We model it using a *categorical distribution* $Z \sim \text{Categorical}(p_{1:C})$, with probability parameters $p_i > 0$, $\sum_{i=1}^C p_i = 1$. Because $|\mathcal{Z}^K| = C^K$ is always finite, the integration in Equation (2) becomes a summation and the log-likelihood is always analytically calculable.

Pairwise similarity is our first example of learning from aggregate observations. In this problem, we only know if a pair of instances belongs to the same class or not. Here $K = 2$. Concretely,

$$Y = T_{\text{sim}}(Z_1, Z_2) = [Z_1 = Z_2], \quad p(Y = 1) = \sum_{i=1}^C p(Z_1 = i)p(Z_2 = i), \quad (5)$$

where $[\cdot]$ denotes the Iverson bracket.² This problem is also considered to be *semi-supervised clustering* in the literature [59, 5, 6, 15]. Recently, Hsu et al. [25] studied this problem thoroughly for several image classification tasks from the perspective of classification, whose method is also based on the maximum likelihood and thus a special case within our framework.

5.2 Classification via triplet comparison

Triplet comparison is of the form “ A (*anchor*) is more similar to P (*positive*) than N (*negative*).” Assuming that $d : \mathcal{Z} \times \mathcal{Z} \mapsto \mathbb{R}$ is a similarity measure between classes, we can instantiate the aggregation function g and Equation (2) for $K = 3$:

$$Y = T_{\text{tri}}(Z_1, Z_2, Z_3) = [d(Z_1, Z_2) < d(Z_1, Z_3)],$$

$$p(Y = 1) = \sum_{\substack{d(i,j) < d(i,k) \\ i,j,k \in \{1, \dots, C\}}} p(Z_1 = i)p(Z_2 = j)p(Z_3 = k), \quad (6)$$

where $[\cdot]$ denotes the Iverson bracket.

Based on Equation (4), the loss function for triplet comparison is in the form of binary cross entropy:

$$\begin{aligned} \ell_N^{\text{tri}}(W) = & -\frac{1}{N} \sum_{i=1}^N [y^{(i)} = 1] \log p(y^{(i)} = 1 | x_{1:K}^{(i)}; W) \\ & -\frac{1}{N} \sum_{i=1}^N [y^{(i)} = 0] \log p(y^{(i)} = 0 | x_{1:K}^{(i)}; W). \end{aligned} \quad (7)$$

Although triplet comparison data has been used for *metric learning* and *representation learning* [50, 46, 39, 48, 32, 51, 3], studies on classification based on solely triplet comparison remain limited. Cui et al. [14] recently showed that it is possible to learn a binary classifier from triplet comparison directly. But so far no result has been given for the multiclass setting, to the best of our knowledge. Existing work either requires labeled data [42] or needs to actively inquire comparison labels from an oracle [23].

Since the parameters of the model given only the pairwise similarity or the triplet comparison are not identifiable, the corresponding MLE cannot be consistent. But that does not mean the learned model does not capture any information. Based on our framework, we prove the following proposition, which suggests that a multiclass classifier is still learnable at most up to a permutation of classes.

Proposition 6 (Classification via triplet comparison is at most consistent up to a permutation). *Let $f(X; W)$ be a C -dimensional vector of probability parameters $p_{1:C}$ for classification, then*

$$\{W \in \mathcal{W} : \exists \text{ permutation matrix } P, \text{ s.t. } Pf(X; W) = f(X; W_0) \text{ a.e.}\} \subseteq [W_0]. \quad (8)$$

Proposition 6 states that the estimator can be consistent up to a permutation, but *not always*. Please refer to Appendix A for more discussion. The same result holds for the pairwise similarity case, which was investigated empirically by Hsu et al. [25]. In Section 6.1, we show that the proposed method works well empirically when the true labels are not too ambiguous.

5.3 Regression via mean observation

In regression problems, the true target is a real value $Z \in \mathbb{R}$. The *mean squared error* (MSE) is the canonical choice for the loss function, which can be derived from the maximum likelihood under an *additive homoscedastic Gaussian noise* model [7]. Thus, we also use a Gaussian distribution for the true target, $Z \sim \mathcal{N}(\mu, \sigma^2)$ with mean $\mu \in \mathbb{R}$ and standard deviation $\sigma \in (0, \infty)$.

Gaussian distributions have desired properties, including *stability* and *decomposability*. Therefore Gaussian distribution is closed under linear combination given independence (See Appendix B). We can model several aggregate observations, e.g., the mean observation and the rank observation, and obtain an analytical expression of the log-likelihood, as discussed below.

²Iverson bracket $[\cdot]$: for any logic expression P , $[P] = 1$ if P is true, otherwise 0.

Mean observation is the arithmetic mean of the set of true targets $Z_{1:K}$. Under the normal distribution assumption, the mean Y is also a Gaussian random variable:

$$Y = T_{\text{mean}}(Z_{1:K}) = \frac{1}{K} \sum_{i=1}^K Z_i, \quad Y \sim \mathcal{N}\left(\frac{1}{K} \sum_{i=1}^K \mu_i, \frac{1}{K^2} \sum_{i=1}^K \sigma_i^2\right). \quad (9)$$

Assuming homoscedastic noise, $Z_i = f(X_i; W) + \varepsilon_i$ for $i = 1, \dots, K$, where $\varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2)$, the loss function realized from Equation (4) becomes

$$\ell_N^{\text{mean}}(W) = \frac{1}{N} \sum_{i=1}^N \left(y^{(i)} - \frac{1}{K} \sum_{j=1}^K f(x_j^{(i)}; W) \right)^2. \quad (10)$$

Theoretically, we can obtain the following proposition, which states that our estimator is consistent:

Proposition 7 (Regression via mean observation is consistent). *The MLE \widehat{W}_N based on Equation (4) for mean observations obtained by Equation (9) is consistent, because*

$$[W_0] = \{W \in \mathcal{W} : f(X; W) = f(X; W_0) \text{ a.e.}\}. \quad (11)$$

In Section 6.2, we validate Proposition 7 and demonstrate that it is feasible to learn solely from mean observations using our method and achieve MSE that is comparable to learning from direct observations. In Appendix C, we provide possible use of the Cauchy distribution for robust regression and the Poisson distribution for count data in addition to the Gaussian distribution.

5.4 Regression via rank observation

Rank observation, or called *pairwise comparison* in the context of regression, indicates the relative order between two real values. Since the difference of two Gaussian random variables is still Gaussian distributed, the likelihood of the rank can be derived from the cumulative distribution function of a Gaussian distribution:

$$Y = T_{\text{rank}}(Z_1, Z_2) = [Z_1 > Z_2], \quad p(Z_1 > Z_2) = \frac{1}{2} \left[1 + \text{erf}\left(\frac{\mu_1 - \mu_2}{\sqrt{2(\sigma_1^2 + \sigma_2^2)}}\right) \right], \quad (12)$$

where $\text{erf}(\cdot)$ is the error function. Note that even though $\text{erf}(\cdot)$ is a special function, its value can be approximated and its gradient is analytically calculable.³ Thus the gradient-based optimization is still applicable.

Without loss of generality, we assume $z_1^{(i)} > z_2^{(i)}$ in the dataset. For a fixed variance σ^2 , the loss function derived from Equations (4) and (12) is

$$\ell_N^{\text{rank}}(W) = -\frac{1}{N} \sum_{i=1}^N \log \frac{1}{2} \left[1 + \text{erf}\left(\frac{f(x_1^{(i)}; W) - f(x_2^{(i)}; W)}{2\sigma}\right) \right]. \quad (13)$$

The rank observation has been studied recently in Xu et al. [60] to solve an uncoupled regression problem, where additional information is required. Here, an important question is how good the estimator can be if we only have pairwise comparison. Intuitively, it should not be consistent. However, surprisingly, it can be theoretically showed that it is still possible to learn solely from rank observations, and the prediction and the true target differ only by a constant under mild conditions.

Proposition 8 (Regression via rank observation is consistent up to an additive constant). *Assuming homoscedastic noise, $Z_i = f(X_i; W) + \varepsilon_i$ for $i = 1, \dots, K$, where $\varepsilon_i \stackrel{\text{i.i.d.}}{\sim} \mathcal{N}(0, \sigma^2)$, the MLE \widehat{W}_N based on Equation (4) for rank observations obtained by Equation (12) is consistent up to an additive constant, because*

$$[W_0] = \{W \in \mathcal{W} : \exists C \in \mathbb{R}, f(X; W) - f(X; W_0) = C \text{ a.e.}\}. \quad (14)$$

As a result, we can guarantee that if we know the mean or can obtain a few direct observations, precise prediction becomes possible. In Section 6.2 we validate this finding. In Appendix D, we provide possible use of the Gumbel distribution, Cauchy distribution, and Exponential distribution for regression via rank observation.

³ $\text{erf}(x) = \frac{1}{\sqrt{\pi}} \int_{-x}^x e^{-t^2} dt$, and $\frac{d}{dx} \text{erf}(x) = \frac{2}{\sqrt{\pi}} e^{-x^2}$ [2, p.110].

Table 2: **Classification via pairwise similarity and triplet comparison.** Means and standard deviations of accuracy (after the optimal permutation) in percentage for 10 trials are reported.

Dataset	Unsupervised	Pairwise Similarity			Triplet Comparison			Supervised
		Siamese	Contrastive	Ours/[25]	Tuplet	Triplet	Ours	
MNIST	52.30	85.82	98.45	98.84	18.42	22.77	94.94	99.04
	(1.15)	(24.86)	(0.11)	(0.10)	(1.08)	(9.38)	(3.68)	(0.08)
Fashion-MNIST	50.94	62.86	88.49	90.59	21.98	27.27	81.49	91.97
	(3.28)	(17.97)	(0.28)	(0.26)	(0.72)	(12.82)	(0.94)	(0.24)
Kuzushiji-MNIST	40.22	61.30	89.65	93.45	16.00	20.39	81.94	94.47
	(0.01)	(17.41)	(0.19)	(0.32)	(0.27)	(2.03)	(4.59)	(0.21)

6 Experiments

In this section, we present the empirical results of the proposed method. All experimental details can be found in Appendix E. More extensive experiments on 20 regression datasets and 30 classification datasets are provided in Appendix F. For each type of aggregate observations, outperforming methods are highlighted in boldface using one-sided t-test with a significance level of 5%.

6.1 Classification via triplet comparison

We demonstrate that a multiclass classifier is learnable using only triplet comparison data introduced in Section 5.2. We evaluate our method on three image classification datasets, namely MNIST,⁴ Fashion-MNIST,⁵ and Kuzushiji-MNIST,⁶ which consist of 28×28 grayscale images in 10 classes.

As for the similarity measure d , we followed Cui et al. [14] and simply used $d = [Z_i \neq Z_j]$ as the similarity measure between classes. We also compared learning from pairwise similarity data, which was studied in Hsu et al. [25]. Both pairwise similarity and triplet comparison observations were generated according to our assumptions in Section 2.2. Since both learning from pairwise similarities and triplet comparisons are only consistent *up to a permutation* at best, we followed Hsu et al. [25] and evaluated the performance by modified accuracy that allows any permutation of classes. The optimal permutation is obtained by solving a linear sum assignment problem using a small amount of individually labeled data [31].

Baseline. We used K-means as the unsupervised clustering baseline and the fully supervised learning method as a reference. We also compared representation learning and metric learning methods such as the Siamese network [29] and contrastive loss [22] for pairwise similarity, the (2+1)-tuplet loss [50] and the triplet loss [46] for triplet comparison. Since the output of such methods is a vector representation, we performed K-means to obtain a prediction so that the results can be directly compared.

Results. Table 2 shows that our method outperforms representation learning methods. It demonstrates that if the goal is classification, directly optimizing a classification-oriented loss is better than combining representation learning and clustering. Representation learning from triplet comparison also suffers from a lack of data because a large amount of triplet comparison data could be in the form of “ Z_1 is equally similar/dissimilar to Z_2 and Z_3 ” if either Z_2 and Z_3 belong to the same class or $Z_{1:3}$ belong to three different classes. Such data cannot be used for representation learning but still can provide some information for the classification task.

6.2 Regression via mean/rank observation

We compare the performance in regression via direct/mean/rank observations introduced in Sections 5.3 and 5.4. We present results on benchmark datasets to show the effectiveness of our method.

Baseline. For the mean observation, we used a method treating the mean as the true label for each instance as the baseline. For the rank observation, we used RankNet [9] for regression to compare different distribution hypotheses.

⁴MNIST [34] <http://yann.lecun.com/exdb/mnist/>

⁵Fashion-MNIST [58] <https://github.com/zalandoresearch/fashion-mnist>

⁶Kuzushiji-MNIST [13] <http://codh.rois.ac.jp/kmnist/>

Table 3: **Regression via mean observation and rank observation on UCI benchmark datasets.** Means and standard deviations of error variance (rank observations) or MSE (otherwise) for 10 trials are reported. We compare linear regression (LR) and gradient boosting machines (GBM) as the regression function.

Dataset	Mean Observation				Rank Observation				Supervised	
	Baseline		Ours		RankNet, Gumbel		Ours, Gaussian		LR	GBM
	LR	GBM	LR	GBM	LR	GBM	LR	GBM		
abalone	7.91 (0.4)	7.89 (0.5)	5.27 (0.4)	4.80 (0.3)	5.81 (0.4)	10.66 (0.7)	5.30 (0.3)	5.04 (0.5)	5.00 (0.3)	4.74 (0.4)
airfoil	38.57 (2.0)	28.65 (2.5)	23.59 (1.8)	4.63 (0.9)	37.15 (1.8)	47.46 (3.7)	27.95 (1.1)	6.18 (1.0)	22.59 (1.9)	3.84 (0.5)
auto-mpg	41.59 (5.7)	36.31 (1.9)	14.61 (3.2)	9.53 (2.4)	27.26 (4.0)	65.39 (7.4)	17.34 (2.0)	9.97 (2.0)	11.73 (2.3)	7.91 (1.6)
concrete	198.51 (12.8)	172.35 (15.2)	115.06 (10.1)	31.84 (3.0)	244.06 (17.1)	268.86 (26.5)	233.93 (20.0)	38.11 (5.4)	111.92 (6.4)	24.80 (5.7)
housing	67.40 (20.8)	52.23 (6.0)	27.54 (6.8)	14.85 (3.0)	52.51 (10.8)	93.07 (8.1)	44.40 (13.4)	23.49 (6.9)	29.66 (6.1)	13.12 (3.7)
power-plant	172.64 (7.1)	170.10 (3.4)	20.73 (0.8)	12.82 (0.6)	163.64 (4.8)	294.07 (4.9)	44.82 (6.1)	26.06 (2.5)	21.17 (1.0)	11.84 (0.9)

Real-world dataset. We conducted experiments on 6 UCI benchmark datasets⁷ and compared linear models and gradient boosting machines as the regression function. Mean observations of four instances and rank observations are generated according to our assumptions in Section 2.2. Since learning from rank observations is only consistent up to an additive constant, we measured the performance by modified MSE that allows any constant shift. This metric coincides with the variance of the error. If the estimator is unbiased, it is equal to MSE. Concretely,

$$\min_C \frac{1}{n} \sum_{i=1}^n \left(Z_i - (\hat{Z}_i + C) \right)^2 = \text{Var}[Z - \hat{Z}]. \quad (15)$$

Results. In Table 3 we report error variance for learning from rank observations, otherwise MSE. It shows that learning from mean observations achieved MSE that is comparable to learning from direct observations, while the error variance of learn from rank observations is slightly higher. Further, our method consistently outperforms the baseline for the mean observation and RankNet for regression via rank observation. The performance ranking of learning from direct/mean/rank observations is roughly maintained regardless of the complexity of the model, while the gradient boosting machine usually performs better than the linear model.

7 Conclusions

We presented a framework for *learning from aggregate observations*, where only supervision signals given to sets of instances are available. We proposed a simple yet effective method based on the *maximum likelihood* principle, which can be simply implemented for various differentiable models, including deep neural networks and gradient boosting machines. We also theoretically analyzed the characteristic of our proposed method based on the concept of consistency up to an equivalent relation. Experiments on classification via pairwise similarity/triplet comparison and regression via mean/rank observation suggested the feasibility and the usefulness of our method.

⁷UCI Machine Learning Repository [17] <https://archive.ics.uci.edu>

8 Broader impact

In this work we proposed a general method that learns from supervision signals given to sets of instances. Such studies could provide new tools for privacy preserving machine learning because individual labels are not needed. This leads to a new way to anonymize data and alleviate potential threats to privacy-sensitive information, in addition to well-known differential privacy techniques [18], which inject noise into the data to guarantee the anonymity of individuals. However, such studies may have some negative consequences because depending on the type of aggregate observations, in the worst case, it may be possible to uncover individual information to some extent from aggregated statistics, even if individual labels are not available in the training data. Nevertheless, a person can deny the uncovered label because of a lack of evidence. So learning from aggregate observations is still arguably safer than the fully-supervised counterparts in terms of privacy preservation.

Our framework also opens possibilities of using machine learning technology in new problem domains where true labels cannot be straightforwardly obtained, but information such as pairwise/triplet comparisons or coarse-grained data are available or possible to collect. Finally, we believe that theoretical understanding could provide a better foundation towards solving learning from aggregate observations more effectively in the future.

9 Acknowledgement

We thank Zhenghang Cui, Takuya Shimada, Liyuan Xu, and Zijian Xu for helpful discussion. We also would like to thank the Supercomputing Division, Information Technology Center, The University of Tokyo, for providing the Reedbush supercomputer system. NC was supported by MEXT scholarship, JST AIP Challenge, and Google PhD Fellowship program. MS was supported by JST CREST Grant Number JPMJCR18A2.

References

- [1] Robert A Amar, Daniel R Dooly, Sally A Goldman, and Qi Zhang. Multiple-instance learning of real-valued data. In *Proceedings of the Eighteenth International Conference on Machine Learning*, ICML '01, pages 3–10, San Francisco, CA, USA, 2001. Morgan Kaufmann Publishers Inc. ISBN 1-55860-778-1.
- [2] Larry C Andrews. *Special functions of mathematics for engineers*, volume 49. Spie Press, 1998.
- [3] Mahdiah Soleymani Baghshah and Saeed Bagheri Shouraki. Kernel-based metric learning for semi-supervised clustering. *Neurocomputing*, 73(7-9):1352–1361, 2010.
- [4] Han Bao, Gang Niu, and Masashi Sugiyama. Classification from pairwise similarity and unlabeled data. In Jennifer Dy and Andreas Krause, editors, *Proceedings of the 35th International Conference on Machine Learning*, volume 80 of *Proceedings of Machine Learning Research*, pages 452–461, Stockholmsmässan, Stockholm Sweden, 10–15 Jul 2018. PMLR.
- [5] Sugato Basu, Mikhail Bilenko, and Raymond J Mooney. A probabilistic framework for semi-supervised clustering. In *Proceedings of the tenth ACM SIGKDD international conference on Knowledge discovery and data mining*, pages 59–68. ACM, 2004.
- [6] Mikhail Bilenko, Sugato Basu, and Raymond J Mooney. Integrating constraints and metric learning in semi-supervised clustering. In *Proceedings of the twenty-first international conference on Machine learning*, page 11. ACM, 2004.
- [7] Christopher M Bishop. *Pattern recognition and machine learning*. Springer, 2006.
- [8] Ralph Allan Bradley and Milton E Terry. Rank analysis of incomplete block designs: I. the method of paired comparisons. *Biometrika*, 39(3/4):324–345, 1952.
- [9] Christopher Burges, Tal Shaked, Erin Renshaw, Ari Lazier, Matt Deeds, Nicole Hamilton, and Gregory N Hullender. Learning to rank using gradient descent. In *Proceedings of the 22nd International Conference on Machine learning*, pages 89–96, 2005.

- [10] Zhe Cao, Tao Qin, Tie-Yan Liu, Ming-Feng Tsai, and Hang Li. Learning to rank: from pairwise approach to listwise approach. In *Proceedings of the 24th international conference on Machine learning*, pages 129–136, 2007.
- [11] Marc-André Carbonneau, Veronika Cheplygina, Eric Granger, and Ghyslain Gagnon. Multiple instance learning: A survey of problem characteristics and applications. *Pattern Recognition*, 77:329–353, 2018.
- [12] Chih-Chung Chang and Chih-Jen Lin. LIBSVM: a library for support vector machines. *ACM transactions on intelligent systems and technology (TIST)*, 2(3):27, 2011.
- [13] Tarin Clanuwat, Mikel Bober-Irizar, Asanobu Kitamoto, Alex Lamb, Kazuaki Yamamoto, and David Ha. Deep learning for classical japanese literature, 2018.
- [14] Zhenghang Cui, Nontawat Charoenphakdee, Issei Sato, and Masashi Sugiyama. Classification from triplet comparison data. *Neural Computation*, 32(3):659–681, 2020.
- [15] Jason V Davis, Brian Kulis, Prateek Jain, Suvrit Sra, and Inderjit S Dhillon. Information-theoretic metric learning. In *Proceedings of the 24th international conference on Machine learning*, pages 209–216. ACM, 2007.
- [16] Thomas G Dietterich, Richard H Lathrop, and Tomás Lozano-Pérez. Solving the multiple instance problem with axis-parallel rectangles. *Artificial intelligence*, 89(1-2):31–71, 1997.
- [17] Dheeru Dua and Casey Graff. UCI machine learning repository, 2017. URL <http://archive.ics.uci.edu/ml>.
- [18] Cynthia Dwork, Aaron Roth, et al. The algorithmic foundations of differential privacy. *Foundations and Trends® in Theoretical Computer Science*, 9(3–4):211–407, 2014.
- [19] Seth R Flaxman, Yu-Xiang Wang, and Alexander J Smola. Who supported Obama in 2012? ecological inference through distribution regression. In *Proceedings of the 21th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, pages 289–298, 2015.
- [20] Jerome H Friedman. Greedy function approximation: a gradient boosting machine. *Annals of statistics*, pages 1189–1232, 2001.
- [21] Pedro Antonio Gutierrez, Maria Perez-Ortiz, Javier Sanchez-Monedero, Francisco Fernandez-Navarro, and Cesar Hervás-Martinez. Ordinal regression methods: survey and experimental study. *IEEE Transactions on Knowledge and Data Engineering*, 28(1):127–146, 2015.
- [22] Raia Hadsell, Sumit Chopra, and Yann LeCun. Dimensionality reduction by learning an invariant mapping. In *2006 IEEE Computer Society Conference on Computer Vision and Pattern Recognition (CVPR’06)*, volume 2, pages 1735–1742. IEEE, 2006.
- [23] Siavash Haghiri, Damien Garreau, and Ulrike von Luxburg. Comparison-based random forests. *arXiv preprint arXiv:1806.06616*, 2018.
- [24] Eric Horvitz and Deirdre Mulligan. Data, privacy, and the greater good. *Science*, 349(6245):253–255, 2015.
- [25] Yen-Chang Hsu, Zhaoyang Lv, Joel Schlosser, Phillip Odom, and Zsolt Kira. Multi-class classification without multi-class labels. In *International Conference on Learning Representations*, 2019.
- [26] Michael I Jordan and Tom M Mitchell. Machine learning: Trends, perspectives, and prospects. *Science*, 349(6245):255–260, 2015.
- [27] Guolin Ke, Qi Meng, Thomas Finley, Taifeng Wang, Wei Chen, Weidong Ma, Qiwei Ye, and Tie-Yan Liu. LightGBM: A highly efficient gradient boosting decision tree. In *Advances in neural information processing systems*, pages 3146–3154, 2017.
- [28] Gary King, Martin A Tanner, and Ori Rosen. *Ecological inference: New methodological strategies*. Cambridge University Press, 2004.
- [29] Gregory Koch, Richard Zemel, and Ruslan Salakhutdinov. Siamese neural networks for one-shot image recognition. In *ICML deep learning workshop*, volume 2. Lille, 2015.
- [30] Hendrik Kück and Nando de Freitas. Learning about individuals from group statistics. In *Proceedings of the Twenty-First Conference on Uncertainty in Artificial Intelligence, UAI’05*, 2005.

- [31] Harold W Kuhn. The hungarian method for the assignment problem. *Naval research logistics quarterly*, 2(1-2):83–97, 1955.
- [32] Nimit Kumar and Krishna Kummamuru. Semisupervised clustering with metric learning using relative comparisons. *IEEE Transactions on Knowledge and Data Engineering*, 20(4):496–503, 2008.
- [33] Ho Chung Law, Dino Sejdinovic, Ewan Cameron, Tim Lucas, Seth Flaxman, Katherine Battle, and Kenji Fukumizu. Variational learning on aggregate outputs with gaussian processes. In *Advances in Neural Information Processing Systems*, pages 6081–6091, 2018.
- [34] Yann LeCun, Léon Bottou, Yoshua Bengio, Patrick Haffner, et al. Gradient-based learning applied to document recognition. *Proceedings of the IEEE*, 86(11):2278–2324, 1998.
- [35] Yann LeCun, Yoshua Bengio, and Geoffrey Hinton. Deep learning. *nature*, 521(7553):436, 2015.
- [36] Tongliang Liu and Dacheng Tao. On the robustness and generalization of cauchy regression. In *2014 4th IEEE International Conference on Information Science and Technology*, pages 100–105. IEEE, 2014.
- [37] Ilya Loshchilov and Frank Hutter. Decoupled weight decay regularization. In *International Conference on Learning Representations*, 2019.
- [38] R Duncan Luce. *Individual choice behavior*. John Wiley, 1959.
- [39] Stefan Mojsilovic and Antti Ukkonen. Relative distance comparisons with confidence judgments. In *Proceedings of the 2019 SIAM International Conference on Data Mining*, pages 459–467. SIAM, 2019.
- [40] Giorgio Patrini, Richard Nock, Paul Rivera, and Tiberio Caetano. (Almost) no label no cry. In *Advances in Neural Information Processing Systems*, pages 190–198, 2014.
- [41] Giorgio Patrini, Alessandro Rozza, Aditya Krishna Menon, Richard Nock, and Lizhen Qu. Making deep neural networks robust to label noise: A loss correction approach. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pages 1944–1952, 2017.
- [42] Michaël Perrot and Ulrike Von Luxburg. Boosting for comparison-based learning. *arXiv preprint arXiv:1810.13333*, 2018.
- [43] Robin L Plackett. The analysis of permutations. *Journal of the Royal Statistical Society: Series C (Applied Statistics)*, 24(2):193–202, 1975.
- [44] Novi Quadrianto, Alex J Smola, Tiberio S Caetano, and Quoc V Le. Estimating labels from label proportions. *Journal of Machine Learning Research*, 10(Oct):2349–2374, 2009.
- [45] Soumya Ray and David Page. Multiple instance regression. In *Proceedings of the Eighteenth International Conference on Machine Learning, ICML '01*, pages 425–432, San Francisco, CA, USA, 2001. Morgan Kaufmann Publishers Inc. ISBN 1-55860-778-1.
- [46] Florian Schroff, Dmitry Kalenichenko, and James Philbin. FaceNet: A unified embedding for face recognition and clustering. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 815–823, 2015.
- [47] Alexander A Schuessler. Ecological inference. *Proceedings of the National Academy of Sciences*, 96(19):10578–10581, 1999.
- [48] Matthew Schultz and Thorsten Joachims. Learning a distance metric from relative comparisons. In *Advances in neural information processing systems*, pages 41–48, 2004.
- [49] Daniel R Sheldon and Thomas G Dietterich. Collective graphical models. In *Advances in Neural Information Processing Systems*, pages 1161–1169, 2011.
- [50] Kihyuk Sohn. Improved deep metric learning with multi-class n-pair loss objective. In *Advances in neural information processing systems*, pages 1857–1865, 2016.
- [51] Omer Tamuz, Ce Liu, Serge Belongie, Ohad Shamir, and Adam Tauman Kalai. Adaptively learning the crowd kernel. *ICML*, 2011.
- [52] Yusuke Tanaka, Tomoharu Iwata, Toshiyuki Tanaka, Takeshi Kurashima, Maya Okawa, and Hiroyuki Toda. Refining coarse-grained spatial data using auxiliary spatial data sets with various granularities. In *Proceedings of the AAAI Conference on Artificial Intelligence*, volume 33, pages 5091–5099, 2019.

- [53] Yusuke Tanaka, Toshiyuki Tanaka, Tomoharu Iwata, Takeshi Kurashima, Maya Okawa, Yasunori Akagi, and Hiroyuki Toda. Spatially aggregated gaussian processes with multivariate areal outputs. In *Advances in Neural Information Processing Systems*, pages 3000–3010, 2019.
- [54] Louis L Thurstone. A law of comparative judgment. *Psychological review*, 34(4):273, 1927.
- [55] Aad W Van der Vaart. *Asymptotic statistics*, volume 3. Cambridge university press, 2000.
- [56] Joaquin Vanschoren, Jan N. van Rijn, Bernd Bischl, and Luis Torgo. OpenML: Networked science in machine learning. *SIGKDD Explorations*, 15(2):49–60, 2013. doi: 10.1145/2641190.2641198. URL <http://doi.acm.org/10.1145/2641190.2641198>.
- [57] Abraham Wald. Note on the consistency of the maximum likelihood estimate. *The Annals of Mathematical Statistics*, 20(4):595–601, 1949.
- [58] Han Xiao, Kashif Rasul, and Roland Vollgraf. Fashion-MNIST: a novel image dataset for benchmarking machine learning algorithms, 2017.
- [59] Eric P Xing, Michael I Jordan, Stuart J Russell, and Andrew Y Ng. Distance metric learning with application to clustering with side-information. In *Advances in neural information processing systems*, pages 521–528, 2003.
- [60] Liyuan Xu, Junya Honda, Gang Niu, and Masashi Sugiyama. Uncoupled regression from pairwise comparison data. In *Advances in Neural Information Processing Systems 32*, pages 3994–4004. Curran Associates, Inc., 2019.
- [61] Jun Yang. Review of multi-instance learning and its applications. *Technical report, School of Computer Science Carnegie Mellon University*, 2005.
- [62] Felix Yu, Dong Liu, Sanjiv Kumar, Jebara Tony, and Shih-Fu Chang. ∞ SVM for learning with label proportions. In *Proceedings of the 30th International Conference on Machine Learning*, pages 504–512, 2013.
- [63] Yivan Zhang, Nontawat Charoenphakdee, and Masashi Sugiyama. Learning from indirect observations. *arXiv preprint arXiv:1910.04394*, 2019.
- [64] Zhi-Hua Zhou. Multi-instance learning: A survey. *Department of Computer Science & Technology, Nanjing University, Tech. Rep*, 2004.
- [65] Zhi-Hua Zhou. A brief introduction to weakly supervised learning. *National Science Review*, 5(1):44–53, 2017.